Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

Rubidium and caesium aluminyls: synthesis, structures and reactivity in C-H activation of benzene

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General procedures

Hexane and C_6H_6 were dried by heating to reflux over sodium benzophenone ketyl and then distilled under nitrogen prior to use. C_6D_6 and THF-d_8 was degassed by freeze-pump-thaw methods and stored over activated 4 Å molecular sieves. [Al(NON^{DIPP})(I)],[S1] RbC_8[S2] and CsC_8[S2] were synthesized according to literature procedures. NMR spectra were recorded on a Bruker AV3 or AV 400 MHz spectrometer operating at 400.13 MHz for ^{1}H, 100.62 MHz for ^{13}C. All ^{13}C spectra were proton decoupled. ^{1}H and ^{13}C{^{1}H} chemical shifts are expressed in parts per million (δ, ppm) and referenced to residual solvent peaks. ^{1}H DOSY measurements were recorded on an AV 400 spectrometer operating at 400.13 MHz, using the pulseprogram dstegp3s. Elemental analysis was by the Elemental Analysis Service at London Metropolitan University.

Synthetic procedures

Synthesis of [Rb{Al(NON^{Dipp})}]$_2$ (**1**):

To a colourless solution of [Al(NON^{DIPP})(I)] (0.311 g, 0.488 mmol) in benzene (15 mL) was added 3 equivalents of RbC_8 (0.266 g, 1.47 mmol) and stirred at room temperature overnight. After filtration of the reaction mixture a yellow solution was obtained, which was evaporated to dryness under high vacuum. Hexane (4 mL) was added and the suspension was heated to 60°C until the yellow solid was completely dissolved. Slow cooling to 5°C overnight gave yellow crystals suitable for x-ray crystallography. Decantation and washing with hexane (1 mL) gave the desired compound (0.201 g, 0.161 mmol) in a 66 % yield.
^{1}H NMR (400 MHz, C_6D_6, 25°C): δH = 0.36 (s, 12 H, Si(CH_3)$_2$), 1.13 (d, ^3J(H,H) = 6.7 Hz, 12 H, CH_3), 1.27 (d, ^3J(H,H) = 7.0 Hz, 12 H, CH_3), 4.06 (sept, ^3J(H,H) = 6.8 Hz, 4 H, CH), 6.72 (t, ^3J(H,H) = 7.4 Hz, 2 H, CH_{arom}), 6.90 (d, ^3J(H,H) = 7.5 Hz, 4 H, CH_{arom}).
^{13}C NMR (100 MHz, C_6D_6, 25°C): δC = 3.4 (Si(CH$_3$)$_2$, 24.1 (CH$_3$), 25.6 (CH$_3$), 27.6 (CH), 122.0 (CH$_{arom}$), 123.2 (CH$_{arom}$), 148.9 (CH$_{arom}$), 149.4 (CH$_{arom}$).
^{29}Si NMR (80 MHz, C_6D_6, 25°C): δSi: -15.1.
Elemental Analysis: Calculated: C: 57.62 H: 8.38 N: 4.48; Obtained: C: 56.50 H: 7.97 N: 4.16.

Synthesis of [Cs{Al(NON^{Dipp})}]$_2$ (**2**):

To a colourless solution of [Al(NON^{DIPP})(I)] (0.256 g, 0.402 mmol) in benzene (15 mL) was added 3 equivalents of CsC_8 (0.276 g, 1.21 mmol) and stirred at room temperature overnight. After filtration of the reaction mixture a yellow solution was obtained, which was evaporated to dryness under high vacuum. Hexane (10 mL) was added and the suspension was heated to 60°C until the yellow solid was completely dissolved. Slow cooling to 5°C overnight gave yellow crystals suitable for x-ray crystallography. Decantation and washing with hexane (1 mL) gave the desired compound (0.168 g, 0.124 mmol) in a 62 % yield.
^{1}H NMR (400 MHz, C_6D_6, 25°C): δH = 0.36 (s, 12 H, Si(CH_3)$_2$), 1.19 (d, ^3J(H,H) = 6.8 Hz, 12 H, CH_3), 1.29 (d, ^3J(H,H) = 6.9 Hz, 12 H, CH_3), 4.14 (sept, ^3J(H,H) = 6.8 Hz, 4 H, CH), 6.71 (t, ^3J(H,H) = 7.5 Hz, 2 H, CH_{arom}), 6.90 (d, ^3J(H,H) = 7.6 Hz, 4 H, CH_{arom}).
^{13}C NMR (100 MHz, C_6D_6, 25°C): δC = 3.3 (Si(CH$_3$)$_2$, 24.1 (CH$_3$), 25.5 (CH$_3$), 27.7 (CH), 122.0 (CH$_{arom}$), 123.6 (CH$_{arom}$), 148.7 (CH$_{arom}$), 150.4 (CH$_{arom}$).
^{29}Si NMR (80 MHz, C_6D_6, 25°C): δSi: -15.1.
Elemental Analysis: Calculated: C: 53.56 H: 7.79 N: 4.16; Obtained: C: 52.35 H: 7.29 N: 3.83.

Synthesis of [Cs{Al(NON^{Dipp})(C_6H_5)(H)}]$_n$:

[Cs{Al(NON^{Dipp})}]$_2$ (**2**) (105 mg, 0.0780 mmol) was dissolved in C_6H_6 (2 mL) and the resulting yellow solution was heated at 80°C. After 5 days the yellow colour disappeared and a colourless precipitate was formed, which was collected by filtration and dried in high vacuum to yield the title compound (35 mg, 0.0238 mmol) in a 31 % yield.
^{1}H NMR (400 MHz, C_6D_6/THF-d_8 (4/1), 25°C): δH = 0.45 (s, 6 H, Si(CH_3)$_2$), 0.60 (s, 6 H, Si(CH_3)$_2$), 0.63 (d, ^3J(H,H) = 6.7 Hz, 6 H, CH_3), 1.31 (d, ^3J(H,H) = 6.8 Hz, 6 H, CH_3), 1.45 (d, ^3J(H,H) = 6.8 Hz, 6 H, CH_3), 1.54 (d, ^3J(H,H) = 6.7 Hz, 6 H, CH_3), 4.21 (sept, ^3J(H,H) = 6.7 Hz, 2 H, CH), 4.56 (sept, ^3J(H,H) = 6.7 Hz, 2 H, CH), 6.79-6.88 (m, 4 H, CH_{arom}), 6.93-6.99 (m, 3 H, CH_{arom}), 7.07-7.10 (m, 2 H, CH_{arom}), 7.57-7.61 (m, 2 H, CH_{arom}).
^{13}C NMR (100 MHz, C_6D_6/THF-d_8 (4/1), 25°C): δC = 2.8 (Si(CH_3)$_2$, 4.1 (Si(CH_3)$_2$, 25.6 (CH_3), 25.7(CH_3), 25.8 (CH_3), 27.3 (CH), 27.9 (CH), 121.8 (CH_{arom}), 123.6 (CH_{arom}), 123.9 (CH_{arom}), 126.0 (CH_{arom}), 126.7 (CH_{arom}), 127.9 (CH_{arom}), 139.2 (CH_{arom}), 148.0 (CH_{arom}), 148.6 (CH_{arom}).
^{27}Al NMR (104 MHz, C_6D_6/THF-d_8 (4/1), 25°C): δAl: 119.9.
^{29}Si NMR (80 MHz, C_6D_6/THF-d_8 (4/1), 25°C): δSi: -11.9.
Elemental Analysis: Calculated: C: 57.58 H: 7.79 N: 3.73; Obtained: C: 57.09 H: 6.91 N: 3.28.

NMR characterization

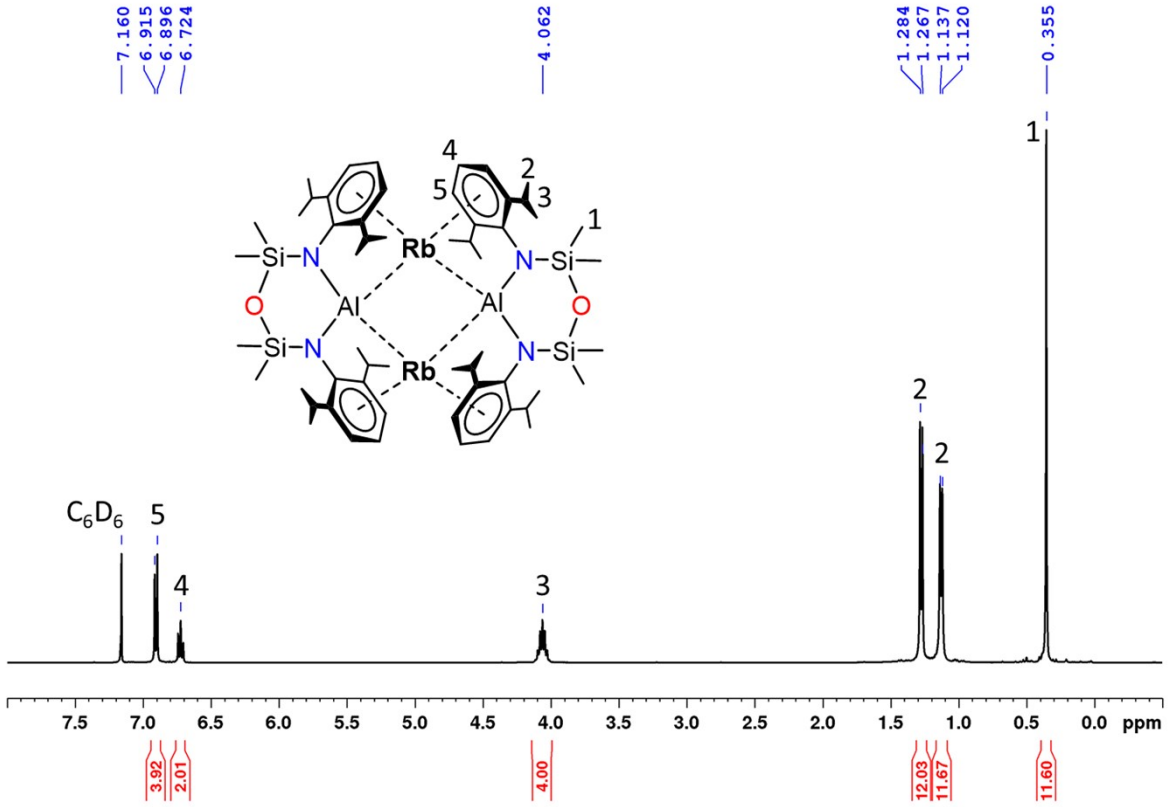


Figure S1: ^{1}H NMR spectrum of [Rb{Al(NON^{Dipp}}]$_2$ (**1**) in C_6D_6.

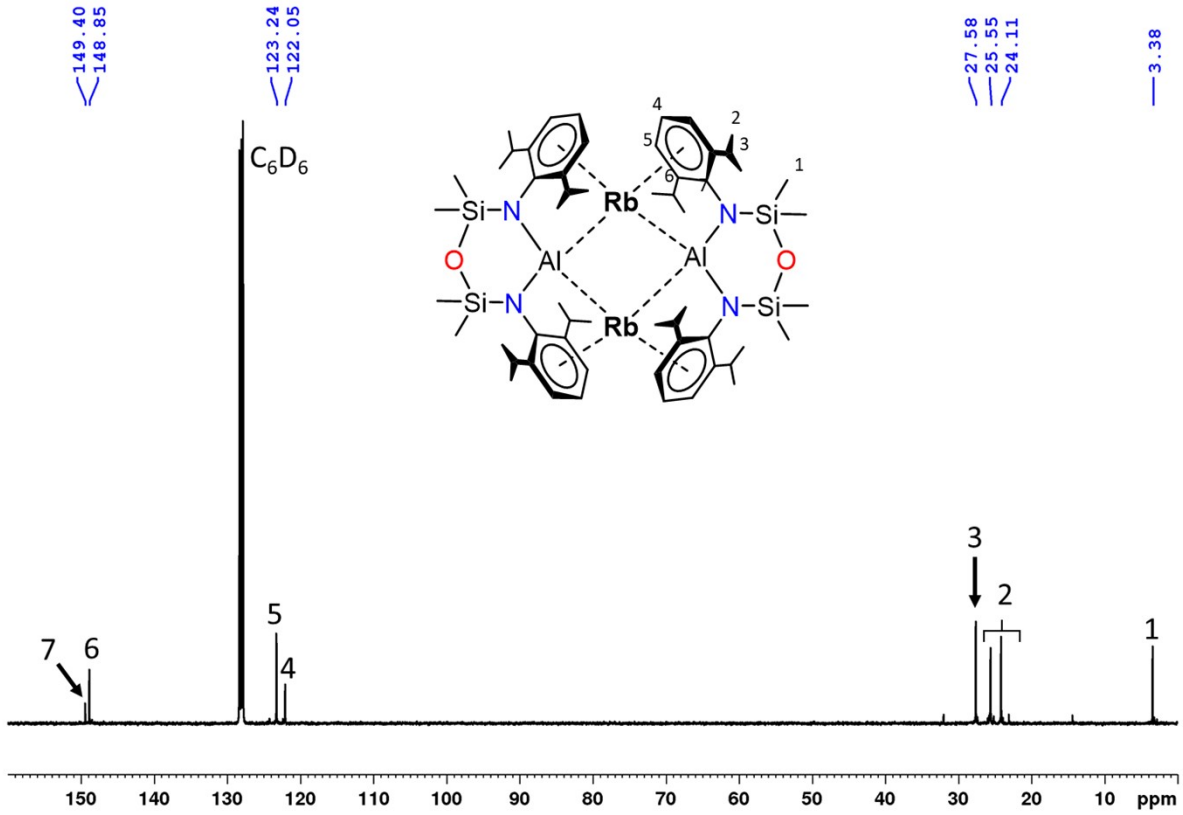


Figure S2: ^{13}C NMR spectrum of [Rb{Al(NON^{Dipp}}]$_2$ (**1**) in C_6D_6.

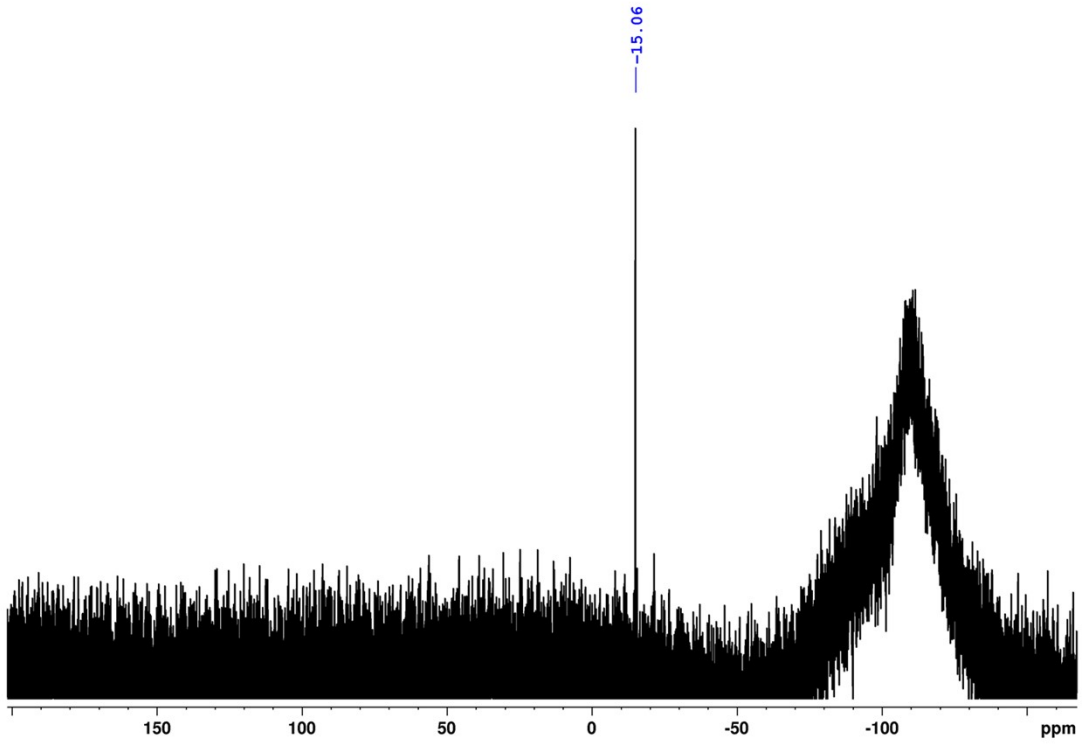


Figure S3: ^{29}Si NMR spectrum of [Rb{Al(NON^{Dipp}}]$_2$ (**1**) in C_6D_6.

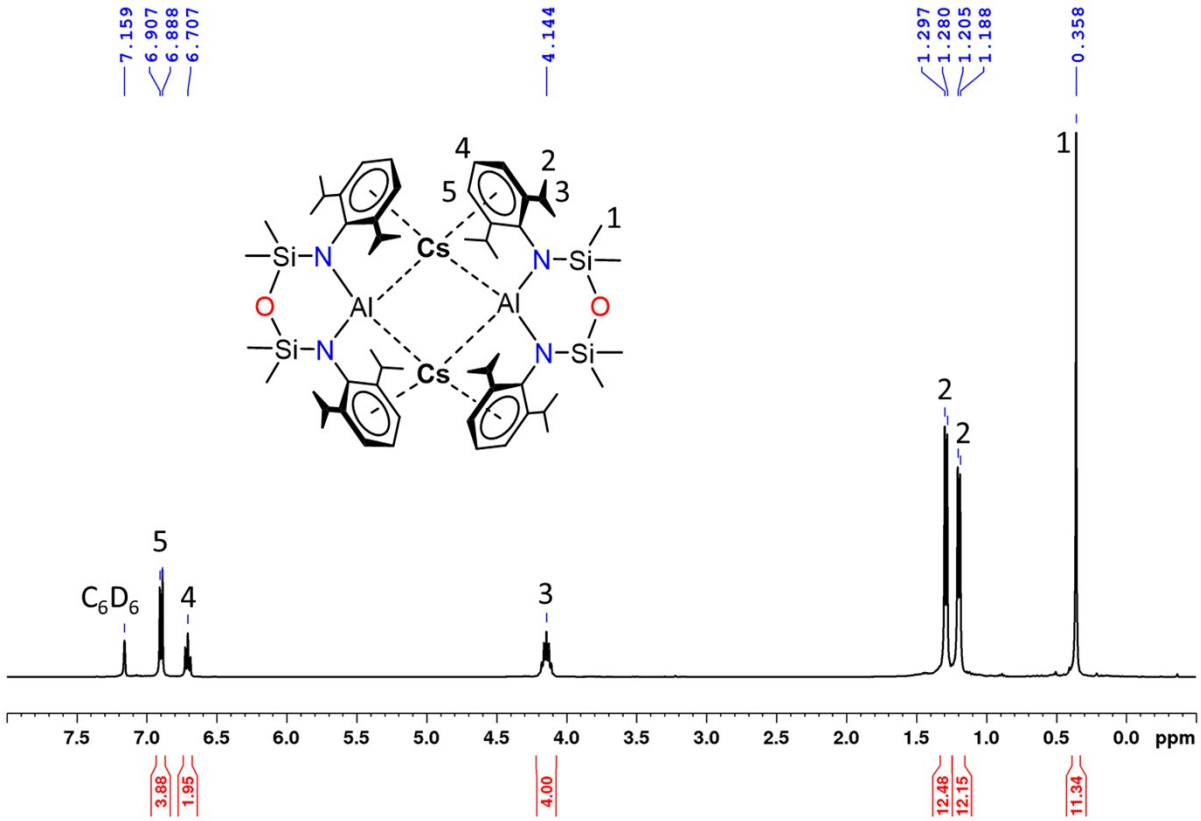


Figure S4: ^{1}H NMR spectrum of [Cs{Al(NON^{Dipp})}]$_2$ (**2**) in C_6D_6.

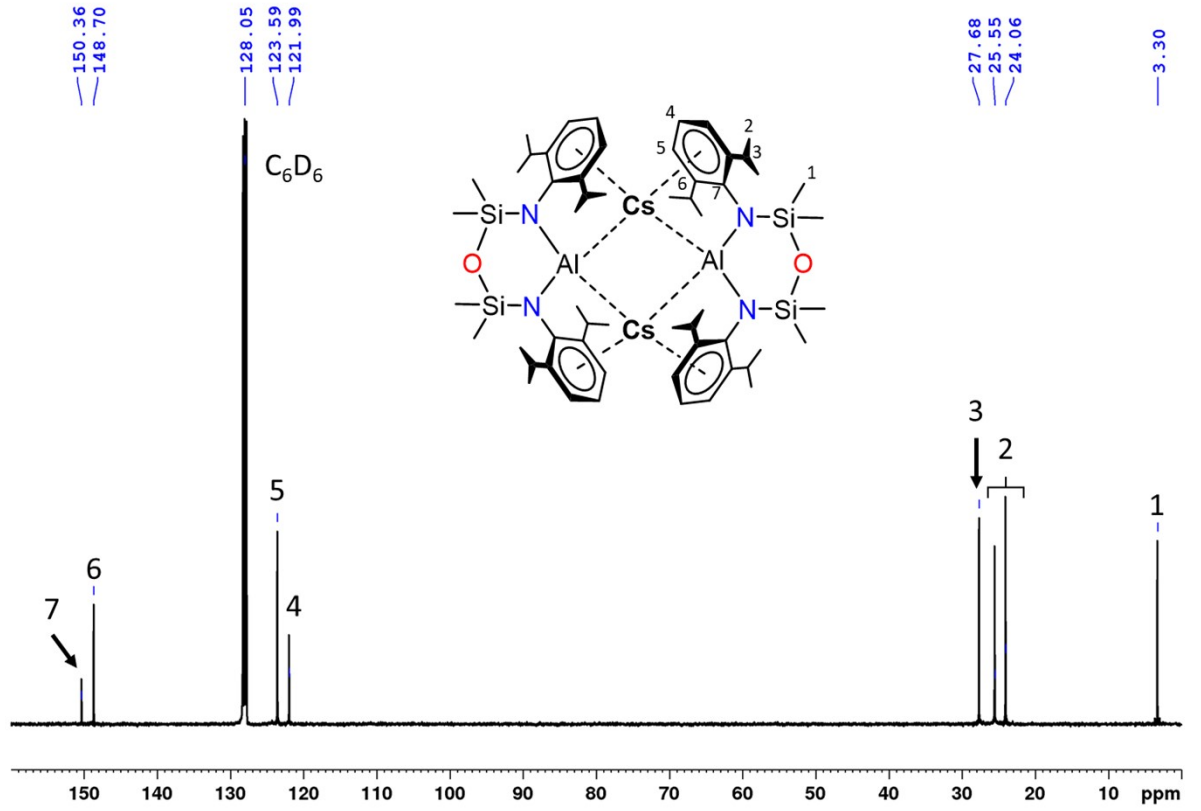


Figure S5: ^{13}C NMR spectrum of [Cs{Al(NON^{Dipp})}]$_2$ (**2**) in C_6D_6.

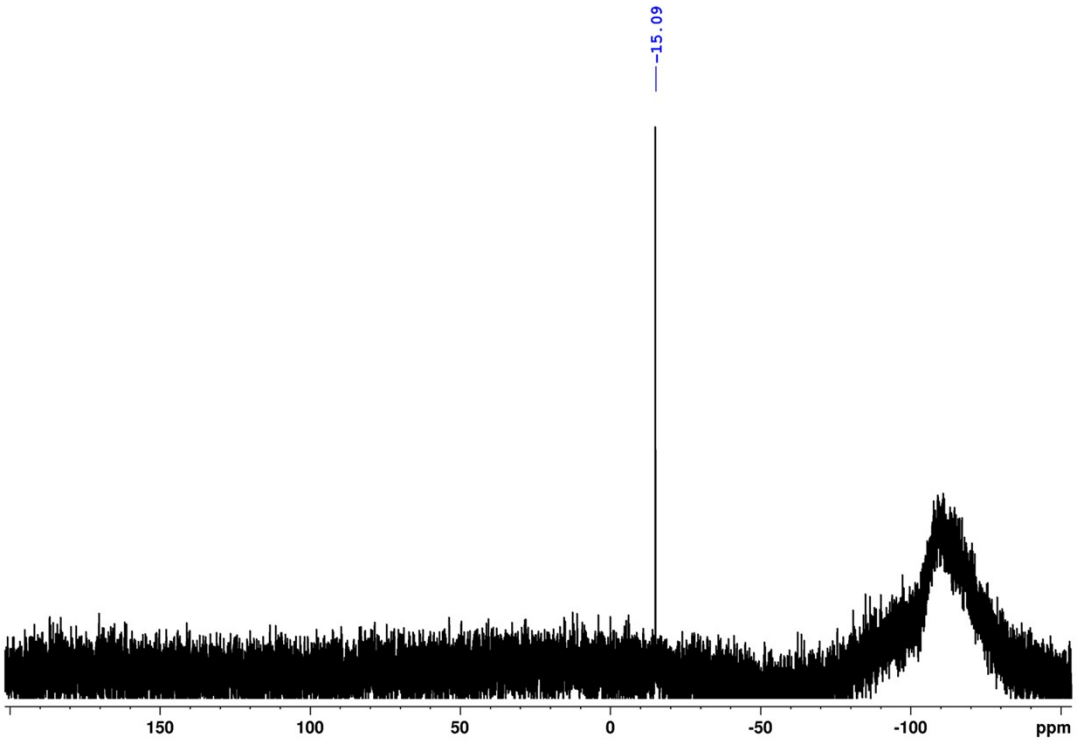


Figure S6: ^{29}Si NMR spectrum of [Cs{Al(NON^{Dipp}}]$_2$ (2) in C_6D_6.

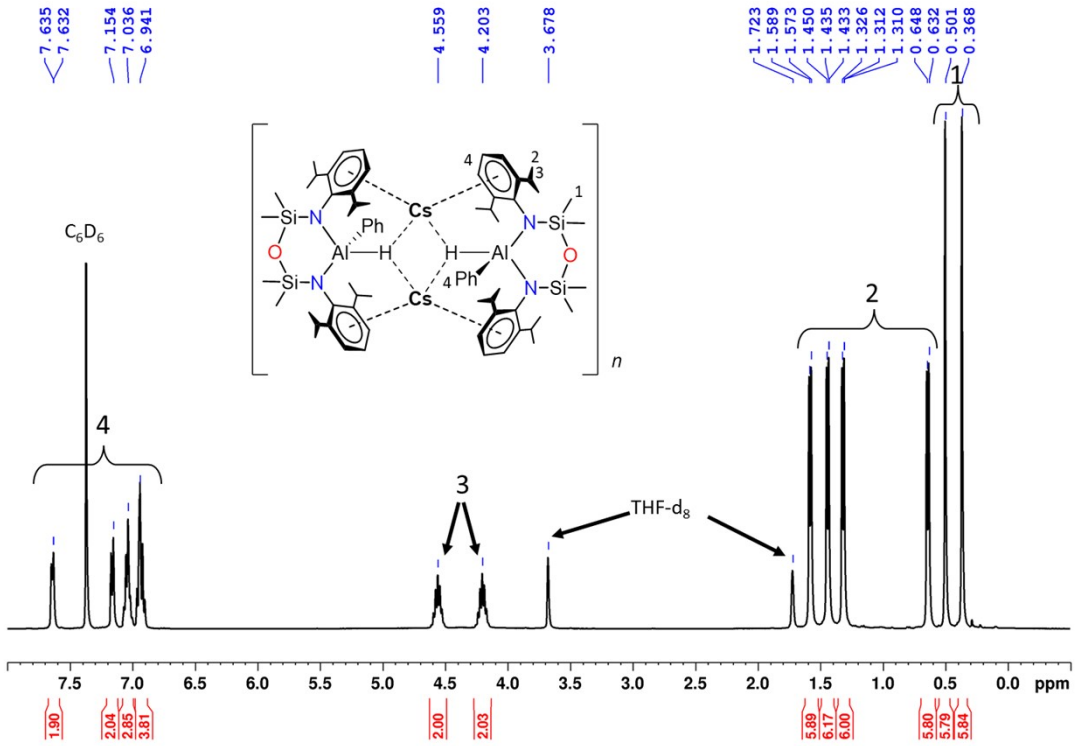


Figure S7: ^{1}H NMR spectrum of [Cs{Al(NON^{Dipp})(C_6H_5)(H)}]$_2$ in C_6D_6/THF-d_8 (4/1).

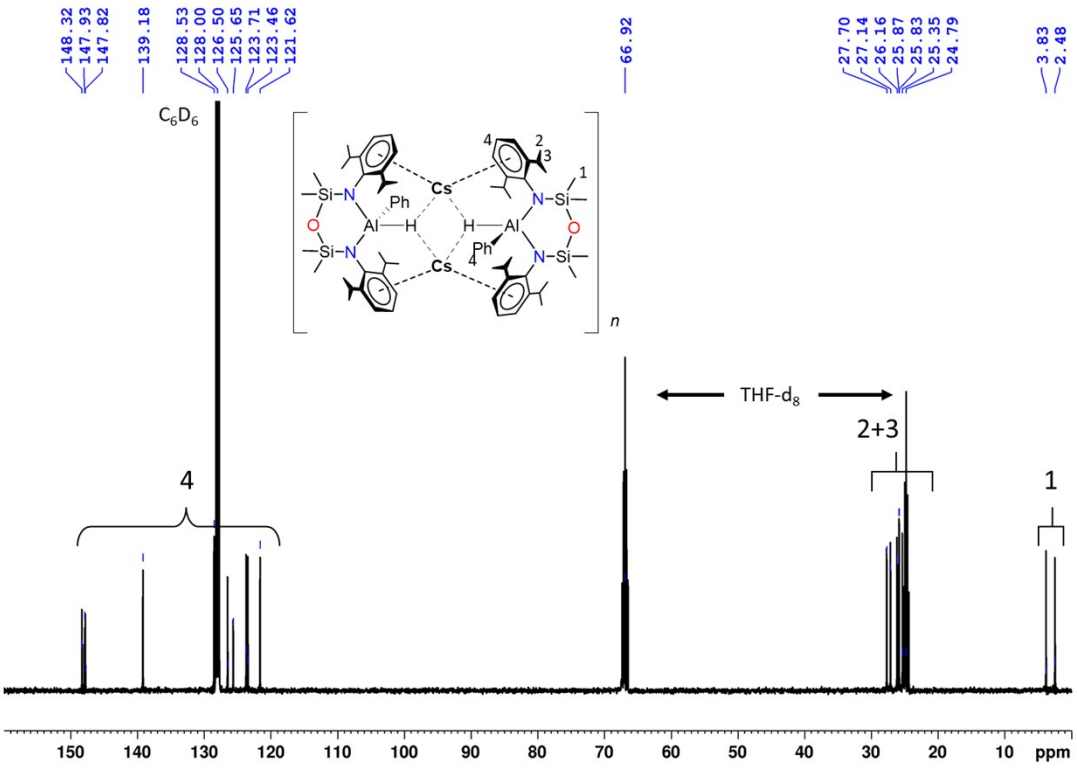


Figure S8: ^{13}C NMR spectrum of $[Cs\{Al(NON^{Dipp})(C_6H_5)(H)\}]_2$ in C_6D_6/THF-d_8 (4/1).

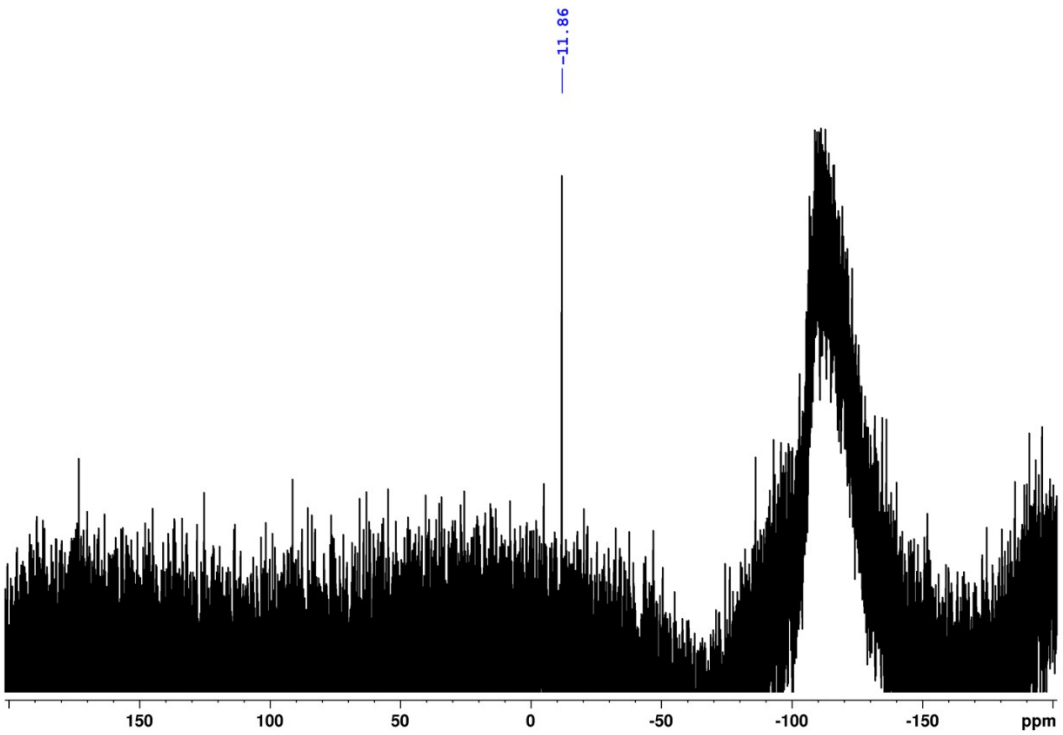


Figure S9: ^{29}Si NMR spectrum of $[Cs\{Al(NON^{Dipp})(C_6H_5)(H)\}]_2$ in C_6D_6/THF-d_8 (4/1).

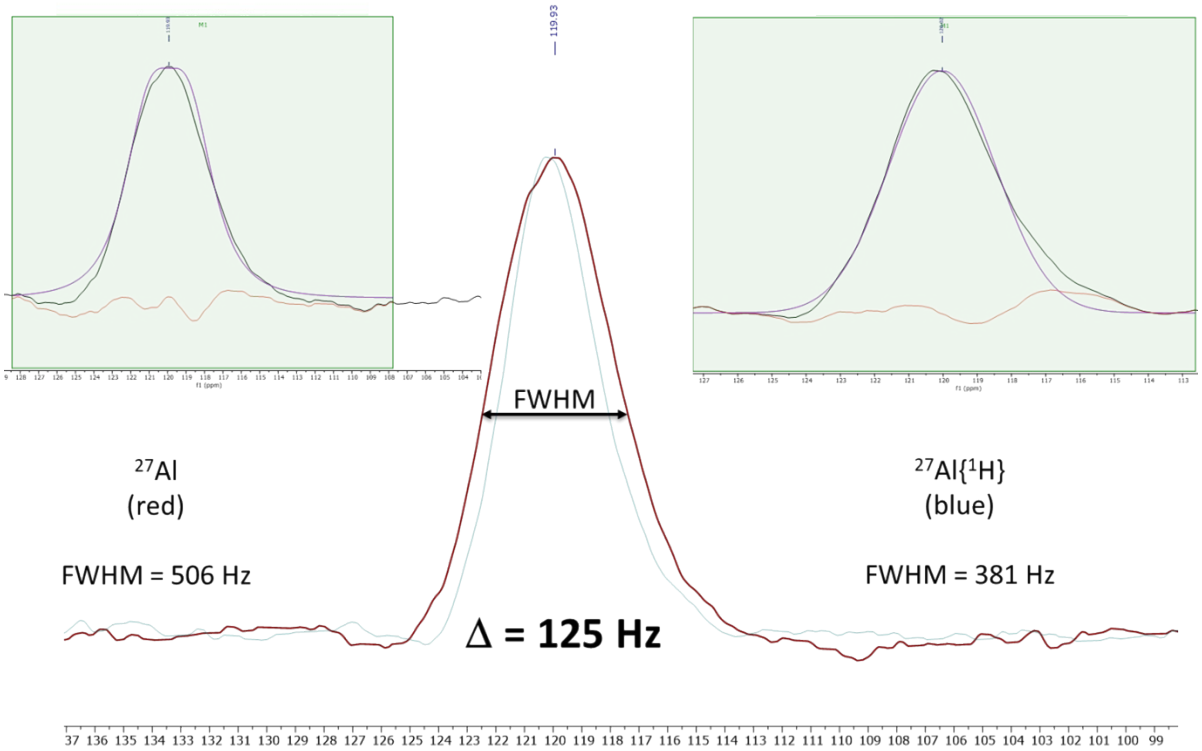


Figure S10: top left: ^{27}Al NMR spectrum of [Cs{Al(NON^{Dipp})(C_6H_5)(H)}]$_2$ in C_6D_6/THF-d_8 (4/1); top right: ^{27}Al{^{1}H} NMR spectrum of [Cs{Al(NON^{Dipp})(C_6H_5)(H)}]$_2$ in C_6D_6/THF-d_8 (4/1); middle: stacked ^{27}Al and ^{27}Al{^{1}H} NMR spectra of [Cs{Al(NON^{Dipp})(C_6H_5)(H)}]$_2$ in C_6D_6/THF-d_8 (4/1) to show the change in the FWHM (Full Width Half Maximum) consistent with the presence of a hydride ligand.

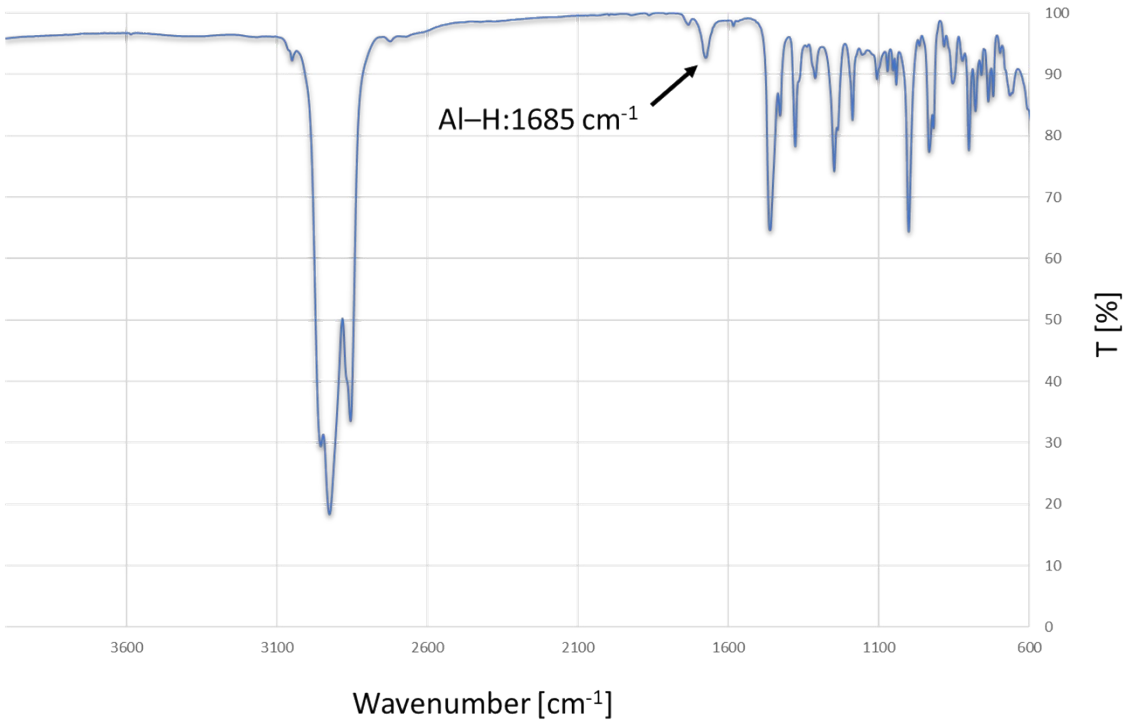


Figure S11: IR spectrum of [Cs{Al(NON)(H)(C_6H_5)}]$_n$.

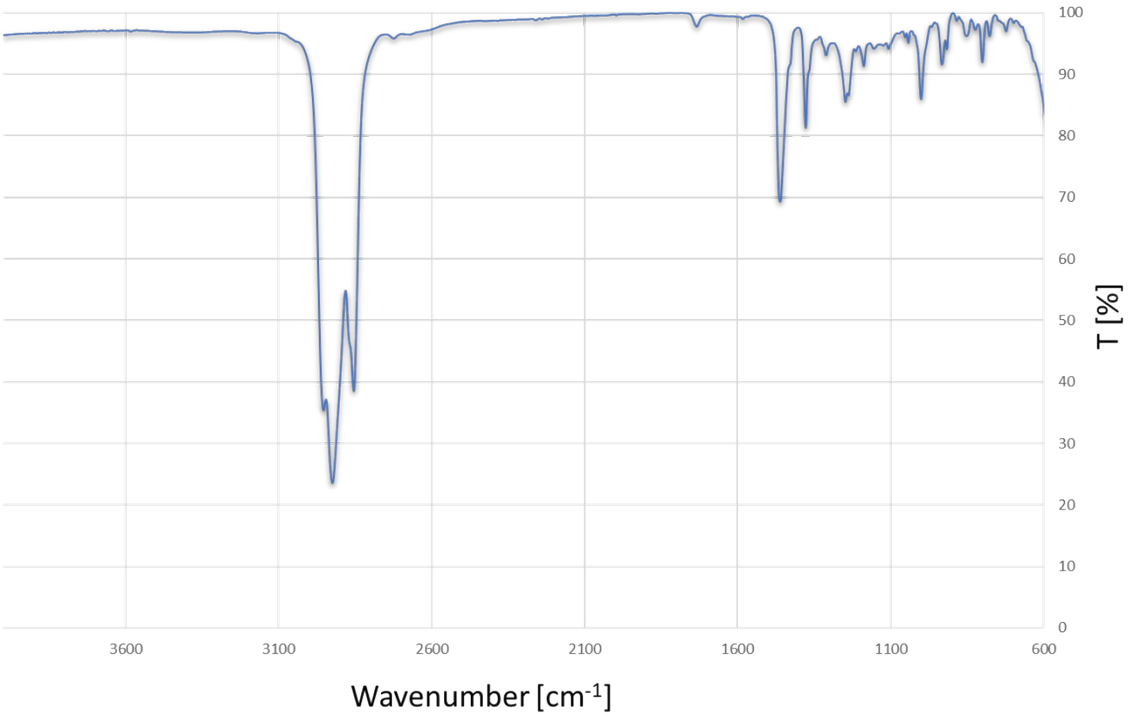


Figure S12: IR spectrum of $[Cs\{Al(NON)(D)(C_6D_5)\}]_n$.

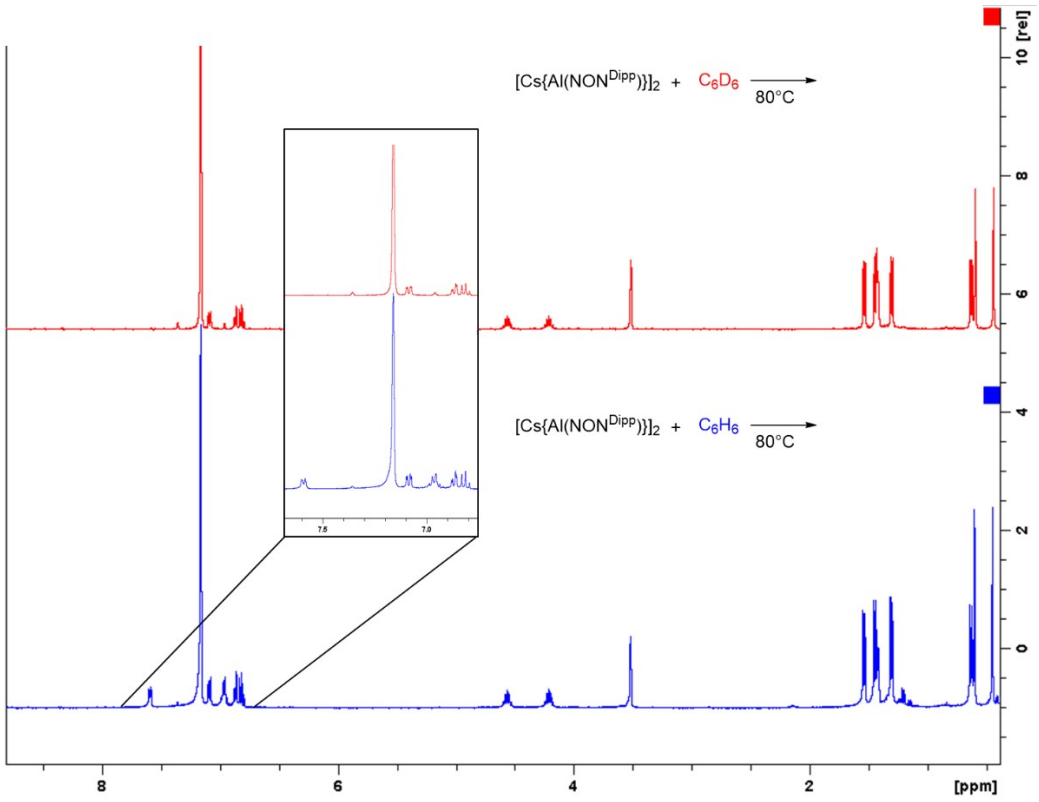


Figure S13: ^1H NMR spectrum of $[Cs\{Al(NON^{Dipp})(C_6D_5)(D)\}]_2$ (top) and $[Cs\{Al(NON^{Dipp})(C_6H_5)(H)\}]_2$ (bottom) (both in C_6D_6/THF-d_8 (4/1)) to show the presence of the phenyl ligand.

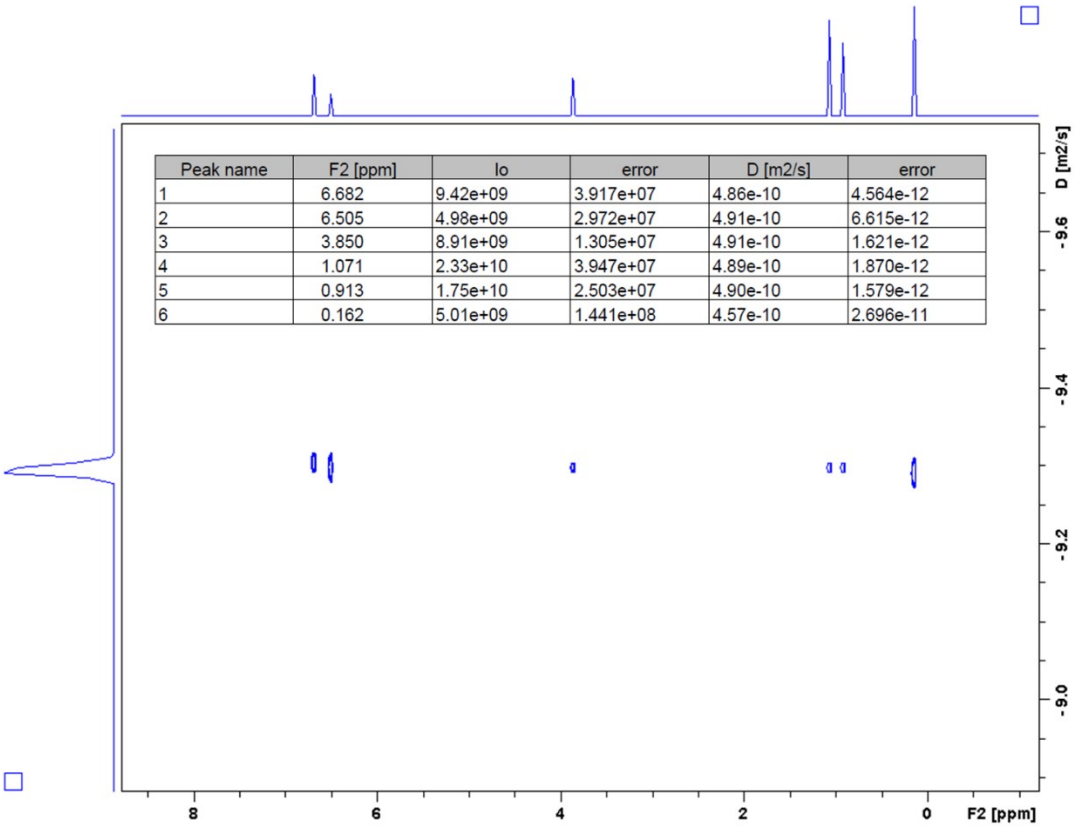


Figure S14: ^{1}H DOSY NMR spectrum of [Rb{Al(NON^{Dipp}}]$_2$ (**1**) in C_6D_6

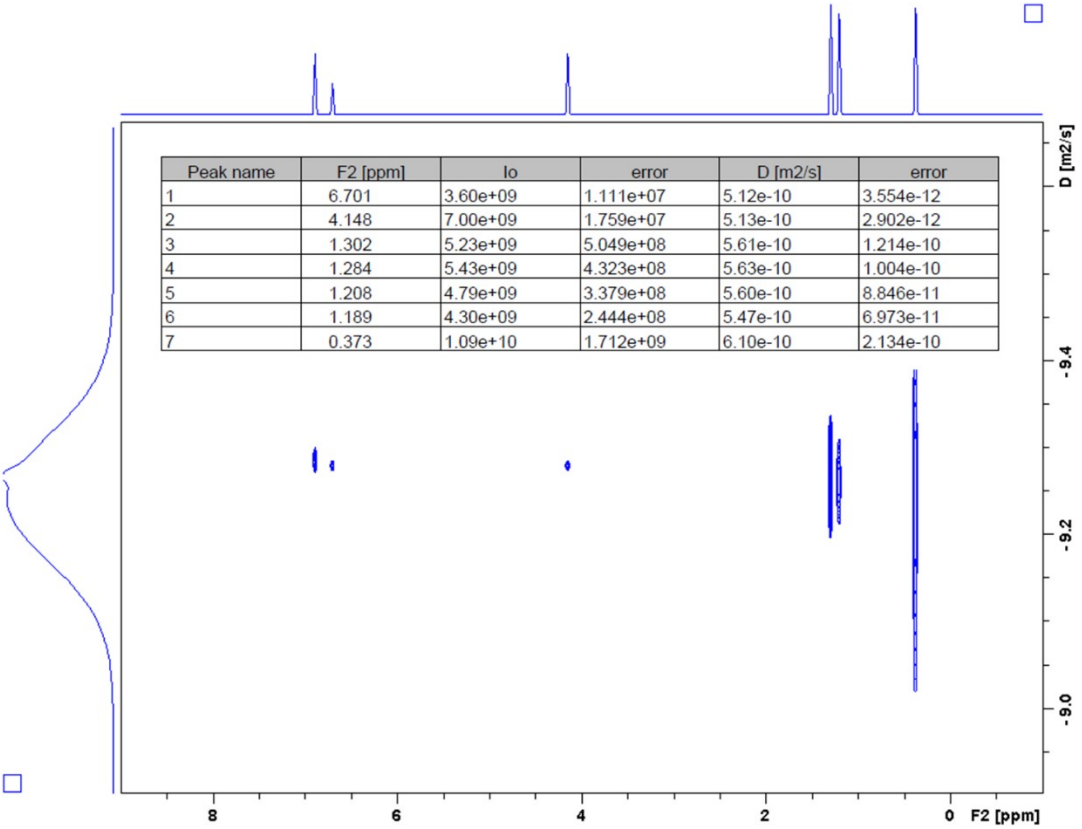


Figure S15: ^{1}H DOSY NMR spectrum of [Cs{Al(NON^{Dipp})}]$_2$ (**2**) in C_6D_6.

Crystal structure determination

Experimental Technique, Single Crystal Diffraction

Single crystal x-ray diffraction data for **1** and **2** were measured with a Rigaku Synergy-I instrument using Cu (λ = 1.54184 Å) radiation. Data collection and processing used CrysalisPro software.[S3] The structures were refined to convergence on F^2 using all independent reflections and the OLEX program suite.[S4] All non-H atoms were refined anisotropically but H atoms were placed in idealised positions and refined in riding modes. Selected crystallographic data and refinement parameters are presented in Table **S1**. Views of the molecular structures are given in Figures **S16** and **S17**. CCDC deposition numbers CCDC 2111090 and 2111091 contain the full supplementary crystallographic data for this paper in cif format. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.

Table S1: Selected crystallographic data and refinement parameters.

Compound	**1**	**2**
CCDC	2111090	2111091
Formula	$C_{59}H_{99}Al_2N_4O_2Rb_2Si_4$	$C_{59}H_{99}Al_2Cs_2N_4O_2Si_4$
Solvate	0.5 hexane	0.5 hexane
Form. Wt.	1233.68	1328.56
Space Group	I2/a	I2/a
Crystal system	Monoclinic	Monoclinic
Temp. (K)	100(2)	100(2)
a (Å)	23.3817(2)	23.57265(17)
b (Å)	17.46640(10)	17.60387(9)
c (Å)	36.1000(3)	36.1042(2)
β (°)	108.3720(10)	108.7249(8)
Volume (Å^3)	13991.6(2)	14189.15(17)
Z	8	8
λ (Å)	1.54184	1.54184
Measured Reflections	75098	106812
Unique Reflections	13840	14056
2θmax (°)	145.292	145.370
R_{int}	0.0689	0.1063
Observed Reflections [I>2σI]	13196	13626
No. Parameters	683	683
S	1.090	1.056
R [on *F*, obs refls only]	0.0444	0.0581
ωR [on F^2, all data]	0.1198	0.1633
Largest diff. peak /hole (eÅ^{-3})	0.857/-0.968	2.089/-1.572

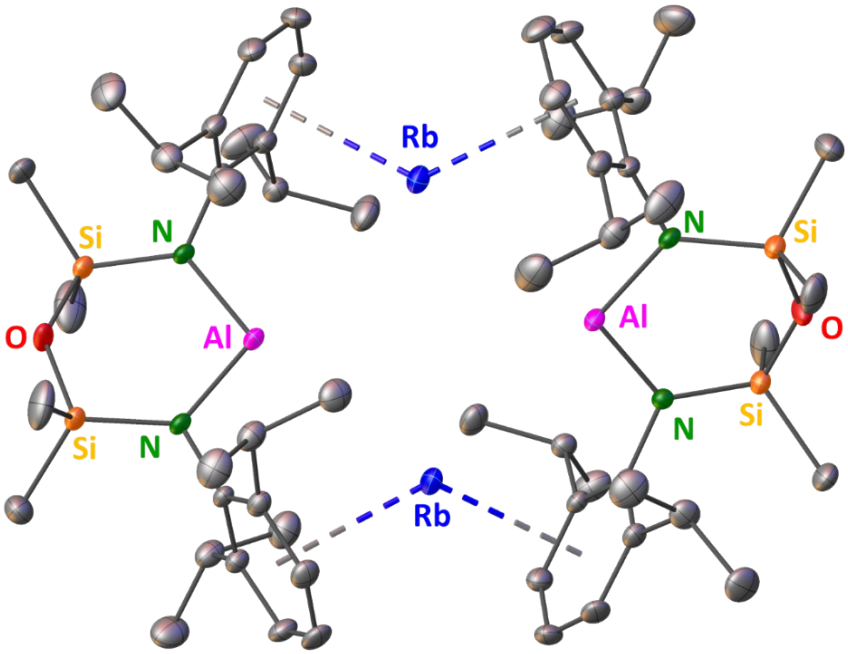


Figure S16: Molecular structure of [Rb{Al(NON^{Dipp}}]$_2$ (**1**). Thermal ellipsoids are drawn at 60% probability and hydrogen atoms and hexane solvate have been omitted for clarity.

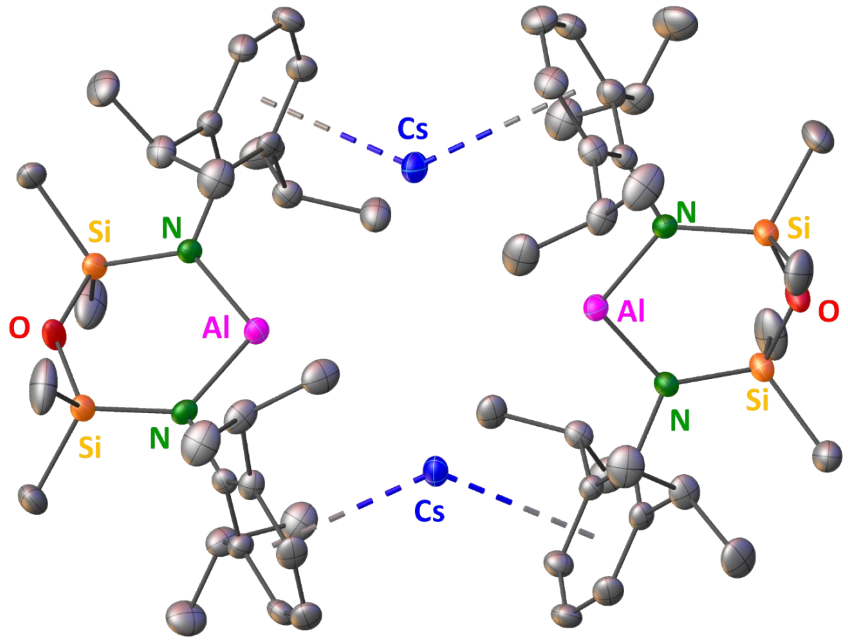


Figure S17: Molecular structure of [Cs{Al(NON^{Dipp}}]$_2$ (**2**). Thermal ellipsoids are drawn at 60% probability and hydrogen atoms and hexane solvate have been omitted for clarity.

Rb and Cs Computational Data

Methodology

DFT calculations were run with Gaussian 16 (A.03).[S5] The Na, Al, Si, K, Cs and Rb centres were described with the Stuttgart RECPs and associated basis sets,[S6] and 6-31G** basis sets were used for all other atoms (BS1).[S7] A polarization function was also added to Al (ζ_d = 0.190), Si (ζ_d = 0.284), K (ζ_d = 1.000), Rb (ζ_d = 0.491) and Cs (ζ_d = 0.306). Initial BP86[S8] optimizations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as minima (all positive eigenvalues) or transition states (one negative eigenvalue). All energies were recomputed with a larger basis set featuring 6-311++G** basis sets on all atoms, with the exception of Rb and Cs, where def2-TVZP was used (BS2). Corrections for the effect of diethyl ether (ε = 4.2400) solvent were run using the polarizable continuum model and BS1.[S9] Single-point dispersion corrections to the BP86/BS1 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[S10] Wiberg Bond Indices (Table S7) were computed using NBO v3.1[S11] as employed in Gaussian 16 and were performed on the BP86-optmised geometries with BS1.

The Quantum Theory of Atoms in Molecules (QTAIM, AIMALL program)[S12] and Natural Bonding Orbital (NBO v7)[S13] analyses were performed on the BP86-optmised geometries (Tables S4, S5 and S6), with the QTAIM calculations employing wavefunctions computed using Gaussian 16 (C.01).[S14] For these QTAIM and NBO calculations, the all-electron cc-pVTZ-X2C basis set was used for Rb and Cs,[S15] while the 6-311++G** basis set was used for all other atoms (BS3). Contour plots were generated using threshold values of 0.015 e·Å^{-3} (solid line BCP = strong) and 0.005 e·Å^{-3} (dashed line BCP = weak). The colours for each atom in the QTAIM contour plots are as follows: Rb / Cs = purple, Al = dusty grey, Si = sandy yellow, O = red, N = blue, H = white.

Ether Adduct Stability

Breakdown of Energy Contributions

The following tables detail the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

ΔE_{BSI}	SCF energy computed with the BP86 functional with BS1
ΔH_{BSI}	Enthalpy at 0 K with BS1
ΔG_{BSI}	Free energy at 298.15 K and 1 atm with BS1
$\Delta G_{BSI/Et_2O}$	Free energy corrected for Et_2O solvent with BS1
$\Delta G_{BSI/Et_2O\ +\ D3BJ}$	Free energy corrected for Et_2O and dispersion effects with BS1
ΔE_{BS2}	SCF energy computed with the BP86 functional with BS2
ΔG_{Et_2O}	Free energy corrected for basis set (BS2), dispersion effects and Et_2O solvent
$\Delta G_{BSI/bnz}$	Free energy corrected for benzene solvent with BS1
$\Delta G_{BSI/bnz\ +\ D3BJ}$	Free energy corrected for benzene and dispersion effects with BS1
ΔG_{bnz}	Free energy corrected for basis set (BS2), dispersion effects and benzene solvent

In each case the final data used in the main article are highlighted in bold.

Table S2: Relative energies for BP86-D3BJ/BS2(Et_2O)//BP86/BS1 computed structures. Data in bold are those used in the main text. All energies are quoted relative to each respective group 1 dimer **M_2[II]$_2$** at 0.0 kcal/mol.

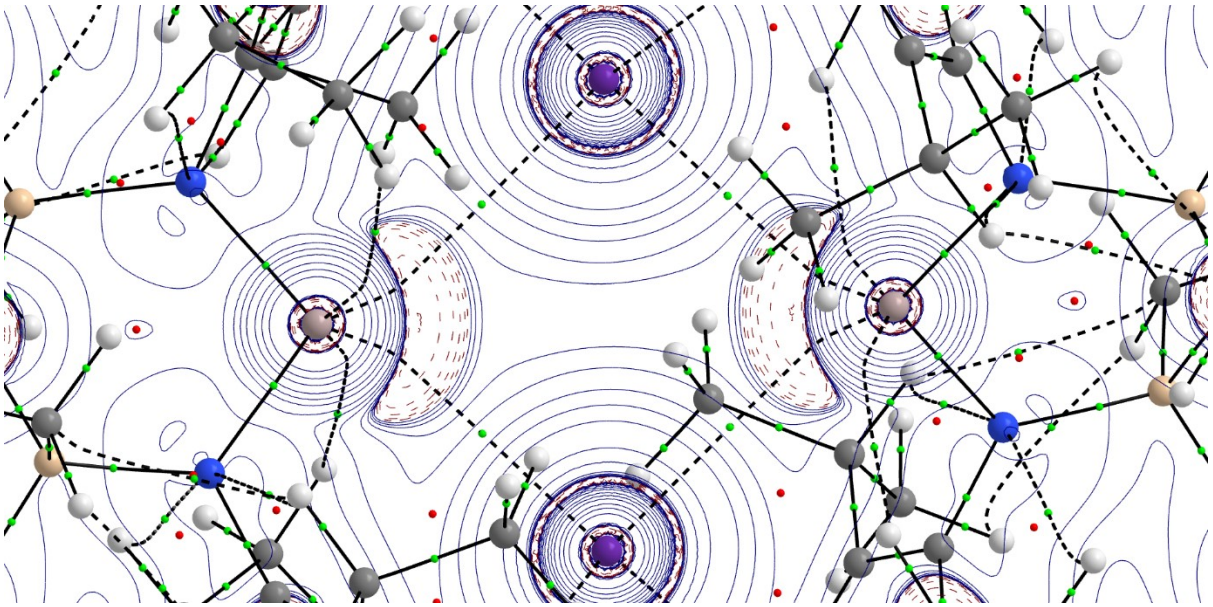
M		ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/Et_2O}$	$\Delta G_{BSI/Et_2O+D3BJ}$	ΔE_{BS2}	ΔG_{Et_2O}
	Li_2[II]$_2$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
Li	**Li[II]**	33.0	31.7	16.6	2.2	30.8	27.6	**25.4**
	[II]Li·2Et_2O	-14.4	-13.3	2.0	2.2	-9.2	-12.2	**-7.0**
	Na_2[II]$_2$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
Na	**Li[II]**	29.1	27.6	13.2	-2.7	21.3	23.7	**15.9**
	[II]Na·2Et_2O	-10.9	-10.3	5.7	5.9	-5.3	-8.7	**-3.2**
	K_2[II]$_2$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
K	**K[II]**	33.8	33.6	22.0	3.9	27.9	29.2	**23.3**
	[II]K·2Et_2O	-0.2	0.6	13.9	11.1	5.4	1.5	**7.0**
	Rb_2[II]$_2$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
Rb	**Rb[II]**	32.4	32.0	19.5	2.4	22.7	29.2	**19.6**
	[II]Rb·2Et_2O	1.5	2.1	14.6	11.6	4.1	3.4	**5.9**
	Cs_2[II]$_2$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
Cs	**Cs[II]**	31.7	31.1	17.8	2.3	20.0	27.3	**15.6**
	[II]Cs·2Et_2O	3.8	4.2	16.0	12.9	3.6	4.9	**4.7**

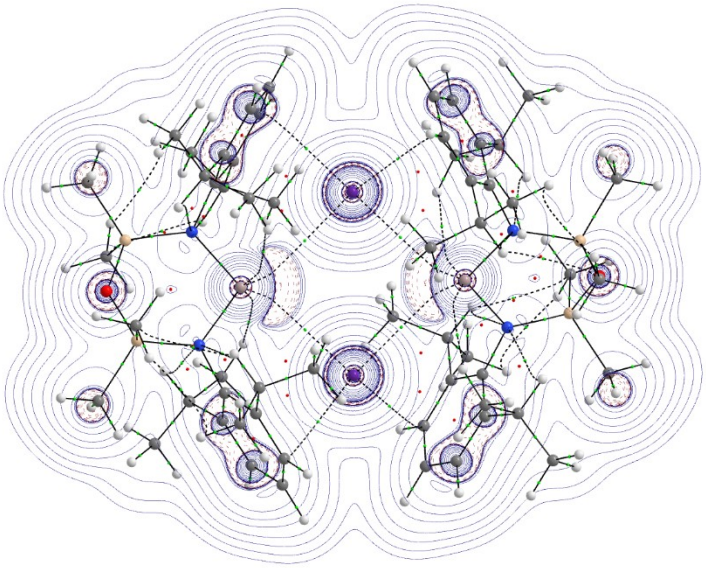
Table S3: Relative energies for BP86-D3BJ/BS2(C_6H_6)//BP86/BS1 computed structures for the C–H activation of benzene. Data in bold are those used in the main text. All energies are quoted relative to each respective group 1 dimer **M**$_2$**[II]**$_2$ at 0.0 kcal/mol.

M		ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/bnz}$	$\Delta G_{BSI/bnz+D3BJ}$	ΔE_{BS2}	ΔG_{bnz}
Rb	**Rb[II]**·C_6H_6	26.3	26.2	21.5	12.4	28.1	24.4	**26.2**
	A-Rb[II]	53.2	52.4	54.6	46.0	50.4	48.4	**45.6**
	TS(A-B)-Rb[II]	63.5	60.5	64.6	53.3	56.6	58.0	**51.1**
	B-Rb[II]	15.5	14.2	17.4	7.0	12.0	12.4	**8.9**
	Rb$_2$**[II]**$_2$·C_6H_6	−1.1	−0.8	5.7	5.8	1.6	−0.1	**2.7**
	A-Rb$_2$**[II]**$_2$	34.6	33.6	46.5	45.5	29.0	32.8	**27.1**
	TS(A-B)-Rb$_2$**[II]**$_2$	37.6	35.0	49.4	48.4	32.6	36.0	**31.0**
	B-Rb$_2$**[II]**$_2$	1.1	0.4	15.9	13.0	−4.4	1.8	**−3.7**
Cs	**Cs[II]**·3C_6H_6	6.1	6.5	26.2	24.9	11.5	7.6	**13.0**
	Cs[II]·2C_6H_6	7.6	7.7	18.3	16.4	11.3	7.5	**11.2**
	Cs[II]·C_6H_6	26.3	26.2	22.8	14.9	27.4	22.7	**23.9**
	A-Cs[II]	51.3	50.4	51.4	44.0	46.3	45.5	**40.5**
	TS(A-B)-Cs[II]	60.8	57.8	58.7	49.3	49.8	54.0	**43.0**
	B-Cs[II]	14.3	12.7	15.0	5.6	7.8	10.3	**3.9**
	Cs$_2$**[II]**$_2$·C_6H_6	−0.2	−0.1	5.5	5.6	3.6	0.6	**4.4**
	A-Cs$_2$**[II]**$_2$	34.0	33.0	47.4	46.4	26.5	32.7	**25.2**
	TS(A-B)-Cs$_2$**[II]**$_2$	37.9	35.1	48.7	47.7	30.3	35.6	**28.1**
	B-Cs$_2$**[II]**$_2$	1.3	0.4	15.1	12.4	−6.3	1.9	**−5.7**

QTAIM and NBO

Figure S19: QTAIM molecular graph and tabulated data of the BP86-optimised geometry of $\mathbf{Rb_2[II]_2}$. The Laplacian contours are computed in the {Al/Am/Al} planes with bond critical points (BCPs) shown as small green spheres.

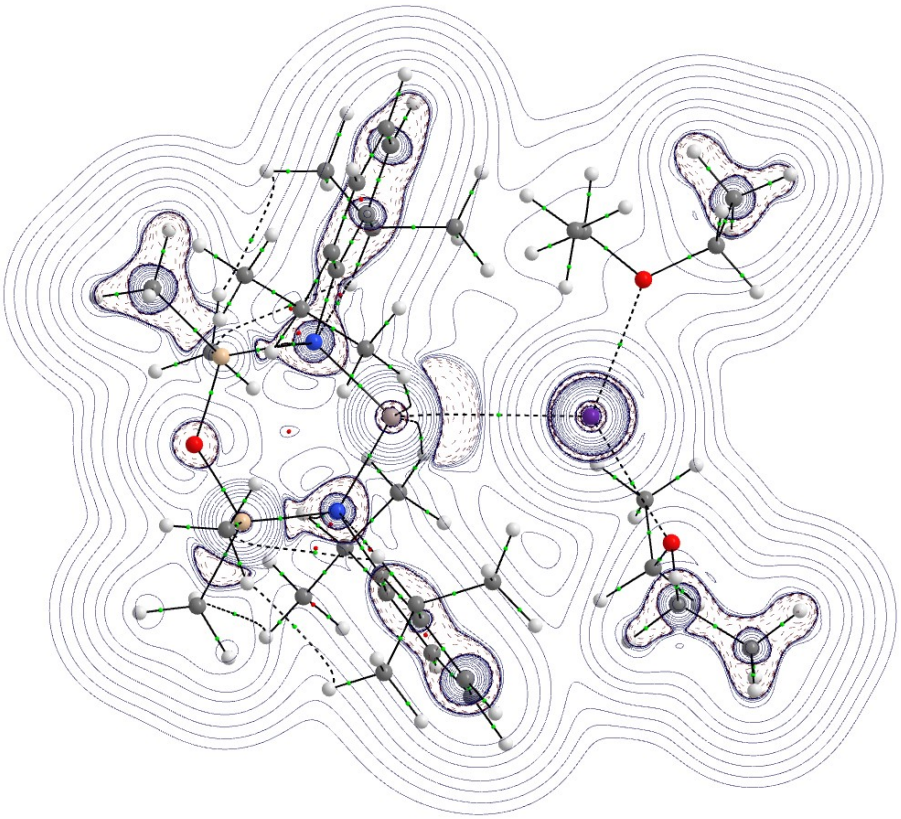




BCP	ρ(r)	$\nabla^2\rho(r)$	E	G(r)	V(r)	H(r)	DI(A|B)
Al1 - Rb3	0.007881	0.012371	0.039669	0.002884	-0.00268	0.000208	0.109715
Al2 - Rb3	0.007877	0.012364	0.039822	0.002883	-0.00267	0.000208	0.109636
Al1 - Rb4	0.007882	0.01237	0.039795	0.002884	-0.00268	0.000208	0.109667
Al2 - Rb4	0.007883	0.012371	0.039756	0.002884	-0.00268	0.000208	0.109741
Rb3 - C21	0.006623	0.021975	8.718961	0.00445	-0.00341	0.001043	0.032014
Rb4 - C54	0.006624	0.021975	8.638467	0.004451	-0.00341	0.001043	0.032067

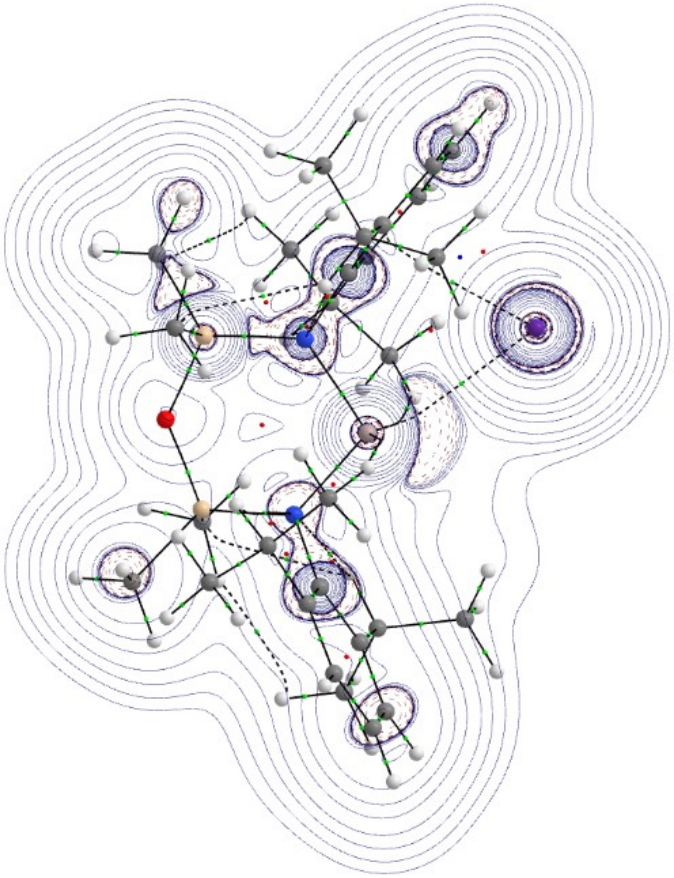
Rb3 - C91	0.00662	0.02197	8.955446	0.004449	-0.00341	0.001043	0.031997
Rb4 - C128	0.006604	0.021913	9.07695	0.004437	-0.0034	0.001042	0.031942

Figure S20: QTAIM molecular graph and tabulated data of the BP86-optimised geometry of **[II]Rb**·2Et_2O. The Laplacian contours are computed in the {Al/N/Am} planes with bond critical points (BCPs) shown as small green spheres.



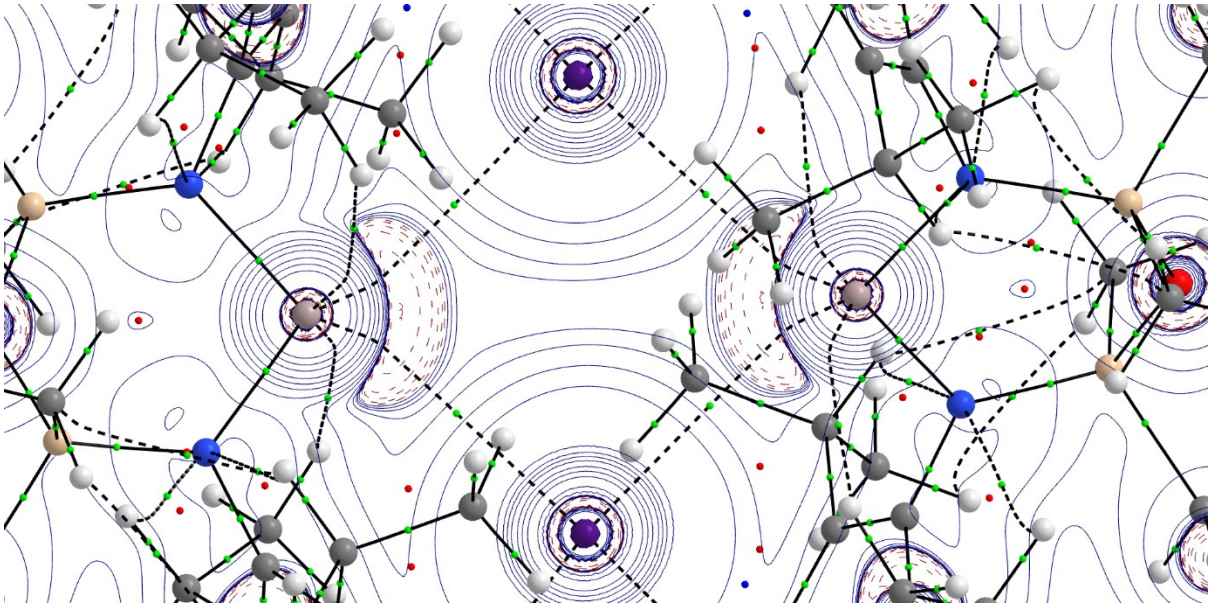
BCP	ρ(r)	∇²ρ(r)	ε	G(r)	V(r)	H(r)	DI(A|B)
Al1 - Rb111	0.01369	0.019207	0.067048	0.005091	-0.00538	-0.00029	0.222233
O81 - Rb111	0.016679	0.06466	0.151214	0.01431	-0.01246	0.001855	0.115117
O82 - Rb111	0.015476	0.056164	0.109559	0.012582	-0.01112	0.001459	0.104147

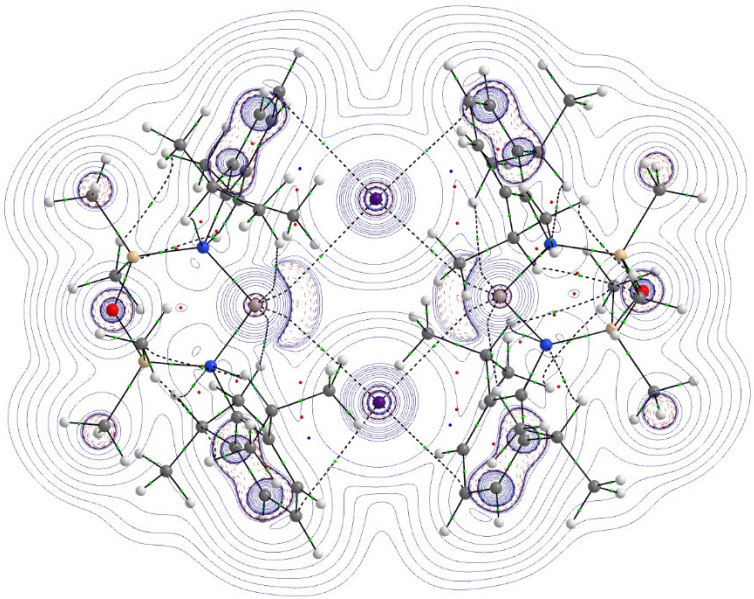
Figure S21: QTAIM molecular graph and tabulated data of the BP86-optimised geometry of **Rb**[**II**]. The Laplacian contours are computed in the {Al/N/Am} planes with bond critical points (BCPs) shown as small green spheres.



BCP	ρ(r)	$\nabla^2\rho(r)$	ε	G(r)	V(r)	H(r)	DI(A|B)
Rb1 - Al4	0.014072	0.018415	0.09079	0.00508	-0.00556	-0.00048	0.239656
Rb1 - C9	0.008458	0.026906	12.28336	0.005589	-0.00445	0.001138	0.037323

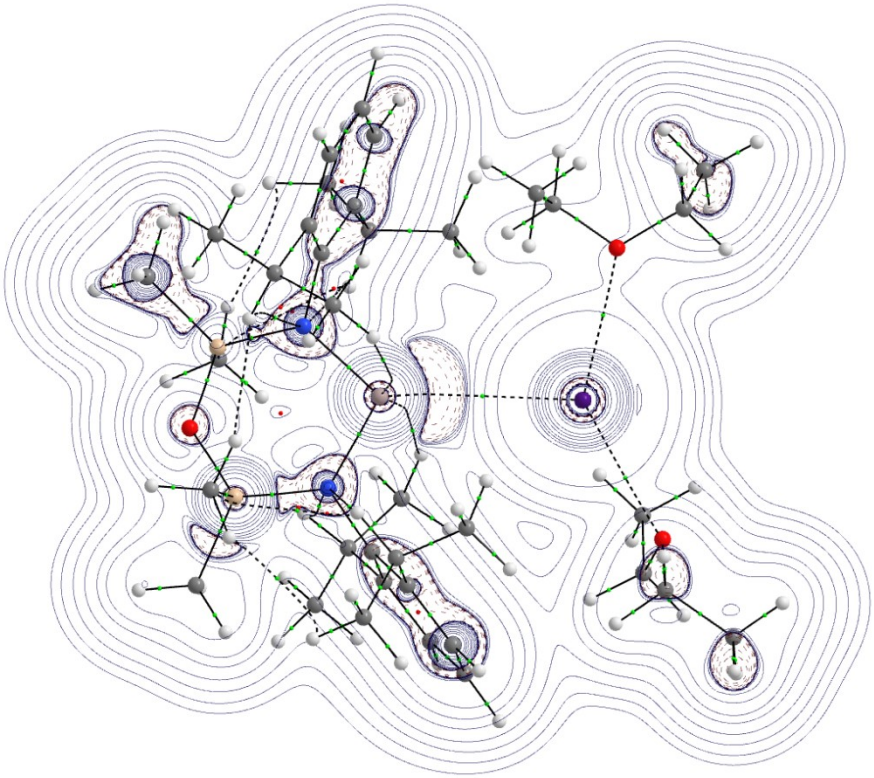
Figure S22: QTAIM molecular graph and tabulated data of the BP86-optimised geometry of **Cs_2[II]$_2$**. The Laplacian contours are computed in the {Al/Am/Al} planes with bond critical points (BCPs) shown as small green spheres.





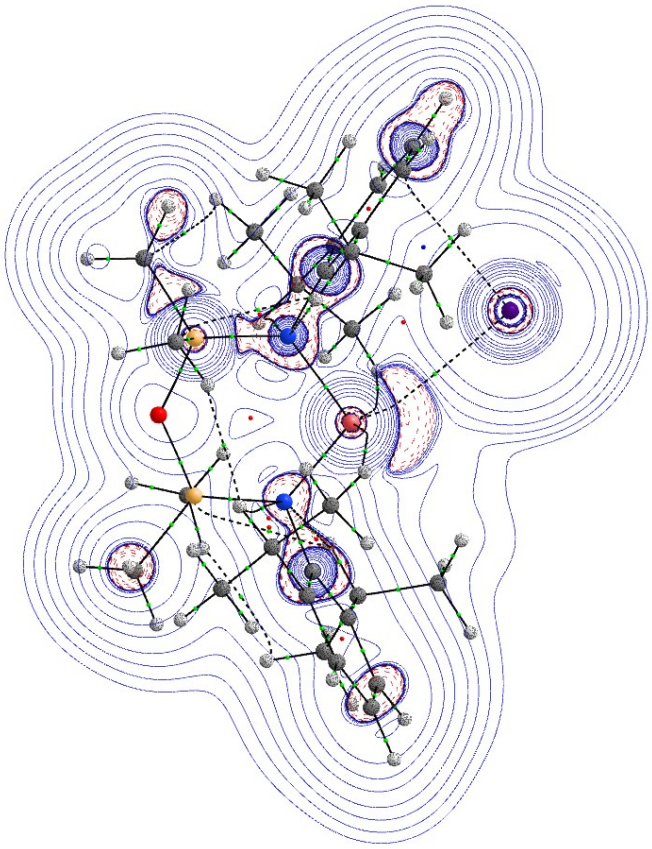
BCP	ρ(r)	∇²ρ(r)	ε	G(r)	V(r)	H(r)	DI(A|B)
Al1 - Cs3	0.008455	0.013606	0.09246	0.003231	-0.00306	0.000171	0.12543
Al2 - Cs3	0.008452	0.0136	0.092716	0.003229	-0.00306	0.000171	0.125403
Al1 - Cs4	0.008439	0.013584	0.09274	0.003224	-0.00305	0.000172	0.125239
Al2 - Cs4	0.008442	0.013588	0.092361	0.003225	-0.00305	0.000171	0.125322
Cs3 - C19	0.007864	0.026675	8.443726	0.00543	-0.00419	0.001239	0.044393
Cs4 - C56	0.007854	0.026636	8.427445	0.005422	-0.00418	0.001237	0.044293
Cs3 - C93	0.007843	0.026597	8.178295	0.005414	-0.00418	0.001236	0.044279
Cs4 - C130	0.007851	0.026623	7.648631	0.005421	-0.00419	0.001235	0.044382

Figure S23: QTAIM molecular graph and tabulated data of the BP86-optimised geometry of **[II]Cs**·2Et_2O. The Laplacian contours are computed in the {Al/N/Am} planes with bond critical points (BCPs) shown as small green spheres.



BCP	ρ(r)	$\nabla^2\rho(r)$	ε	G(r)	V(r)	H(r)	DI(A|B)
Al1 - Cs111	0.014424	0.017231	0.050175	0.004887	-0.00547	-0.000579	0.239731
O82 - Cs111	0.016185	0.051556	0.113776	0.012017	-0.01114	0.00087	0.117912
O81 - Cs111	0.018657	0.061696	0.177277	0.014398	-0.01337	0.00103	0.138214

Figure S24: QTAIM molecular graph and tabulated data of the BP86-optimised geometry of **Cs**[**II**]. The Laplacian contours are computed in the {Al/N/Am} planes with bond critical points (BCPs) shown as small green spheres.

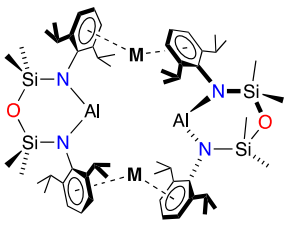


BCP	ρ(r)	$\nabla^2\rho(r)$	ε	G(r)	V(r)	H(r)	DI(A|B)
Cs1 - Al4	0.01545	0.016397	0.0872	0.005001	-0.0059	-0.0009	0.261275
Cs1 - C10	0.009519	0.032195	6.902785	0.006694	-0.00534	0.001354	0.054107

Table S4: Computed Natural atomic charges of the Rb and Cs species at the BP86/BS2 level with BP86/BS1-optimized geometries.

Species	Charge
Cs_2[II]$_2$	
Al1	0.82540
Al2	0.82616
Cs3	0.87463
Cs4	0.87992
[II]**Cs**·$2Et_2O$	
Al1	0.78123
Cs111	0.92199
O81	-0.63955
O82	-0.62743
Cs[II]	
Cs1	0.91507
Al4	0.78344
Rb_2[II]$_2$	
Al1	0.81250
Al2	0.81359
Rb3	0.80847
Rb4	0.80702
[II]**Rb**·$2Et_2O$	
Al1	0.74303
Rb111	0.85536
O81	-0.63593
O82	-0.62690
Rb[II]	
Rb1	0.87868
Al4	0.75006

Table S5: Selected Rb-Al donor acceptor interaction energies, $\Delta E^{(2)}$, for **Cs_2[II]$_2$**.

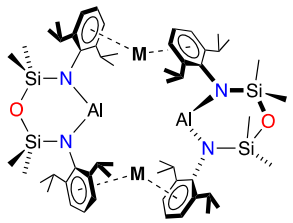


1 **M** = Rb **2** **M** = Cs

Donor NBO (Unit)	Acceptor NBO (Unit)	$\Delta E^{(2)}$ (kcal/mol)
LP_{Al1}	n_{Cs3}*	8.3
LP_{Al1}	r_{Cs3}*	1.5
LP_{Al1}	r_{Cs3}*	0.4
LP_{Al1}	r_{Cs3}*	0.4
LP_{Al1}	n_{Cs4}*	8.4
LP_{Al1}	r_{Cs4}*	1.6
LP_{Al1}	r_{Cs4}*	0.6
LP_{Al1}	r_{Cs4}*	0.4

Donor NBO (Unit)	Acceptor NBO (Unit)	$\Delta E^{(2)}$ (kcal/mol)
LP_{Al2}	n_{Cs3}*	8.3
LP_{Al2}	r_{Cs3}*	1.5
LP_{Al2}	r_{Cs3}*	0.4
LP_{Al2}	r_{Cs3}*	0.4
LP_{Al2}	n_{Cs4}*	8.4
LP_{Al2}	r_{Cs4}*	1.5
LP_{Al2}	r_{Cs4}*	0.6
LP_{Al2}	r_{Cs4}*	0.4

Table S6: Selected Rb-Al donor acceptor interaction energies, $\Delta E^{(2)}$, for **Rb**$_2$**[II]**$_2$.



1 **M** = Rb **2** **M** = Cs

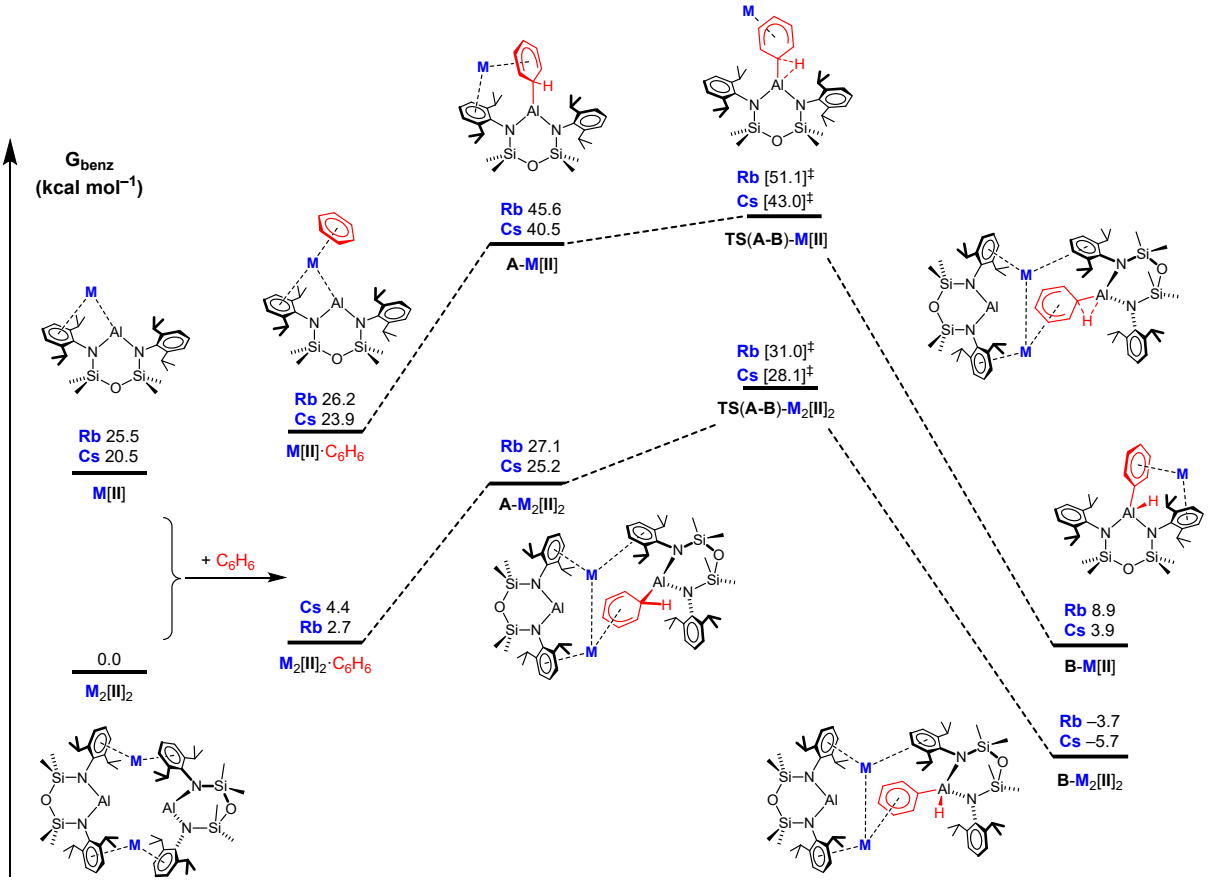
Donor NBO (Unit)	Acceptor NBO (Unit)	$\Delta E^{(2)}$ (kcal/mol)
LP_{Al1}	n_{Rb3}*	10.2
LP_{Al1}	r_{Rb3}*	1.4
LP_{Al1}	r_{Rb3}*	0.8
LP_{Al1}	r_{Rb3}*	0.3
LP_{Al1}	n_{Rb4}*	10.2
LP_{Al1}	r_{Rb4}*	1.4
LP_{Al1}	r_{Rb4}*	0.6
LP_{Al1}	r_{Rb4}*	0.4

Donor NBO (Unit)	Acceptor NBO (Unit)	$\Delta E^{(2)}$ (kcal/mol)
LP_{Al2}	n_{Rb3}*	10.2
LP_{Al2}	r_{Rb3}*	1.4
LP_{Al2}	r_{Rb3}*	0.6
LP_{Al2}	r_{Rb3}*	0.3
LP_{Al2}	n_{Rb4}*	10.2
LP_{Al2}	r_{Rb4}*	1.4
LP_{Al2}	r_{Rb4}*	0.6
LP_{Al2}	r_{Rb4}*	0.3

Table S7: Wiberg Bond Indices (WBI) for Computed Structures at BP86/BS1 level with NBO3.1

M		Al-M	Al1-M1	Al1-M2		Al2-M1	Al2-M2		Al1-Al2	M1-M2
	Li$_2$[**II**]$_2$	-	0.2681	0.0945	0.3626	0.1042	0.2664	0.3706	0.0842	0.0493
Li	**Li**[**II**]	0.3040	-	-		-	-		-	-
	[**II**]**Li**·2Et$_2$O	0.2259	-	-		-	-		-	-
Difference: ***Li**$_2$[**II**]$_2$ – [**II**]Li·2Et$_2$O)*		-	0.0422	-0.1314	0.1367	-0.1217	0.0405	0.1447		
	Na$_2$[**II**]$_2$	-	0.0926	0.1712	0.2638	0.1712	0.0926	0.2638	0.0578	0.0312
Na	**Na**[**II**]	0.3132	-	-		-	-		-	-
	[**II**]**Na**·2Et$_2$O	0.2506	-	-		-	-		-	-
Difference: ***Na**$_2$[**II**]$_2$ – [**II**]Na·2Et$_2$O)*		-	-0.1515	-0.0729	0.0197	-0.0729	-0.1515	0.0197		
	K$_2$[**II**]$_2$	-	0.1296	0.1296	0.2592	0.1296	0.1296	0.2592	0.0474	0.0227
K	**K**[**II**]	0.2639	-	-		-	-		-	-
	[**II**]**K**·2Et$_2$O	0.2237	-	-		-	-		-	-
Difference: ***K**$_2$[**II**]$_2$ – [**II**]K·2Et$_2$O)*			-0.0941	-0.0941	0.0355	-0.0941	-0.0941	0.0355		
	Rb$_2$[**II**]$_2$	-	0.1327	0.1327	0.2654	0.1327	0.1327	0.2654	0.0382	0.0229
Rb	**Rb**[**II**]	0.2596	-	-		-	-		-	-
	[**II**]**Rb**·2Et$_2$O	0.2084	-	-		-	-		-	-
Difference: ***Rb**$_2$[**II**]$_2$ – [**II**]Rb·2Et$_2$O)*			-0.0757	-0.0757	0.0570	-0.0757	-0.0757	0.0570		
	Cs$_2$[**II**]$_2$	-	0.1430	0.1428	0.2858	0.1430	0.1429	0.2859	0.0192	0.0176
Cs	**Cs**[**II**]	0.2463	-	-		-	-		-	-
	[**II**]**Cs**·2Et$_2$O	0.2177	-	-		-	-		-	-
Difference: ***Cs**$_2$[**II**]$_2$ – [II]Cs·2Et$_2$O)*			-0.0747	-0.0749	0.0681	-0.0747	-0.0748	0.0682		

Figure S25 Figure 3 DFT-calculated free energy profile (BP86-D3BJ/BS2(C_6H_6)//BP86/BS1) in kcal mol^{-1} for the C-H activation of benzene relative to 1 (M = Rb) or 2 (M = Cs)



Cartesian Coordinates and Computed Energies (in Hartrees) for Calculated Structures

Rb_2**[II]**$_2$
SCF (BP86) Energy = -2627.33593071
Enthalpy 0K = -2626.004943
Enthalpy 298K = -2625.909983
Free Energy 298K = -2626.145726
Lowest Frequency = 8.7309 cm^{-1}
Second Frequency = 10.6775 cm^{-1}
SCF (BP86-D3BJ) Energy = -2627.78655148
SCF (Et2O) Energy = -2627.34814702
SCF (C6H6) Energy = -2627.34348865
SCF (BS2) Energy = -4251.34800396

Al	-2.96396	-0.00016	0.00024
Al	2.96411	-0.00028	0.00025
Rb	-0.00001	2.43676	0.00211
Rb	-0.00010	-2.43716	0.00395
Si	-5.86555	1.14759	-1.06574
Si	-5.86750	-1.14768	1.06025
Si	5.86667	1.14786	1.06076
Si	5.86660	-1.14690	-1.06583
O	-6.51929	-0.00088	-0.00424
O	6.51935	0.00387	-0.00620
N	-4.16275	1.39550	-0.63068
N	-4.16378	-1.39579	0.62901
N	4.16297	1.39588	0.62957
N	4.16378	-1.39511	-0.63091
C	-3.51774	2.65443	-0.80180
C	-3.43020	3.57500	0.30012
C	-2.68807	4.76566	0.16107
H	-2.63301	5.46175	1.00658
C	-2.03985	5.09239	-1.03971
H	-1.48580	6.03270	-1.13560
C	-2.13899	4.20929	-2.12429
H	-1.65366	4.46779	-3.07357
C	-2.86396	3.00172	-2.03373
C	-4.12381	3.28304	1.63165
H	-4.79787	2.42836	1.44985
C	-4.97260	4.47004	2.13526
H	-4.34860	5.33878	2.41202
H	-5.54130	4.17805	3.03529
H	-5.69150	4.80529	1.36929
C	-3.10863	2.84321	2.71119
H	-2.56603	1.93114	2.39675
H	-3.61743	2.62004	3.66586
H	-2.36560	3.63918	2.90672
C	-2.94116	2.10161	-3.26715
H	-3.56021	1.23415	-2.98647
C	-1.55612	1.55995	-3.68506
H	-0.85489	2.37770	-3.93416
H	-1.64299	0.91704	-4.57870
H	-1.11054	0.95013	-2.87822
C	-3.62430	2.82207	-4.45158
H	-4.62026	3.20458	-4.17109
H	-3.74876	2.13328	-5.30565
H	-3.02706	3.68234	-4.80370
C	-6.87340	2.74535	-0.90634
H	-7.90781	2.57516	-1.25045
H	-6.43913	3.55396	-1.51861
H	-6.91541	3.09081	0.13916
C	-6.13103	0.42759	-2.80529
H	-5.50768	-0.46857	-2.96460
H	-5.89718	1.15427	-3.60110
H	-7.18765	0.12903	-2.91900
C	-3.51912	-2.65463	0.80184
C	-2.86749	-3.00122	2.03509
C	-2.14259	-4.20869	2.12753
H	-1.65884	-4.46663	3.07777
C	-2.04164	-5.09240	1.04363
H	-1.48778	-6.03266	1.14099
C	-2.68786	-4.76639	-0.15843
H	-2.63146	-5.46302	-1.00340
C	-3.42970	-3.57578	-0.29944
C	-2.94710	-2.10051	3.26791
H	-3.56581	-1.23331	2.98566
C	-3.63232	-2.82052	4.45143
H	-4.62774	-3.20320	4.16929
H	-3.75836	-2.13137	5.30497
H	-3.03566	-3.68060	4.80499
C	-1.56296	-1.55832	3.68806
H	-0.86189	-2.37578	3.93864
H	-1.65154	-0.91513	4.58133
H	-1.11625	-0.94865	2.88172
C	-4.12076	-3.28427	-1.63239
H	-4.79556	-2.42985	-1.45210
C	-3.10351	-2.84403	-2.70981
H	-2.35976	-3.63972	-2.90379
H	-2.56191	-1.93176	-2.39420
H	-3.61039	-2.62102	-3.66553
C	-4.96800	-4.47164	-2.13770
H	-4.34308	-5.34014	-2.41315
H	-5.53495	-4.17992	-3.03891
H	-5.68836	-4.80714	-1.37321
C	-6.13625	-0.42575	2.79851
H	-5.51334	0.47070	2.95795
H	-5.90358	-1.15155	3.59548
H	-7.19312	-0.12731	2.91013
C	-6.87481	-2.74578	0.90085
H	-7.90984	-2.57538	1.24300
H	-6.44144	-3.55363	1.51476
H	-6.91495	-3.09241	-0.14433
C	3.51796	2.65446	0.80260
C	2.86591	3.00053	2.03577
C	2.14081	4.20786	2.12839
H	1.65671	4.46540	3.07856
C	2.04003	5.09189	1.04473
H	1.48597	6.03202	1.14223
C	2.68665	4.76637	-0.15725
H	2.63036	5.46325	-1.00202
C	3.42871	3.57592	-0.29842
C	2.94548	2.09944	3.26831
H	3.56385	1.23213	2.98565
C	3.63127	2.81893	4.45182
H	4.62686	3.20110	4.16955
H	3.75708	2.12962	5.30527
H	3.03513	3.67930	4.80553
C	1.56127	1.55761	3.68870
H	0.86059	2.37520	3.93987
H	1.64993	0.91400	4.58165

H	1.11401	0.94847	2.88226
C	4.12023	3.28487	-1.63124
H	4.79524	2.43063	-1.45094
C	4.96722	4.47260	-2.13612
H	4.34210	5.34093	-2.41167
H	5.53457	4.18120	-3.03718
H	5.68720	4.80828	-1.37136
C	3.10339	2.84452	-2.70901
H	2.56204	1.93199	-2.39375
H	3.61058	2.62190	-3.66466
H	2.35943	3.64000	-2.90301
C	6.87318	2.74676	0.90470
H	7.90845	2.57602	1.24594
H	6.43976	3.55301	1.52066
H	6.91267	3.09579	-0.13971
C	6.13492	0.42265	2.79773
H	5.51232	-0.47438	2.95507
H	5.90133	1.14682	3.59592
H	7.19187	0.12454	2.90948
C	3.51894	-2.65412	-0.80246
C	2.86480	-3.00087	-2.03435
C	2.13982	-4.20841	-2.12522
H	1.65422	-4.46649	-3.07447
C	2.04110	-5.09204	-1.04106
H	1.48708	-6.03233	-1.13721
C	2.68972	-4.76587	0.15965
H	2.63499	-5.46236	1.00485
C	3.43179	-3.57521	0.29905
C	2.94158	-2.10025	-3.26742
H	3.56098	-1.23305	-2.98671
C	1.55645	-1.55814	-3.68441
H	0.85496	-2.37567	-3.93354
H	1.64299	-0.91484	-4.57780
H	1.11138	-0.94867	-2.87703
C	3.62392	-2.82040	-4.45253
H	4.61983	-3.20347	-4.17268
H	3.74827	-2.13121	-5.30629
H	3.02616	-3.68023	-4.80483
C	4.12554	-3.28375	1.63061
H	4.79950	-2.42893	1.44910
C	3.11042	-2.84444	2.71042
H	2.56770	-1.93230	2.39637
H	3.61927	-2.62158	3.66513
H	2.36750	-3.64058	2.90571
C	4.97451	-4.47085	2.13366
H	4.35064	-5.33980	2.41007
H	5.54320	-4.17919	3.03380
H	5.69343	-4.80564	1.36751
C	6.87538	-2.74386	-0.90388
H	7.90930	-2.57397	-1.24961
H	6.44077	-3.55407	-1.51380
H	6.91881	-3.08690	0.14235
C	6.13246	-0.42936	-2.80632
H	5.50960	0.46694	-2.96681
H	5.89830	-1.15694	-3.60122
H	7.18924	-0.13150	-2.92033

Rb**[II]**SCF (BP86) Energy = -1313.64215778
Enthalpy 0K = -1312.976984
Enthalpy 298K = -1312.930195
Free Energy 298K = -1313.057310
Lowest Frequency = 15.5489 cm^{-1}
Second Frequency = 20.4748 cm^{-1}
SCF (BP86-D3BJ) Energy = -1313.85125899
SCF (Et2O) Energy = -1313.66191386
SCF (C6H6) Energy = -1313.65486116
SCF (BS2) Energy = -2125.65071951

Rb	-2.39997	-1.91466	-2.28783
Si	-0.73719	1.86027	1.80814
Si	2.00994	0.40001	2.06122
Al	0.15912	-0.29748	-0.52993
O	0.71742	1.39800	2.53717
N	-1.16044	0.63084	0.59841
N	1.83265	0.02714	0.33574
C	-2.49960	0.26300	0.31343
C	-3.26768	0.94422	-0.69664
C	-4.53780	0.45116	-1.06642
H	-5.11362	0.98796	-1.83090
C	-5.08729	-0.69420	-0.47052
H	-6.08178	-1.05214	-0.76039
C	-4.35678	-1.34845	0.53393
H	-4.79067	-2.22720	1.02671
C	-3.08815	-0.88996	0.94682
C	-2.74673	2.20857	-1.38086
H	-1.74736	2.40363	-0.95976
C	-3.65000	3.42463	-1.07367
H	-3.76550	3.57536	0.01285
H	-3.22034	4.34610	-1.50429
H	-4.66170	3.29790	-1.49972
C	-2.57439	2.02995	-2.90583
H	-3.52879	1.76676	-3.39948
H	-2.21147	2.96430	-3.36840
H	-1.83055	1.24338	-3.12999
C	-2.36298	-1.63608	2.06820
H	-1.48021	-1.02648	2.32632
C	-3.23763	-1.78432	3.33246
H	-4.10750	-2.44339	3.15898
H	-2.64917	-2.22844	4.15407
H	-3.62088	-0.80850	3.67375
C	-1.84670	-3.01582	1.60049
H	-1.12994	-2.90778	0.76448
H	-1.32686	-3.54087	2.42121
H	-2.67957	-3.66383	1.26632
C	-2.05493	1.99050	3.16679
H	-1.80442	2.81405	3.85713
H	-3.05246	2.19441	2.74140
H	-2.11496	1.06122	3.75589
C	-0.44010	3.59233	1.08242
H	0.25835	3.55452	0.22963
H	-1.37480	4.06864	0.74119
H	0.00611	4.24057	1.85648
C	3.62932	1.31371	2.42597
H	3.72410	1.49155	3.51085
H	4.50150	0.72524	2.09577
H	3.66229	2.28926	1.91484
C	1.88901	-1.12102	3.19592
H	0.97055	-1.69590	2.98755
H	2.74990	-1.79923	3.07474
H	1.85499	-0.79758	4.25083
C	3.01223	-0.16655	-0.46542
C	3.57677	0.94242	-1.17692
C	4.71041	0.74414	-1.98637
H	5.13486	1.59606	-2.52968
C	5.30673	-0.51636	-2.11421
H	6.19087	-0.65089	-2.74699
C	4.75399	-1.60112	-1.42697
H	5.21110	-2.59276	-1.53033
C	3.61810	-1.45548	-0.60513
C	2.93468	2.32837	-1.11191
H	2.29210	2.33781	-0.21439
C	3.95429	3.47814	-0.97880
H	4.57230	3.59377	-1.88712
H	3.43025	4.43721	-0.82040
H	4.63781	3.31655	-0.12810

C	2.01547	2.55312	-2.33476
H	1.23384	1.77171	-2.39028
H	1.51701	3.53867	-2.28404
H	2.59371	2.50937	-3.27525
C	3.05884	-2.69775	0.08888
H	2.21968	-2.36295	0.72179
C	4.10507	-3.37906	0.99880
H	4.51902	-2.67322	1.73895
H	3.65456	-4.22620	1.54648
H	4.95376	-3.77759	0.41452
C	2.49122	-3.70596	-0.93630
H	2.06299	-4.58716	-0.42373
H	1.69851	-3.23504	-1.54377
H	3.27732	-4.06566	-1.62448

Rb**[II]**·Et_2O
SCF (BP86) Energy = -1780.97552045
Enthalpy 0K = -1780.043005
Enthalpy 298K = -1779.977873
Free Energy 298K = -1780.154142
Lowest Frequency = 9.8913 cm^{-1}
Second Frequency = 11.0329 cm^{-1}
SCF (BP86-D3BJ) Energy = -1781.24095156
SCF (Et2O) Energy = -1780.98996196
SCF (BS2) Energy = -2593.10687777

Al	0.47550	-0.44087	-0.01276
Si	3.10895	-2.10094	0.99661
Si	0.94208	-3.63345	-0.62894
O	2.38494	-3.43752	0.24081
N	2.36273	-0.62038	0.36809
N	-0.13123	-2.26968	-0.26010
C	3.14704	0.56458	0.19588
C	3.75446	0.84468	-1.07405
C	4.47580	2.03995	-1.25505
H	4.93950	2.24057	-2.22820
C	4.62423	2.97185	-0.21895
H	5.20046	3.89077	-0.37504
C	4.03787	2.70166	1.02268
H	4.15643	3.42182	1.84193
C	3.30446	1.52001	1.25344
C	3.60762	-0.12307	-2.24819
H	3.25492	-1.07880	-1.82378
C	2.52166	0.36893	-3.23218
H	2.79542	1.34874	-3.66443
H	1.54974	0.48782	-2.71723
H	2.38648	-0.34494	-4.06516
C	4.93388	-0.38975	-2.99038
H	5.72635	-0.71847	-2.29706
H	5.30311	0.50792	-3.51839
H	4.79459	-1.17851	-3.75051
C	2.70533	1.29477	2.64185
H	2.19048	0.32000	2.61217
C	1.64898	2.36516	2.99570
H	0.83470	2.36418	2.24932
H	2.08925	3.37858	3.01919
H	1.20722	2.16743	3.98931
C	3.79680	1.23392	3.73422
H	4.32604	2.19903	3.83173
H	4.55436	0.46578	3.50437
H	3.35446	0.99626	4.71830
C	4.97002	-2.16352	0.63849
H	5.16775	-2.19130	-0.44520
H	5.40928	-3.06995	1.08918
H	5.48843	-1.28531	1.05863
C	2.83630	-2.37234	2.85998
H	3.16879	-3.38721	3.13945
H	1.76828	-2.28202	3.12109
H	3.39993	-1.64922	3.47283
C	1.46215	-3.74114	-2.45566
H	2.26619	-4.48944	-2.56600
H	1.84872	-2.77308	-2.81618
H	0.62712	-4.04151	-3.11045
C	0.17729	-5.29316	-0.11966
H	0.03366	-5.34864	0.97146
H	0.84319	-6.12092	-0.41814
H	-0.80186	-5.44959	-0.60294
C	-1.54576	-2.46045	-0.19836
C	-2.37126	-2.33298	-1.36478
C	-3.76999	-2.46675	-1.24952
H	-4.38775	-2.38263	-2.15268
C	-4.38558	-2.72157	-0.01783
H	-5.47298	-2.84162	0.04820
C	-3.58404	-2.84865	1.12529
H	-4.05679	-3.06220	2.09148
C	-2.18255	-2.73044	1.06050
C	-1.77650	-2.07207	-2.74888
H	-0.68242	-2.02632	-2.62104
C	-2.10263	-3.21482	-3.73702
H	-3.18756	-3.28299	-3.93562
H	-1.77886	-4.19255	-3.34220
H	-1.59727	-3.05127	-4.70554
C	-2.22863	-0.71392	-3.32995
H	-1.90557	0.11328	-2.67232
H	-3.32770	-0.66318	-3.43747
H	-1.78465	-0.54524	-4.32744
C	-1.36358	-2.87599	2.34308
H	-0.31221	-2.99683	2.02993
C	-1.44034	-1.59022	3.19746
H	-2.48231	-1.38078	3.50270
H	-1.07039	-0.71906	2.62418
H	-0.82981	-1.68372	4.11390
C	-1.76018	-4.10959	3.18139
H	-1.73185	-5.03335	2.57946
H	-2.77744	-4.01662	3.60293
H	-1.06653	-4.23299	4.03159
O	-0.43887	4.65059	-0.70352
O	-4.72775	1.74986	0.40581
C	-0.82943	6.03572	-0.71032
H	-1.87944	6.05322	-1.05619
H	-0.23435	6.59644	-1.45788
C	-0.71549	6.68902	0.67016
H	0.32356	6.67894	1.03891
H	-1.34552	6.16321	1.40752
H	-1.04552	7.74140	0.62485
C	0.99051	4.44095	-0.84730
H	1.19248	3.44087	-0.42427
H	1.54221	5.17286	-0.22620
C	1.44991	4.49670	-2.30316
H	1.28719	5.48957	-2.75680
H	0.91703	3.74438	-2.90801
H	2.52779	4.26881	-2.35080
C	-5.37533	1.22839	-0.77519
H	-5.30349	0.12177	-0.77742
H	-4.77344	1.59821	-1.62581
C	-6.82535	1.69263	-0.93512
H	-7.47752	1.30369	-0.13610
H	-7.22922	1.32963	-1.89578
H	-6.88714	2.79364	-0.92844
C	-5.14842	1.07981	1.61206
H	-4.95406	-0.00852	1.51562
H	-6.23748	1.21961	1.76394
C	-4.38431	1.66430	2.79428
H	-4.53332	2.75548	2.86029
H	-3.30359	1.45107	2.72521
H	-4.74476	1.21392	3.73374

Rb -1.87743 2.24200 -0.08510

Cs_2**[II]**$_2$
SCF (BP86) Energy = -2619.47428475
Enthalpy 0K = -2618.143284
Enthalpy 298K = -2618.048495
Free Energy 298K = -2618.283671
Lowest Frequency = 7.7543 cm^{-1}
Second Frequency = 10.5226 cm^{-1}
SCF (BP86-D3BJ) Energy = -2619.92295439
SCF (Et2O) Energy = -2619.48607978
SCF (C6H6) Energy = -2619.48154800
SCF (BS2) Energy = -4243.48686915

Al	3.05446	0.00015	0.00038
Al	-3.05473	-0.00039	-0.00102
Cs	-0.00014	2.56123	-0.00135
Cs	-0.00005	-2.56311	-0.00457
Si	5.96498	1.12217	1.08899
Si	5.96721	-1.11975	-1.08334
Si	-5.96705	1.11956	-1.08579
Si	-5.96542	-1.12100	1.08800
O	6.62706	0.00022	0.00453
O	-6.62721	-0.00081	0.00151
N	4.26465	1.38422	0.65044
N	4.26621	-1.38303	-0.64831
N	-4.26628	1.38289	-0.65000
N	-4.26494	-1.38366	0.65049
C	3.64487	2.65285	0.84228
C	3.58210	3.59629	-0.24212
C	2.88039	4.80767	-0.07777
H	2.84444	5.52081	-0.90996
C	2.24733	5.13263	1.13177
H	1.72374	6.08832	1.24732
C	2.32038	4.22571	2.19855
H	1.84438	4.48025	3.15365
C	3.00556	2.99753	2.08231
C	4.25725	3.30282	-1.58266
H	4.92628	2.44205	-1.41088
C	5.10886	4.48197	-2.09867
H	4.48871	5.35394	-2.37431
H	5.66724	4.18203	-3.00246
H	5.83715	4.81572	-1.34092
C	3.22352	2.87061	-2.64757
H	2.68279	1.95918	-2.32717
H	3.71626	2.64793	-3.61091
H	2.48121	3.67088	-2.82908
C	3.05304	2.06988	3.29666
H	3.66031	1.19814	3.00374
C	1.65297	1.54271	3.68153
H	0.96029	2.36757	3.93205
H	1.71402	0.88323	4.56536
H	1.21423	0.95323	2.85614
C	3.73186	2.74945	4.50711
H	4.73690	3.12358	4.24868
H	3.83531	2.03701	5.34440
H	3.14357	3.60938	4.87498
C	6.97576	2.72232	0.97484
H	8.01076	2.53889	1.31031
H	6.54556	3.51341	1.61221
H	7.01561	3.09897	-0.05998
C	6.21940	0.36061	2.81276
H	5.58993	-0.53512	2.94879
H	5.98650	1.07014	3.62418
H	7.27378	0.05325	2.92368
C	3.64748	-2.65186	-0.84206
C	3.01050	-2.99606	-2.08348
C	2.32633	-4.22460	-2.20177
H	1.85216	-4.47878	-3.15789
C	2.25203	-5.13232	-1.13575
H	1.72935	-6.08832	-1.25293
C	2.88276	-4.80781	0.07515
H	2.84579	-5.52156	0.90677
C	3.58338	-3.59607	0.24162
C	3.05946	-2.06750	-3.29708
H	3.66546	-1.19546	-3.00240
C	3.74107	-2.74561	-4.50677
H	4.74601	-3.11894	-4.24678
H	3.84533	-2.03253	-5.34342
H	3.15427	-3.60588	-4.87622
C	1.65963	-1.54124	-3.68412
H	0.96819	-2.36649	-3.93675
H	1.72175	-0.88084	-4.56718
H	1.21882	-0.95298	-2.85895
C	4.25579	-3.30291	1.58361
H	4.92497	-2.44191	1.41352
C	3.21975	-2.87126	2.64650
H	2.47734	-3.67181	2.82634
H	2.67936	-1.95996	2.32513
H	3.71045	-2.64858	3.61088
C	5.10661	-4.48202	2.10101
H	4.48610	-5.35421	2.37515
H	5.66308	-4.18219	3.00602
H	5.83652	-4.81540	1.34466
C	6.22419	-0.35545	-2.80553
H	5.59461	0.54022	-2.94137
H	5.99279	-1.06396	-3.61829
H	7.27864	-0.04761	-2.91439
C	6.97831	-2.71975	-0.97010
H	8.01412	-2.53515	-1.30240
H	6.55010	-3.50956	-1.61041
H	7.01555	-3.09874	0.06396
C	-3.64721	2.65168	-0.84323
C	-3.00911	2.99587	-2.08413
C	-2.32429	4.22415	-2.20158
H	-1.84920	4.47830	-3.15725
C	-2.25045	5.13168	-1.13531
H	-1.72714	6.08741	-1.25186
C	-2.88244	4.80723	0.07495
H	-2.84583	5.52079	0.90675
C	-3.58372	3.59574	0.24059
C	-3.05764	2.06763	-3.29798
H	-3.66406	1.19569	-3.00384
C	-3.73845	2.74627	-4.50783
H	-4.74345	3.11972	-4.24829
H	-3.84239	2.03348	-5.34477
H	-3.15124	3.60653	-4.87668
C	-1.65778	1.54105	-3.68442
H	-0.96595	2.36614	-3.93648
H	-1.71965	0.88089	-4.56769
H	-1.21758	0.95248	-2.85915
C	-4.25734	3.30255	1.58196
H	-4.92699	2.44209	1.41104
C	-5.10771	4.48201	2.09927
H	-4.48682	5.35367	2.37421
H	-5.66501	4.18218	3.00377
H	-5.83688	4.81618	1.34254
C	-3.22235	2.86965	2.64535
H	-2.68225	1.95825	2.32377
H	-3.71385	2.64660	3.60925
H	-2.47962	3.66968	2.82625
C	-6.97830	2.71948	-0.97285
H	-8.01403	2.53481	-1.30537
H	-6.54999	3.50926	-1.61313
H	-7.01579	3.09857	0.06116
C	-6.22305	0.35537	-2.80817

H	-5.59302	-0.54002	-2.94377
H	-5.99153	1.06406	-3.62074
H	-7.27732	0.04710	-2.91758
C	-3.64519	-2.65204	0.84401
C	-3.00555	-2.99493	2.08442
C	-2.32036	-4.22295	2.20224
H	-1.84411	-4.47610	3.15759
C	-2.24768	-5.13146	1.13678
H	-1.72416	-6.08703	1.25362
C	-2.88106	-4.80825	-0.07308
H	-2.84531	-5.52259	-0.90425
C	-3.58269	-3.59702	-0.23907
C	-3.05286	-2.06566	3.29753
H	-3.65966	-1.19402	3.00331
C	-1.65260	-1.53875	3.68209
H	-0.96060	-2.36363	3.93436
H	-1.71362	-0.87768	4.56473
H	-1.21305	-0.95112	2.85582
C	-3.73229	-2.74337	4.50868
H	-4.73747	-3.11731	4.25050
H	-3.83555	-2.02986	5.34508
H	-3.14450	-3.60316	4.87769
C	-4.25785	-3.30527	-1.58000
H	-4.92716	-2.44450	-1.40926
C	-3.22417	-2.87387	-2.64529
H	-2.68386	-1.96183	-2.32590
H	-3.71689	-2.65250	-3.60895
H	-2.48155	-3.67408	-2.82582
C	-5.10904	-4.48523	-2.09483
H	-4.48859	-5.35729	-2.36953
H	-5.66746	-4.18640	-2.99897
H	-5.83727	-4.81844	-1.33678
C	-6.97628	-2.72125	0.97588
H	-8.01145	-2.53714	1.31043
H	-6.54654	-3.51130	1.61486
H	-7.01556	-3.09966	-0.05831
C	-6.22011	-0.35712	2.81069
H	-5.59035	0.53853	2.94581
H	-5.98755	-1.06578	3.62299
H	-7.27441	-0.04931	2.92108

Cs**[II]**
SCF (BP86) Energy = -1309.71188222
Enthalpy 0K = -1309.046848
Enthalpy 298K = -1309.000030
Free Energy 298K = -1309.127669
Lowest Frequency = 15.9626 cm^{-1}
Second Frequency = 19.6774 cm^{-1}
SCF (BP86-D3BJ) Energy = -1309.92209700
SCF (Et2O) Energy = -1309.73013274
SCF (C6H6) Energy = -1309.72362370
SCF (BS2) Energy = -2121.72167525

Cs	-2.64051	-2.37092	-1.26733
Si	-0.30995	2.59683	1.09488
Si	2.32503	1.07571	1.77256
Al	0.26208	-0.34507	-0.32486
O	1.15587	2.30665	1.88692
N	-0.90037	1.05454	0.44240
N	2.01022	0.12559	0.30960
C	-2.28015	0.74383	0.36313
C	-3.06265	1.07978	-0.79874
C	-4.39757	0.63270	-0.90180
H	-4.98167	0.90572	-1.78978
C	-4.99856	-0.13677	0.10590
H	-6.04107	-0.46218	0.01354
C	-4.25030	-0.45102	1.25161
H	-4.71949	-1.03036	2.05628
C	-2.91650	-0.01983	1.40722
C	-2.48446	1.92319	-1.93550
H	-1.44932	2.16834	-1.64799
C	-3.26644	3.24403	-2.11377
H	-3.30996	3.81551	-1.17141
H	-2.78549	3.87904	-2.87830
H	-4.30679	3.06209	-2.43914
C	-2.41583	1.14490	-3.26852
H	-3.41480	0.79522	-3.59152
H	-2.01478	1.78521	-4.07355
H	-1.74304	0.27185	-3.18011
C	-2.16581	-0.38338	2.68919
H	-1.22918	0.19981	2.67512
C	-2.95321	-0.00845	3.96308
H	-3.87052	-0.61396	4.07810
H	-2.33297	-0.18235	4.85949
H	-3.25217	1.05278	3.95386
C	-1.77162	-1.87769	2.71179
H	-1.10732	-2.12271	1.86079
H	-1.23018	-2.12971	3.64073
H	-2.66566	-2.52887	2.66077
C	-1.52033	3.33444	2.35691
H	-1.16137	4.32348	2.68944
H	-2.52520	3.46632	1.92044
H	-1.61296	2.69140	3.24699
C	0.05406	3.91011	-0.23136
H	0.69203	3.50190	-1.03317
H	-0.86705	4.30562	-0.69199
H	0.59121	4.75682	0.23025
C	4.03566	1.89041	1.73902
H	4.21198	2.43334	2.68334
H	4.83267	1.13757	1.62033
H	4.11991	2.61042	0.90924
C	2.14618	0.08687	3.38766
H	1.17467	-0.43490	3.42497
H	2.94210	-0.66777	3.50171
H	2.19780	0.77094	4.25253
C	3.11693	-0.44589	-0.40927
C	3.70736	0.27663	-1.49760
C	4.76501	-0.30113	-2.22380
H	5.20829	0.25648	-3.05685
C	5.26227	-1.57125	-1.90719
H	6.08850	-2.00372	-2.48214
C	4.68529	-2.28073	-0.84954
H	5.06473	-3.27955	-0.60152
C	3.62221	-1.74733	-0.09330
C	3.17331	1.64678	-1.91524
H	2.58084	2.02694	-1.06500
C	4.28219	2.67479	-2.22089
H	4.86055	2.40678	-3.12317
H	3.84105	3.67064	-2.40343
H	4.99387	2.76368	-1.38268
C	2.21166	1.50788	-3.11805
H	1.37147	0.83001	-2.87572
H	1.79299	2.48882	-3.40948
H	2.73567	1.08541	-3.99436
C	3.02880	-2.59920	1.02900
H	2.25714	-1.98565	1.52394
C	4.08515	-2.98936	2.08660
H	4.58988	-2.10034	2.50170
H	3.61741	-3.54030	2.92231
H	4.86748	-3.64118	1.65805
C	2.32912	-3.85855	0.46876
H	1.87619	-4.45134	1.28505
H	1.53283	-3.57407	-0.24126
H	3.04287	-4.51132	-0.06551

Cs**[II]**·Et_2O

SCF (BP86) Energy = -1777.04106501
Enthalpy 0K = -1776.108831
Enthalpy 298K = -1776.043598
Free Energy 298K = -1776.220871
Lowest Frequency = 5.5688 cm^{-1}
Second Frequency = 9.8885 cm^{-1}
SCF (BP86-D3BJ) Energy = -1777.30849632
SCF (Et2O) Energy = -1777.05532247
SCF (BS2) Energy = -2589.17393918

Al	0.64548	-0.45657	-0.00911
Si	3.39306	-1.87366	1.07279
Si	1.43216	-3.59948	-0.61150
O	2.82871	-3.27320	0.29397
N	2.53688	-0.47058	0.41109
N	0.22753	-2.34247	-0.27108
C	3.22040	0.77537	0.24735
C	3.84181	1.09312	-1.00695
C	4.46333	2.34403	-1.18150
H	4.94005	2.57360	-2.14184
C	4.49782	3.29635	-0.15357
H	4.99774	4.25981	-0.30416
C	3.89762	2.98988	1.07293
H	3.92811	3.72619	1.88589
C	3.26157	1.75179	1.29653
C	3.81652	0.10071	-2.16949
H	3.55529	-0.88067	-1.73727
C	2.70392	0.46487	-3.17905
H	2.88004	1.46448	-3.61669
H	1.71422	0.48302	-2.68469
H	2.66308	-0.26686	-4.00662
C	5.17599	-0.03936	-2.88559
H	5.98599	-0.27279	-2.17403
H	5.46003	0.88240	-3.42478
H	5.13188	-0.85102	-3.63298
C	2.63986	1.48853	2.66821
H	2.21404	0.47178	2.63429
C	1.48112	2.46345	2.97308
H	0.69595	2.37949	2.20077
H	1.82763	3.51272	2.99585
H	1.02624	2.23790	3.95496
C	3.69577	1.53456	3.79551
H	4.13671	2.54273	3.89672
H	4.52356	0.83204	3.60040
H	3.24342	1.27023	4.76823
C	5.26478	-1.76288	0.78795
H	5.50617	-1.76572	-0.28721
H	5.76821	-2.62745	1.25354
H	5.68290	-0.84282	1.22978
C	3.07228	-2.16439	2.92555
H	3.48217	-3.14405	3.22687
H	1.99043	-2.16799	3.14131
H	3.54299	-1.39044	3.55472
C	2.00353	-3.65594	-2.42536
H	2.87448	-4.32800	-2.51705
H	2.30852	-2.65582	-2.77648
H	1.21433	-4.02977	-3.09911
C	0.81263	-5.32604	-0.12470
H	0.64301	-5.39978	0.96157
H	1.56194	-6.08622	-0.40478
H	-0.13292	-5.57198	-0.63682
C	-1.16207	-2.66822	-0.25500
C	-1.96257	-2.59916	-1.44385
C	-3.34500	-2.86684	-1.37294
H	-3.94215	-2.82528	-2.29282
C	-3.96763	-3.20386	-0.16490
H	-5.03930	-3.43191	-0.13412
C	-3.19052	-3.27547	1.00016
H	-3.66793	-3.55409	1.94724
C	-1.80606	-3.02134	0.97999
C	-1.35458	-2.26215	-2.80594
H	-0.27130	-2.13275	-2.64711
C	-1.56229	-3.40493	-3.82528
H	-2.63211	-3.55290	-4.05939
H	-1.17483	-4.36270	-3.43908
H	-1.04254	-3.18197	-4.77409
C	-1.89611	-0.93041	-3.37156
H	-1.63393	-0.09355	-2.69900
H	-2.99530	-0.95507	-3.48860
H	-1.45598	-0.71519	-4.36186
C	-1.01144	-3.10952	2.28316
H	0.05341	-3.15888	1.99725
C	-1.19478	-1.82875	3.12866
H	-2.25645	-1.68635	3.40361
H	-0.86531	-0.93762	2.56097
H	-0.60516	-1.87959	4.06208
C	-1.34215	-4.36435	3.11793
H	-1.24084	-5.28582	2.52028
H	-2.37088	-4.33834	3.52087
H	-0.65813	-4.43889	3.98145
O	-0.68184	4.58620	-0.72038
O	-5.05468	1.05139	0.48981
C	-1.10523	5.96038	-0.75638
H	-2.15135	5.94614	-1.11455
H	-0.51542	6.52349	-1.50655
C	-1.02472	6.64108	0.61343
H	0.01003	6.66574	0.99335
H	-1.64832	6.11099	1.35308
H	-1.38247	7.68316	0.54524
C	0.75396	4.40855	-0.83709
H	0.97204	3.41841	-0.39854
H	1.27890	5.15941	-0.21555
C	1.23832	4.45766	-2.28517
H	1.06035	5.44097	-2.75388
H	0.73474	3.68563	-2.89039
H	2.32206	4.25525	-2.30925
C	-5.62453	0.47485	-0.70366
H	-5.36247	-0.60155	-0.75804
H	-5.11465	0.98041	-1.54509
C	-7.13631	0.68562	-0.82531
H	-7.69469	0.15696	-0.03551
H	-7.49084	0.29751	-1.79565
H	-7.38711	1.75793	-0.76892
C	-5.31712	0.26236	1.66798
H	-4.90001	-0.75699	1.53021
H	-6.41012	0.16389	1.82465
C	-4.68610	0.95128	2.87240
H	-5.06415	1.98199	2.97896
H	-3.58579	0.98013	2.79427
H	-4.93339	0.39831	3.79353
Cs	-2.16817	2.02361	-0.13548

C-H Activation Mechanism

C_6H_6
SCF (BP86) Energy = -232.242070159
Enthalpy 0K = -232.144365
Enthalpy 298K = -232.138889
Free Energy 298K = -232.171907
Lowest Frequency = 397.4324 cm^{-1}
Second Frequency = 397.5218 cm^{-1}
SCF (BP86-D3) Energy = -232.258991628
SCF (C6H6) Energy = -232.243164330
SCF (BS2) Energy = -232.299995204

C	-1.39698	0.14820	0.00000
C	-0.82679	-1.13574	-0.00001
C	0.57013	-1.28391	0.00001
C	1.39699	-0.14815	-0.00000
C	0.82683	1.13570	-0.00001
C	-0.57018	1.28388	0.00001
H	-2.48620	0.26369	-0.00000
H	-1.47152	-2.02121	-0.00000
H	1.01475	-2.28493	0.00001
H	2.48619	-0.26379	0.00001
H	1.47144	2.02127	-0.00001
H	-1.01466	2.28497	0.00002

Cs**[II]**·$2C_6H_6$
SCF (BP86) Energy = -1774.20925404
Enthalpy 0K = -1773.348044
Enthalpy 298K = -1773.287275
Free Energy 298K = -1773.456421
Lowest Frequency = 5.7696 cm^{-1}
Second Frequency = 8.2054 cm^{-1}
SCF (BP86-D3) Energy = -1774.47565499
SCF (C6H6) Energy = -1774.21813603
SCF (BS2) Energy = -2586.33147077

Cs	-2.72372	0.30843	0.32156
Al	1.01780	0.02928	0.04650
N	1.00083	-1.93963	0.23867
N	2.82043	0.38556	-0.54550
C	-0.30748	-2.47024	0.36227
C	3.26910	1.73782	-0.37349
C	-0.95746	-2.58316	1.64146
C	-1.06603	-2.81415	-0.81287
C	-1.33941	3.09547	2.31033
C	-2.25417	2.61121	3.26372
C	-3.63337	2.83527	3.09662
C	-0.21135	-2.29421	2.94395
C	3.95810	2.11371	0.82688
C	3.00000	2.74694	-1.35344
C	-3.04936	-3.28386	0.55884
C	-3.18255	4.04991	1.03314
C	-1.80559	3.81730	1.19581
C	-2.30922	-2.98138	1.71133
C	-4.09858	3.55399	1.98051
C	-2.41557	-3.20178	-0.69083
C	4.23396	1.08958	1.92774
C	-0.13331	-3.54971	3.84136
C	3.41613	4.07289	-1.11837
C	3.17213	1.19705	3.04626
C	-0.82272	-1.10653	3.71883
C	4.35013	3.45185	1.01604
C	-0.43067	-2.75953	-2.20282
C	4.08842	4.43471	0.05332
C	2.25224	2.43716	-2.65041
C	-0.91831	-1.52874	-2.99947
C	0.87819	3.14350	-2.69251
C	5.65683	1.18487	2.51599
C	3.08567	2.79142	-3.90191
C	-0.65269	-4.05616	-3.01025
H	-0.26794	2.90567	2.42380
H	-1.89069	2.06148	4.13808
H	-4.34328	2.46617	3.84521
H	0.81362	-2.00529	2.66017
H	-4.09382	-3.60715	0.63548
H	-3.54203	4.62701	0.17416
H	-1.08955	4.19302	0.45801
H	-2.78682	-3.07011	2.69548
H	-5.17042	3.74620	1.86106
H	-2.97770	-3.46352	-1.59566
H	4.12021	0.09341	1.46599
H	-1.13470	-3.86830	4.18371
H	0.47708	-3.34879	4.73946
H	0.31808	-4.40049	3.30374
H	3.20411	4.83850	-1.87500
H	3.19623	2.19633	3.51793
H	3.34481	0.44198	3.83525
H	2.15576	1.04289	2.63614
H	-0.77640	-0.18143	3.11621
H	-0.26431	-0.92298	4.65396
H	-1.87731	-1.29699	3.99423
H	4.87268	3.73020	1.93864
H	0.65357	-2.63197	-2.04166
H	4.40452	5.47098	0.21654
H	2.06315	1.35049	-2.65824
H	-2.01618	-1.55360	-3.13774
H	-0.45394	-1.49563	-4.00134
H	-0.65492	-0.59134	-2.47269
H	0.25959	2.82836	-1.83363
H	0.33669	2.89332	-3.62385
H	0.98877	4.24251	-2.65232
H	6.42495	1.13665	1.72566
H	5.83654	0.35322	3.22007
H	5.81338	2.12375	3.07696
H	3.27604	3.87769	-3.96961
H	2.55601	2.49033	-4.82371
H	4.06658	2.28650	-3.88977
H	-0.31837	-4.94335	-2.44720
H	-0.08685	-4.01780	-3.95745
H	-1.71614	-4.20670	-3.27141
O	3.62367	-2.31669	-0.69693
Si	2.44866	-2.95769	0.33904
Si	3.85412	-0.77939	-1.38743
C	5.69268	-0.34020	-1.23954
H	5.89327	0.66965	-1.63486
H	6.02757	-0.36828	-0.19013
H	6.30029	-1.06147	-1.81248
C	3.42674	-1.00451	-3.22828
H	2.35357	-1.22526	-3.35886
H	3.66444	-0.10622	-3.82229
H	4.00057	-1.85068	-3.64473
C	2.09793	-4.74069	-0.21183
H	1.27924	-5.18948	0.37642
H	1.81924	-4.78338	-1.27716
H	2.99855	-5.36283	-0.07190
C	3.24882	-3.01096	2.06434
H	3.40256	-1.99467	2.46442
H	2.64150	-3.57816	2.78991
H	4.23608	-3.49992	1.99456
C	-6.12669	-0.55538	-1.33365
C	-5.24077	-0.67018	-2.42002
C	-4.66340	0.48276	-2.98219
C	-4.97397	1.75117	-2.45912

C	-5.86144	1.86588	-1.37405
C	-6.43659	0.71267	-0.81024
H	-6.58502	-1.45240	-0.90415
H	-5.00635	-1.65619	-2.83369
H	-3.98046	0.39348	-3.83322
H	-4.53476	2.64927	-2.90608
H	-6.11425	2.85406	-0.97619
H	-7.13890	0.80327	0.02543

Cs**[II]**·$3C_6H_6$

SCF (BP86) Energy = -2006.45370311
Enthalpy 0K = -2005.494362
Enthalpy 298K = -2005.426685
Free Energy 298K = -2005.615885
Lowest Frequency = 6.8178 cm^{-1}
Second Frequency = 7.5316 cm^{-1}
SCF (BP86-D3) Energy = -2006.75013626
SCF (C6H6) Energy = -2006.46267264
SCF (BS2) Energy = -2818.63129260

Cs	2.26325	-0.25651	0.34347
Al	-1.50703	-0.01065	-0.09083
N	-1.66624	-1.95727	-0.40105
N	-3.33361	0.51357	0.24458
C	-0.42555	-2.63954	-0.34266
C	-3.61736	1.91373	0.10146
C	0.42194	-2.76248	-1.49954
C	0.06668	-3.14691	0.91243
C	1.38230	3.16571	-1.35020
C	2.13190	3.26522	-2.53645
C	3.26488	4.09698	-2.58842
C	-0.03982	-2.29540	-2.88012
C	-4.06404	2.42660	-1.16106
C	-3.42046	2.83101	1.18318
C	2.18856	-3.79870	-0.14066
C	2.90321	4.73252	-0.26565
C	1.77057	3.90128	-0.21571
C	1.70518	-3.33511	-1.37312
C	3.65154	4.82983	-1.45199
C	1.36001	-3.70228	0.98861
C	-4.25347	1.50123	-2.36309
C	-0.08119	-3.46258	-3.89156
C	-3.66681	4.20430	0.98371
C	-3.01778	1.55689	-3.29042
C	0.81984	-1.13240	-3.42256
C	-4.29337	3.80680	-1.31042
C	-0.79262	-3.08172	2.17558
C	-4.10139	4.70031	-0.24936
C	-2.93018	2.37059	2.55609
C	-0.33701	-1.93534	3.10593
C	-1.51856	2.91903	2.86456
C	-5.54493	1.78129	-3.15907
C	-3.91837	2.74422	3.68314
C	-0.83851	-4.42140	2.94020
H	0.49000	2.52622	-1.30170
H	1.81774	2.71109	-3.42809
H	3.83785	4.18615	-3.51786
H	-1.06425	-1.90960	-2.75259
H	3.18286	-4.25362	-0.06575
H	3.19174	5.32112	0.61241
H	1.16750	3.84071	0.69713
H	2.33333	-3.43244	-2.26778
H	4.52547	5.48910	-1.49633
H	1.71906	-4.08689	1.95092
H	-4.31496	0.47414	-1.96323
H	0.92757	-3.86940	-4.08783
H	-0.49652	-3.12493	-4.85740
H	-0.70590	-4.29289	-3.52152
H	-3.51071	4.89926	1.81812
H	-2.86771	2.57753	-3.68661
H	-3.13169	0.86915	-4.14867
H	-2.10083	1.27469	-2.73899
H	0.74875	-0.25233	-2.75742
H	0.47004	-0.82187	-4.42307
H	1.88360	-1.42204	-3.51880
H	-4.62982	4.19056	-2.28053
H	-1.81565	-2.83808	1.84123
H	-4.28719	5.77155	-0.38427
H	-2.85312	1.27107	2.51612
H	0.71300	-2.07546	3.42632
H	-0.96340	-1.89002	4.01493
H	-0.41623	-0.95802	2.59136
H	-0.80085	2.57757	2.09742
H	-1.16831	2.56707	3.85290
H	-1.50954	4.02410	2.87719
H	-6.43329	1.77175	-2.50502
H	-5.68642	1.01416	-3.94084
H	-5.51569	2.76123	-3.66847
H	-4.00999	3.83930	3.79761
H	-3.57921	2.33736	4.65291
H	-4.92863	2.34967	3.48062
H	-1.14567	-5.25088	2.28167
H	-1.56022	-4.35985	3.77327
H	0.14150	-4.68592	3.37758
O	-4.43709	-2.08139	0.05699
Si	-3.17390	-2.79601	-0.81324
Si	-4.60665	-0.57247	0.82432
C	-6.34097	0.08645	0.43426
H	-6.49331	1.08864	0.86853
H	-6.50640	0.15719	-0.65285
H	-7.10452	-0.59089	0.85366
C	-4.50363	-0.95598	2.68566
H	-3.49065	-1.29494	2.96188
H	-4.74828	-0.07575	3.30351
H	-5.21375	-1.76123	2.94241
C	-3.10867	-4.63545	-0.34579
H	-2.25536	-5.14255	-0.82786
H	-3.01773	-4.77103	0.74404
H	-4.03385	-5.13961	-0.67395
C	-3.66303	-2.66479	-2.64704
H	-3.64706	-1.61711	-2.99144
H	-2.99588	-3.25214	-3.30056
H	-4.68953	-3.04864	-2.77992
C	4.90762	-0.68005	3.06479
C	3.80966	-0.80341	3.93513
C	2.97653	0.30351	4.17790
C	3.24438	1.53547	3.55421
C	4.34374	1.65963	2.68519
C	5.17443	0.55094	2.43796
H	5.56183	-1.53952	2.88311
H	3.60801	-1.75853	4.43118
H	2.12385	0.20847	4.85762
H	2.59998	2.39855	3.75080
H	4.55230	2.61916	2.20043
H	6.02519	0.64493	1.75515
C	6.49352	-1.36879	-1.76679
C	5.28931	-0.95201	-2.36033
C	4.90718	0.40067	-2.29895
C	5.72826	1.33656	-1.64442
C	6.93557	0.91898	-1.05795
C	7.31747	-0.43293	-1.11851
H	6.79637	-2.41980	-1.82226
H	4.65629	-1.67762	-2.88252
H	3.98139	0.73716	-2.77957
H	5.42373	2.38795	-1.60692
H	7.58669	1.64973	-0.56570

H 8.26325 -0.75543 -0.67000

Cs**[II]**·C_6H_6
SCF (BP86) Energy = -1541.96262208
Enthalpy 0K = -1541.199015
Enthalpy 298K = -1541.145501
Free Energy 298K = -1541.291538
Lowest Frequency = 11.1022 cm^{-1}
Second Frequency = 15.4649 cm^{-1}
SCF (BP86-D3) Energy = -1542.19800521
SCF (C6H6) Energy = -1541.97189325
SCF (BS2) Energy = -2354.02896210

Cs -3.15291 0.66871 -0.37164
Al 0.46809 0.03108 0.02532
N 0.17672 -1.92149 0.12145
N 2.37465 0.18646 -0.20298
C -1.18301 -2.29483 -0.02002
C 2.92496 1.47827 0.10061
C -2.06743 -2.36409 1.11430
C -1.74615 -2.51410 -1.32840
C -2.18128 3.94681 0.86433
C -3.14280 3.60590 1.83396
C -4.50953 3.59508 1.49996
C -1.55031 -2.18811 2.54226
C 3.39963 1.75787 1.42471
C 2.96645 2.52357 -0.87747
C -3.98791 -2.79007 -0.35996
C -3.95770 4.27884 -0.77305
C -2.59137 4.28752 -0.43827
C -3.44398 -2.60709 0.92021
C -4.91811 3.92747 0.19454
C -3.12998 -2.74491 -1.47013
C 3.33796 0.69756 2.52431
C -1.78614 -3.45829 3.39004
C 3.46985 3.79048 -0.51951
C 2.10101 0.92227 3.42416
C -2.15508 -0.94768 3.23683
C 3.89024 3.04026 1.73284
C -0.86759 -2.49058 -2.58005
C 3.93271 4.05853 0.77253
C 2.46129 2.31913 -2.30600
C -1.08502 -1.19894 -3.40063
C 1.20213 3.17023 -2.58800
C 4.62294 0.61642 3.37416
C 3.55622 2.60530 -3.35757
C -1.06507 -3.73884 -3.46665
H -1.11710 3.94164 1.11861
H -2.82450 3.35205 2.85045
H -5.25726 3.34193 2.25964
H -0.46417 -2.01939 2.46293
H -5.05752 -2.99182 -0.48890
H -4.27588 4.55797 -1.78361
H -1.84208 4.55915 -1.18879
H -4.10155 -2.66545 1.79692
H -5.98332 3.93545 -0.06139
H -3.54180 -2.91108 -2.47322
H 3.20166 -0.27366 2.01780
H -2.86345 -3.65889 3.53338
H -1.33265 -3.34726 4.39070
H -1.34526 -4.34859 2.91087
H 3.49616 4.58478 -1.27571
H 2.15414 1.90416 3.92866
H 2.02689 0.14102 4.20295
H 1.17096 0.90500 2.82492
H -1.87377 -0.02245 2.70121
H -1.77710 -0.85665 4.27039
H -3.25868 -1.00619 3.29198
H 4.24688 3.24567 2.74886
H 0.17692 -2.47793 -2.22435
H 4.32141 5.04996 1.03019
H 2.16740 1.25974 -2.39331
H -2.13578 -1.11115 -3.73835
H -0.44478 -1.18968 -4.30058
H -0.83168 -0.30431 -2.79977
H 0.39542 2.90642 -1.88139
H 0.83531 2.99898 -3.61704
H 1.41452 4.24963 -2.48090
H 5.51737 0.48125 2.74280
H 4.56553 -0.23553 4.07461
H 4.77759 1.52567 3.98238
H 3.86083 3.66730 -3.34865
H 3.19219 2.37433 -4.37484
H 4.46173 2.00286 -3.17238
H -0.92540 -4.66827 -2.89012
H -0.33679 -3.73701 -4.29626
H -2.07361 -3.77274 -3.91734
O 2.86346 -2.58941 -0.34469
Si 1.45582 -3.10913 0.43644
Si 3.42351 -1.07354 -0.87445
C 5.22326 -0.87995 -0.31053
H 5.62211 0.11136 -0.58345
H 5.31420 -0.99579 0.78146
H 5.85326 -1.64858 -0.79010
C 3.38694 -1.18763 -2.77327
H 2.35034 -1.26600 -3.14314
H 3.85480 -0.31171 -3.25259
H 3.93347 -2.08872 -3.10202
C 1.01117 -4.82254 -0.24854
H 0.05132 -5.18221 0.16004
H 0.93272 -4.80570 -1.34762
H 1.79242 -5.55250 0.02440
C 1.91041 -3.29438 2.27423
H 2.10305 -2.31271 2.73876
H 1.11769 -3.79877 2.85234
H 2.83036 -3.89781 2.36461

A-Cs**[II]**
SCF (BP86) Energy = -1541.92266716
Enthalpy 0K = -1541.160427
Enthalpy 298K = -1541.108182
Free Energy 298K = -1541.246081
Lowest Frequency = 12.7994 cm^{-1}
Second Frequency = 23.5573 cm^{-1}
SCF (BP86-D3) Energy = -1542.17437271
SCF (C6H6) Energy = -1541.93100806
SCF (BS2) Energy = -2353.99266082

Cs 3.72553 -1.83403 -0.14223
Al -0.58408 -0.07860 -0.16460
N -2.35688 0.27991 0.23868
N 0.50604 1.42640 0.06623
C -3.37197 -0.61796 -0.27947
C 1.90320 1.35797 0.37964
C -3.85923 -0.43765 -1.61348
C -3.89003 -1.68708 0.51371
C -0.02605 -1.88831 -0.74587
C 0.60737 -2.70560 0.39378
C 1.30721 -3.86810 0.07568
C -3.31751 0.66909 -2.51759
C 2.90129 1.66118 -0.60895
C 2.33588 1.02654 1.71052
C -5.33617 -2.37126 -1.34482
C 1.64561 -3.08735 -2.20278
C 0.95183 -1.91344 -1.92822
C -4.82737 -1.32377 -2.12073

```
C   1.79238 -4.13021 -1.23818
C  -4.86536 -2.54076 -0.03994
C   2.54596  1.97109 -2.06507
C  -4.41239  1.39922 -3.32321
C   3.71209  1.04669  2.01927
C   3.17149  0.94158 -3.03449
C  -2.22774  0.11643 -3.46613
C   4.26356  1.67406 -0.24264
C  -3.41726 -1.96402  1.94101
C   4.68049  1.38301  1.06338
C   1.35710  0.67204  2.83297
C  -2.73069 -3.34455  2.05673
C   1.66420 -0.70873  3.45551
C   2.96046  3.40405 -2.47048
C   1.32493  1.75916  3.93152
C  -4.57888 -1.85821  2.95616
H  -1.00452 -2.35958 -1.04815
H   0.27885 -2.55076  1.42881
H   1.57831 -4.55760  0.89205
H  -2.83930  1.41241 -1.85638
H  -6.09065 -3.05048 -1.75579
H   2.18395 -3.16856 -3.16132
H   0.89784 -1.13369 -2.69855
H  -5.18998 -1.18891 -3.14566
H   2.32863 -5.05419 -1.47456
H  -5.25592 -3.36361  0.56989
H   1.44992  1.88668 -2.15376
H  -4.87352  0.74498 -4.08393
H  -3.98046  2.26293 -3.85861
H  -5.21844  1.76958 -2.66764
H   4.02621  0.81970  3.04499
H   2.82776 -0.08136 -2.79796
H   4.27635  0.96902 -2.99697
H   2.87375  1.16026 -4.07499
H  -1.39993 -0.36577 -2.91308
H  -1.79961  0.91951 -4.09331
H  -2.64766 -0.65322 -4.13748
H   5.01192  1.93404 -1.00106
H  -2.66935 -1.19296  2.19359
H   5.74126  1.42603  1.33444
H   0.34701  0.62844  2.38577
H  -3.43406 -4.16119  1.81531
H  -2.37157 -3.51113  3.08855
H  -1.86835 -3.43011  1.37490
H   1.66852 -1.50222  2.68721
H   0.89852 -0.97127  4.20612
H   2.64150 -0.71271  3.97170
H   2.51662  4.16567 -1.80811
H   2.64009  3.62120 -3.50466
H   4.05719  3.53063 -2.43088
H   2.31289  1.86534  4.41415
H   0.59472  1.49395  4.71588
H   1.04212  2.74251  3.52366
H  -5.10039 -0.88828  2.88587
H  -4.20678 -1.97604  3.98948
H  -5.33234 -2.64736  2.78445
O  -1.73001  2.94197  0.89348
Si -0.28029  3.04308  0.02825
Si -2.87016  1.71189  1.17407
C  -2.85251  1.46704  3.05438
H  -3.64079  0.77673  3.39461
H  -1.88084  1.07363  3.39715
H  -3.01457  2.44124  3.54738
C  -4.57738  2.31081  0.62597
H  -4.57364  2.62668 -0.42947
H  -5.33368  1.51719  0.74317
H  -4.88390  3.17298  1.24228
C  -0.72310  3.61472 -1.72641
H   0.16785  3.92734 -2.29507
H  -1.23356  2.82457 -2.30107
H  -1.40565  4.47967 -1.66289
C   0.79663  4.35152  0.86646
H   0.91209  4.15131  1.94311
H   1.80326  4.40726  0.42144
H   0.31524  5.33784  0.75383
```

TS(A-B)-Cs**[II]**

SCF (BP86) Energy = -1541.90756926
Enthalpy 0K = -1541.148719
Enthalpy 298K = -1541.096992
Free Energy 298K = -1541.234314
Lowest Frequency = -655.4479 cm^{-1}
Second Frequency = 6.3222 cm^{-1}
SCF (BP86-D3) Energy = -1542.16226593
SCF (C6H6) Energy = -1541.91915686
SCF (BS2) Energy = -2353.97909813

```
Cs  0.00032  4.41412 -0.34696
Al -0.00341 -0.57604  0.22101
N  -1.58370 -1.47124 -0.20364
N   1.57963 -1.45693 -0.22745
C  -2.85597 -0.80149 -0.08898
C   2.85450 -0.80372 -0.04419
C  -3.62522 -0.87810  1.11493
C  -3.36127 -0.03443 -1.18894
C  -0.01218  1.17527  1.06397
C  -1.24464  1.97529  1.31244
C  -1.24405  3.02650  2.23290
C  -3.13705 -1.63520  2.35024
C   3.58145 -0.93444  1.18199
C   3.40491  0.00127 -1.09505
C  -5.35012  0.55132  0.11586
C   1.17980  3.02823  2.27050
C   1.21096  1.97636  1.35138
C  -4.85675 -0.19717  1.18932
C  -0.04047  3.56121  2.76796
C  -4.59688  0.62871 -1.06160
C   3.03761 -1.71662  2.37837
C  -4.16498 -2.68038  2.83858
C   4.64658  0.63709 -0.90326
C   2.61250 -0.76123  3.51835
C  -2.77444 -0.66218  3.49621
C   4.81981 -0.27643  1.32139
C  -2.56300  0.13828 -2.48217
C   5.36087  0.50108  0.29273
C   2.64525  0.25516 -2.39872
C  -1.89476  1.53395 -2.51634
C   2.00221  1.66304 -2.37404
C   4.04431 -2.76155  2.90950
C   3.51166  0.08636 -3.66409
C  -3.40104 -0.08719 -3.75787
H  -0.02428  0.13146  1.95841
H  -2.20131  1.64043  0.89701
H  -2.20347  3.50495  2.48285
H  -2.21461 -2.16573  2.06121
H  -6.31201  1.06964  0.19507
H   2.13033  3.50748  2.55090
H   2.18119  1.64115  0.96877
H  -5.43706 -0.25259  2.11762
H  -0.05232  4.37549  3.49896
H  -4.97756  1.21603 -1.90557
H   2.13501 -2.24907  2.03468
H  -5.08360 -2.19842  3.21854
H  -3.74377 -3.27940  3.66502
H  -4.46595 -3.37105  2.03241
H   5.06188  1.25241 -1.71005
```

H	3.48208	-0.20064	3.90696
H	2.17765	-1.33184	4.35831
H	1.86347	-0.02828	3.17531
H	-2.01337	0.06962	3.17843
H	-2.37851	-1.21879	4.36430
H	-3.66390	-0.10036	3.83499
H	5.36726	-0.37409	2.26586
H	-1.75384	-0.61206	-2.46481
H	6.32802	0.99908	0.42205
H	1.82269	-0.47891	-2.44207
H	-2.66286	2.32996	-2.52628
H	-1.26532	1.65058	-3.41752
H	-1.26191	1.67221	-1.62074
H	1.35583	1.76438	-1.48346
H	1.39397	1.83621	-3.28085
H	2.78458	2.44370	-2.32722
H	4.39869	-3.43768	2.11345
H	3.57858	-3.37681	3.69922
H	4.93340	-2.27927	3.35369
H	4.30978	0.84790	-3.72225
H	2.89124	0.19522	-4.57146
H	3.99208	-0.90468	-3.69663
H	-3.89930	-1.07019	-3.74439
H	-2.75710	-0.04164	-4.65407
H	-4.18403	0.68262	-3.87925
O	-0.00764	-3.36771	-1.46825
Si	1.57146	-3.10109	-0.91165
Si	-1.54580	-3.15154	-0.78418
C	2.00842	-4.47071	0.32712
H	3.06713	-4.41206	0.62953
H	1.39186	-4.42847	1.23939
H	1.84868	-5.45385	-0.14900
C	2.72279	-3.28458	-2.40253
H	2.34799	-2.72261	-3.27238
H	3.74046	-2.93062	-2.16801
H	2.78952	-4.34885	-2.68604
C	-2.82042	-3.47024	-2.14480
H	-3.82350	-3.12633	-1.84275
H	-2.54140	-2.95461	-3.07732
H	-2.87812	-4.55157	-2.35581
C	-1.76476	-4.45633	0.57715
H	-1.08322	-4.28391	1.42647
H	-2.79565	-4.46326	0.96806
H	-1.55204	-5.45813	0.16530

B-Cs**[II]**
SCF (BP86) Energy = -1541.98176032
Enthalpy 0K = -1541.220553
Enthalpy 298K = -1541.168668
Free Energy 298K = -1541.304039
Lowest Frequency = 20.9812 cm^{-1}
Second Frequency = 23.9407 cm^{-1}
SCF (BP86-D3) Energy = -1542.23362979
SCF (C6H6) Energy = -1541.99332346
SCF (BS2) Energy = -2354.04872657

Cs	-3.37646	1.94949	0.24369
Al	0.51224	-0.01820	-0.88503
N	2.31100	-0.45130	-0.38235
N	-0.68177	-1.42842	-0.21879
C	3.19039	0.49031	0.24832
C	-2.08436	-1.30309	-0.08539
C	3.79382	1.56248	-0.48973
C	3.47000	0.39627	1.65289
C	-0.06117	1.83678	-0.22361
C	-0.06031	2.33212	1.10782
C	-0.47531	3.63881	1.43621
C	3.64171	1.69790	-2.00590
C	-2.95513	-1.19047	-1.23598
C	-2.71229	-1.28845	1.21742
C	4.82411	2.43700	1.55815
C	-0.89237	4.08005	-0.91400
C	-0.47617	2.76668	-1.21768
C	4.59051	2.51102	0.18139
C	-0.90437	4.51806	0.42354
C	4.26790	1.37412	2.27741
C	-2.42435	-1.22571	-2.67091
C	4.99830	1.47571	-2.71576
C	-4.11441	-1.17901	1.33596
C	-2.61206	0.13620	-3.37664
C	3.04832	3.06035	-2.42686
C	-4.35064	-1.06904	-1.05886
C	2.93946	-0.75506	2.50630
C	-4.94571	-1.06806	0.21166
C	-1.89400	-1.39672	2.50412
C	1.89481	-0.28534	3.54196
C	-2.00527	-0.11592	3.36294
C	-3.08114	-2.34535	-3.51041
C	-2.30363	-2.62591	3.34659
C	4.07509	-1.52035	3.22311
H	0.36876	0.10779	-2.50437
H	0.30248	1.68962	1.91844
H	-0.44052	3.98060	2.47799
H	2.94368	0.91014	-2.33756
H	5.44157	3.18941	2.06112
H	-1.18458	4.76713	-1.71816
H	-0.44941	2.44998	-2.26945
H	5.04065	3.32741	-0.39637
H	-1.21018	5.54139	0.67063
H	4.46135	1.29323	3.35424
H	-1.33946	-1.41553	-2.61284
H	5.71694	2.27394	-2.45545
H	4.87381	1.48177	-3.81350
H	5.45745	0.51540	-2.42703
H	-4.56396	-1.19854	2.33686
H	-3.68307	0.40828	-3.45008
H	-2.20650	0.10024	-4.40243
H	-2.07073	0.93931	-2.84818
H	2.07732	3.24337	-1.94016
H	2.89849	3.09369	-3.52108
H	3.72130	3.89543	-2.16006
H	-4.98936	-1.00740	-1.94878
H	2.43458	-1.44502	1.80986
H	-6.03479	-1.01077	0.32143
H	-0.84092	-1.50874	2.19668
H	2.32147	0.46664	4.23007
H	1.53662	-1.13423	4.15311
H	1.01836	0.16742	3.04957
H	-1.63849	0.77220	2.81796
H	-1.39721	-0.20542	4.27974
H	-3.04981	0.06966	3.67786
H	-2.99275	-3.32729	-3.01945
H	-2.59486	-2.41122	-4.49922
H	-4.15562	-2.15334	-3.68546
H	-3.32521	-2.51512	3.75382
H	-1.61851	-2.75567	4.20231
H	-2.28644	-3.55219	2.74974
H	4.84832	-1.85690	2.51416
H	3.67627	-2.40946	3.74456
H	4.57123	-0.88972	3.98258
O	1.44980	-2.90677	-1.22071
Si	0.06877	-3.04367	-0.25105
Si	2.85679	-1.93812	-1.15982
C	3.35581	-1.81685	-2.98662
H	4.31891	-1.29986	-3.12680
H	3.44889	-2.83232	-3.40988

H	2.58253	-1.27595	-3.55623
C	4.24537	-2.81665	-0.21178
H	5.08694	-2.12681	-0.02726
H	3.89909	-3.20186	0.76009
H	4.62674	-3.66589	-0.80418
C	-1.04879	-4.33318	-1.07965
H	-2.07731	-4.30578	-0.68143
H	-1.08971	-4.16583	-2.16753
H	-0.64415	-5.34518	-0.90714
C	0.59391	-3.76267	1.43114
H	1.16679	-3.04779	2.04246
H	-0.27339	-4.10085	2.02201
H	1.23377	-4.64384	1.24791

Cs_2**[II]$_2$**$\cdot C_6H_6$

SCF (BP86) Energy = SCF
Enthalpy 0K = -2850.287774
Enthalpy 298K = -2850.185731
Free Energy 298K = -2850.446842
Lowest Frequency = 4.5598 cm^{-1}
Second Frequency = 5.4762 cm^{-1}
SCF (BP86-D3BJ) Energy = -2852.1855901
SCF (C6H6) Energy = -2851.72485410
SCF (BS2) Energy = -4475.78590668

Al	2.80470	-0.63259	-0.70498
Al	-3.25644	0.00880	-0.02787
Cs	-0.27302	-2.37330	1.12247
Cs	-0.17546	1.75337	-1.86653
Si	5.50299	-2.46852	-1.20081
Si	5.86000	0.61180	-0.84318
Si	-5.99263	-0.00515	1.82211
Si	-6.27213	0.62885	-1.22119
O	6.33670	-0.99721	-1.08486
O	-6.78624	0.38213	0.37530
N	3.88165	-2.24710	-0.51221
N	4.11823	0.73175	-1.16423
N	-4.38444	-0.64309	1.42327
N	-4.51970	0.91272	-1.20588
C	3.22276	-3.30808	0.17326
C	3.29813	-3.39737	1.60727
C	2.56324	-4.38890	2.28817
H	2.63321	-4.44861	3.38087
C	1.76415	-5.31475	1.60032
H	1.21667	-6.09183	2.14542
C	1.70035	-5.24491	0.20148
H	1.09266	-5.97637	-0.34567
C	2.41048	-4.26602	-0.52565
C	4.15691	-2.42344	2.41495
H	4.79871	-1.89817	1.68679
C	5.06820	-3.13275	3.43906
H	4.48935	-3.61244	4.24884
H	5.74845	-2.40404	3.91336
H	5.68253	-3.91317	2.95997
C	3.28499	-1.35351	3.11094
H	2.70479	-0.77154	2.36923
H	3.90970	-0.64284	3.68099
H	2.57501	-1.81906	3.82057
C	2.29678	-4.26495	-2.05025
H	2.93507	-3.44327	-2.41385
C	0.85670	-3.97240	-2.52685
H	0.14202	-4.73141	-2.15812
H	0.80251	-3.97695	-3.62992
H	0.52100	-2.97772	-2.18211
C	2.81285	-5.58794	-2.65970
H	3.84429	-5.80638	-2.33533
H	2.80281	-5.53795	-3.76278
H	2.18391	-6.44586	-2.36087
C	6.49217	-3.78168	-0.25652
H	7.47266	-3.93496	-0.73873
H	5.96280	-4.74953	-0.24372
H	6.67054	-3.47429	0.78656
C	5.51473	-2.90670	-3.05136
H	4.88808	-2.20774	-3.63079
H	5.15305	-3.93064	-3.24310
H	6.54672	-2.83423	-3.43641
C	3.55567	1.91687	-1.72176
C	3.12608	3.00866	-0.89172
C	2.49101	4.12443	-1.47774
H	2.17718	4.95527	-0.83377
C	2.26532	4.20350	-2.85921
H	1.78419	5.08584	-3.29604
C	2.69093	3.14505	-3.67611
H	2.53498	3.20758	-4.75973
C	3.33698	2.01245	-3.14060
C	3.34143	3.00540	0.62208
H	3.88146	2.07540	0.86276
C	4.20660	4.20170	1.07835
H	5.17249	4.22700	0.54560
H	4.40846	4.14422	2.16206
H	3.70005	5.16528	0.88941
C	2.00661	2.97267	1.39982
H	1.37343	3.84705	1.15965
H	2.19035	2.98912	2.48827
H	1.43843	2.05287	1.16936
C	3.78575	0.89750	-4.08624
H	4.44940	0.24049	-3.49809
C	2.58648	0.03929	-4.54955
H	1.84951	0.65156	-5.10294
H	2.07426	-0.42466	-3.68471
H	2.91659	-0.77348	-5.22103
C	4.57937	1.42341	-5.30117
H	3.94903	2.02456	-5.98104
H	4.97927	0.57951	-5.88989
H	5.42748	2.05416	-4.98674
C	6.35674	1.01299	0.94828
H	5.74387	0.44359	1.66753
H	6.25281	2.08547	1.18281
H	7.41245	0.73141	1.10565
C	6.86739	1.70940	-2.01579
H	7.93868	1.65333	-1.75768
H	6.55363	2.76467	-1.94458
H	6.75273	1.38713	-3.06331
C	-3.77489	-1.64913	2.22753
C	-2.97343	-1.31329	3.37230
C	-2.31144	-2.33398	4.08726
H	-1.71138	-2.06448	4.96528
C	-2.41366	-3.68126	3.71285
H	-1.90375	-4.46078	4.29003
C	-3.20298	-4.01699	2.60237
H	-3.30340	-5.07044	2.31506
C	-3.89100	-3.03543	1.86069
C	-2.81836	0.13085	3.84970
H	-3.43770	0.75172	3.18233
C	-3.33081	0.31255	5.29605
H	-4.37295	-0.03334	5.40150
H	-3.29028	1.37581	5.59143
H	-2.71921	-0.25583	6.01981
C	-1.36295	0.63237	3.72022
H	-0.66484	0.01950	4.32032
H	-1.27594	1.67466	4.07474
H	-1.03161	0.61226	2.66621
C	-4.74513	-3.46807	0.66817
H	-5.35707	-2.59253	0.39071
C	-5.69707	-4.63583	1.00350
H	-5.14931	-5.57306	1.20947

H	-6.37171	-4.83414	0.15253
H	-6.31712	-4.40996	1.88698
C	-3.86539	-3.81627	-0.55420
H	-3.25557	-2.94570	-0.86365
H	-4.48662	-4.11602	-1.41712
H	-3.18221	-4.65620	-0.32613
C	-7.04354	-1.28242	2.74882
H	-8.01436	-0.83978	3.02985
H	-6.54197	-1.61957	3.67180
H	-7.24186	-2.16754	2.12310
C	-5.96838	1.61005	2.82592
H	-5.30776	2.36006	2.35884
H	-5.63068	1.45463	3.86416
H	-6.98765	2.03240	2.86088
C	-3.91025	1.79006	-2.14904
C	-3.47122	1.32366	-3.43562
C	-2.78999	2.20305	-4.30388
H	-2.47005	1.83681	-5.28730
C	-2.52567	3.53298	-3.94732
H	-2.00787	4.20411	-4.64177
C	-2.95964	3.99721	-2.69627
H	-2.77286	5.04118	-2.41761
C	-3.65192	3.16093	-1.79723
C	-3.72647	-0.10976	-3.90218
H	-4.28857	-0.60879	-3.09620
C	-2.41305	-0.89874	-4.10001
H	-1.76421	-0.42789	-4.86175
H	-2.62379	-1.92901	-4.43749
H	-1.84902	-0.96845	-3.15226
C	-4.58328	-0.14752	-5.18752
H	-5.52954	0.40439	-5.05801
H	-4.82770	-1.18905	-5.46107
H	-4.05198	0.30412	-6.04463
C	-4.10733	3.73053	-0.45304
H	-4.80733	2.99262	-0.02466
C	-2.92193	3.86046	0.53055
H	-2.44947	2.87608	0.71329
H	-3.25710	4.25887	1.50490
H	-2.15062	4.54845	0.13562
C	-4.84954	5.07673	-0.59131
H	-4.18210	5.88598	-0.93846
H	-5.25802	5.38900	0.38556
H	-5.68667	5.00442	-1.30546
C	-7.21715	2.11540	-1.92230
H	-8.29601	1.88892	-1.96870
H	-6.87578	2.36203	-2.94199
H	-7.08398	3.00840	-1.29052
C	-6.80366	-0.93499	-2.16358
H	-6.22110	-1.81337	-1.83781
H	-6.68357	-0.82955	-3.25470
H	-7.86862	-1.14024	-1.95814
C	3.39237	3.55516	6.05232
C	2.34054	4.45568	6.29043
C	2.52086	5.82728	6.04508
C	3.75276	6.29845	5.56174
C	4.62496	4.02631	5.56885
C	4.80497	5.39826	5.32364
H	1.38090	4.08882	6.67019
H	1.70124	6.52935	6.23225
H	3.89379	7.36787	5.37182
H	5.44657	3.32519	5.38742
H	5.76656	5.76601	4.94997
H	3.25354	2.48652	6.24857

A-Cs_2**[II]$_2$**
SCF (BP86) Energy = SCF
Enthalpy 0K = -2850.235044
Enthalpy 298K = -2850.134651
Free Energy 298K = -2850.380084
Lowest Frequency = 6.9187 cm^{-1}
Second Frequency = 12.2478 cm^{-1}
SCF (BP86-D3BJ) Energy = -2852.1594316
SCF (C6H6) Energy = -2851.67200580
SCF (BS2) Energy = -4475.73471671

Al	4.07570	-0.03146	-0.20664
Al	-3.67886	0.12273	0.07136
Cs	-0.60092	2.92352	-0.34108
Cs	-0.81910	-2.56219	-1.00018
Si	6.64490	0.27891	1.68843
Si	6.13446	-2.37462	0.11743
Si	-6.70561	1.40996	-0.17061
Si	-6.37747	-1.20770	1.48139
O	6.84777	-1.35144	1.26477
O	-7.18013	0.14682	0.85766
N	5.39418	0.97836	0.61109
N	4.43554	-1.85133	-0.08790
N	-4.94522	1.60667	-0.04503
N	-4.81864	-1.37117	0.64396
C	5.43084	2.41131	0.39165
C	6.14710	2.94868	-0.72490
C	6.16217	4.34256	-0.92307
H	6.70366	4.75116	-1.78341
C	5.49912	5.21503	-0.05268
H	5.52911	6.29666	-0.22249
C	4.79475	4.68738	1.03438
H	4.26612	5.36644	1.71337
C	4.74453	3.30016	1.27622
C	6.84236	2.05209	-1.75025
H	6.89304	1.04104	-1.30953
C	8.28462	2.49912	-2.07259
H	8.30390	3.47310	-2.59271
H	8.77112	1.76652	-2.74028
H	8.89838	2.59481	-1.16165
C	6.00607	1.96254	-3.04990
H	4.95613	1.68495	-2.85099
H	6.44403	1.22870	-3.75001
H	5.98183	2.94143	-3.56166
C	3.89730	2.79010	2.44266
H	4.12185	1.71783	2.56385
C	2.39054	2.90593	2.10974
H	2.10283	3.96703	1.98669
H	1.77402	2.47551	2.92031
H	2.16186	2.37801	1.16519
C	4.21305	3.49883	3.77677
H	5.28754	3.44706	4.02083
H	3.65026	3.03347	4.60502
H	3.93275	4.56680	3.75028
C	8.30115	1.16991	1.49997
H	9.01195	0.78066	2.24872
H	8.19694	2.25604	1.65679
H	8.73307	1.00423	0.50059
C	6.16825	0.25427	3.52440
H	5.19208	-0.23251	3.68650
H	6.12456	1.26681	3.95774
H	6.92863	-0.32011	4.08157
C	3.41498	-2.85962	-0.09259
C	3.04360	-3.53789	-1.29575
C	2.10517	-4.59042	-1.23035
H	1.85273	-5.13247	-2.15029
C	1.51459	-4.97501	-0.01890
H	0.81244	-5.81592	0.01662
C	1.84777	-4.27989	1.15456
H	1.39421	-4.58359	2.10385
C	2.78989	-3.23343	1.14376
C	3.62895	-3.16026	-2.65598

H	4.33764	-2.33289	-2.48072
C	4.40563	-4.33181	-3.29812
H	5.20059	-4.71007	-2.63305
H	4.87393	-4.01209	-4.24539
H	3.73802	-5.18111	-3.53019
C	2.53287	-2.64103	-3.61524
H	1.79708	-3.43521	-3.84572
H	2.97706	-2.32116	-4.57375
H	1.99731	-1.77558	-3.18721
C	3.14310	-2.49973	2.43811
H	4.18853	-2.15986	2.33251
C	2.26910	-1.23445	2.60350
H	1.20243	-1.50200	2.70567
H	2.35052	-0.55569	1.73160
H	2.56422	-0.66052	3.49953
C	3.05831	-3.37365	3.70474
H	2.01813	-3.64951	3.95459
H	3.46080	-2.82145	4.57102
H	3.63901	-4.30508	3.59560
C	7.13747	-2.21205	-1.48280
H	7.06337	-1.19405	-1.90138
H	6.79202	-2.92094	-2.25347
H	8.20318	-2.41695	-1.28242
C	6.22510	-4.14224	0.77814
H	7.28123	-4.41810	0.93734
H	5.78505	-4.86294	0.06928
H	5.69608	-4.24262	1.73933
C	-4.37089	2.91087	-0.07314
C	-4.07079	3.57608	-1.31180
C	-3.45177	4.84377	-1.29399
H	-3.24396	5.34602	-2.24693
C	-3.10692	5.47941	-0.09277
H	-2.63912	6.47059	-0.10041
C	-3.39602	4.83570	1.11943
H	-3.14607	5.33338	2.06426
C	-4.02735	3.57579	1.15580
C	-4.41730	2.95445	-2.66486
H	-4.86135	1.96765	-2.45459
C	-5.45819	3.80627	-3.42692
H	-6.36581	3.97471	-2.82305
H	-5.75763	3.30838	-4.36618
H	-5.04960	4.79802	-3.69245
C	-3.16697	2.72367	-3.54175
H	-2.66201	3.67515	-3.79101
H	-3.44640	2.24207	-4.49559
H	-2.43044	2.06964	-3.04307
C	-4.34085	2.94603	2.51375
H	-4.99677	2.08170	2.31101
C	-5.09259	3.90877	3.45822
H	-4.46399	4.76444	3.76429
H	-5.39671	3.38114	4.37904
H	-5.99990	4.31562	2.98147
C	-3.06166	2.40678	3.19377
H	-2.56993	1.64424	2.56044
H	-3.29791	1.93912	4.16643
H	-2.33730	3.22176	3.38171
C	-7.62371	2.97229	0.38484
H	-8.71128	2.83510	0.25942
H	-7.31842	3.85154	-0.20710
H	-7.42841	3.19083	1.44719
C	-7.32244	0.91307	-1.90027
H	-6.74110	0.06848	-2.30678
H	-7.26369	1.74524	-2.62091
H	-8.37778	0.59657	-1.83275
C	-4.25740	-2.66200	0.43360
C	-3.43494	-3.29851	1.42693
C	-2.84166	-4.54882	1.15139
H	-2.22812	-5.02736	1.92470
C	-3.02694	-5.19828	-0.07747
H	-2.57341	-6.17815	-0.26519
C	-3.82690	-4.58338	-1.05272
H	-3.99158	-5.09210	-2.01020
C	-4.44970	-3.33989	-0.82206
C	-3.17771	-2.65380	2.78907
H	-3.78335	-1.73410	2.82235
C	-1.70071	-2.23002	2.95142
H	-1.01770	-3.09476	2.85376
H	-1.52911	-1.78047	3.94574
H	-1.42597	-1.47426	2.19224
C	-3.61467	-3.56776	3.95509
H	-4.66822	-3.87755	3.85165
H	-3.50425	-3.04349	4.92055
H	-3.00341	-4.48685	4.00681
C	-5.31875	-2.72965	-1.92179
H	-5.88087	-1.90691	-1.44745
C	-4.45162	-2.10658	-3.03978
H	-3.79524	-1.31177	-2.63584
H	-5.08272	-1.65389	-3.82524
H	-3.81580	-2.87238	-3.52392
C	-6.33363	-3.73020	-2.51410
H	-5.83862	-4.53915	-3.08121
H	-7.01382	-3.21325	-3.21307
H	-6.94483	-4.20000	-1.72557
C	-7.47681	-2.73043	1.21485
H	-8.42137	-2.61412	1.77328
H	-6.98230	-3.65106	1.56842
H	-7.72604	-2.86237	0.14949
C	-6.24723	-0.87176	3.34927
H	-5.55448	-0.03845	3.55634
H	-5.90596	-1.75302	3.91732
H	-7.24195	-0.58594	3.73324
C	1.19330	0.15992	-1.11787
C	0.27722	0.49456	-2.12432
C	0.57826	1.51728	-3.07134
C	1.63460	2.42082	-2.72172
C	2.62963	0.62341	-1.36542
C	2.54634	2.10240	-1.72377
H	-0.76605	0.12988	-2.08290
H	-0.10028	1.73418	-3.90201
H	1.65463	3.42202	-3.18127
H	2.97770	0.08287	-2.30228
H	3.23918	2.84651	-1.31697
H	0.88035	-0.29387	-0.16496

TS(A-B)-Cs_2**[II]$_2$**
SCF (BP86) Energy = -2851.65602321
Enthalpy 0K = -2850.231800
Enthalpy 298K = -2850.131809
Free Energy 298K = -2850.378046
Lowest Frequency = -614.1043 cm^{-1}
Second Frequency = 5.7691 cm^{-1}
SCF (BP86-D3) Energy = -2852.14937104
SCF (C6H6) Energy = -2851.66586171
SCF (BS2) Energy = -4475.73012731

Al	4.23135	-0.07809	-0.23438
Al	-3.83900	0.19270	0.11293
Cs	-0.53724	2.42721	-0.24480
Cs	-1.08447	-2.42098	-0.74982
Si	6.84816	0.11375	1.59896
Si	6.10743	-2.54140	0.09751
Si	-6.69344	1.76295	-0.13165
Si	-6.73000	-1.01382	1.28283
O	6.89494	-1.53658	1.21174
O	-7.22811	0.56947	0.94944
N	5.60862	0.87790	0.56832

N	4.43882	-1.92903	-0.08761
N	-4.92250	1.79089	-0.05499
N	-5.10194	-1.22344	0.59438
C	5.65112	2.31327	0.38499
C	6.34217	2.87882	-0.73480
C	6.35240	4.27742	-0.90109
H	6.87550	4.70442	-1.76423
C	5.70809	5.13100	0.00056
H	5.73324	6.21613	-0.14670
C	5.02783	4.57818	1.09058
H	4.51352	5.24129	1.79607
C	4.98411	3.18607	1.30325
C	7.02756	2.01793	-1.79756
H	7.03205	0.98036	-1.42007
C	8.49100	2.44033	-2.05706
H	8.54963	3.44527	-2.51155
H	8.97235	1.73792	-2.76026
H	9.08515	2.45852	-1.12890
C	6.22648	2.03689	-3.12135
H	5.18684	1.69807	-2.97321
H	6.69948	1.37720	-3.87083
H	6.19256	3.05696	-3.54457
C	4.16685	2.65774	2.48331
H	4.37202	1.57744	2.56195
C	2.65111	2.82091	2.21684
H	2.38200	3.89044	2.13677
H	2.05878	2.38019	3.03993
H	2.37338	2.32673	1.26887
C	4.54833	3.32151	3.82399
H	5.63076	3.24872	4.02186
H	4.01354	2.83997	4.66168
H	4.28277	4.39357	3.83847
C	8.56141	0.86380	1.31654
H	9.26971	0.45912	2.05944
H	8.54142	1.96105	1.42428
H	8.94229	0.62145	0.31205
C	6.47826	0.15455	3.46055
H	5.48601	-0.26820	3.69064
H	6.52361	1.17440	3.87582
H	7.23422	-0.45709	3.98331
C	3.35250	-2.85930	-0.05377
C	2.98226	-3.60902	-1.21845
C	1.95565	-4.57179	-1.12360
H	1.70237	-5.16437	-2.01151
C	1.28014	-4.81192	0.08146
H	0.51557	-5.59545	0.14568
C	1.61899	-4.05498	1.21449
H	1.10578	-4.24896	2.16332
C	2.64308	-3.08822	1.17330
C	3.67730	-3.40850	-2.56584
H	4.42019	-2.60539	-2.42475
C	4.41795	-4.68626	-3.02238
H	5.14333	-5.03438	-2.26773
H	4.96552	-4.50039	-3.96306
H	3.71215	-5.51575	-3.20927
C	2.69221	-2.93727	-3.65990
H	1.91224	-3.69731	-3.85537
H	3.22860	-2.76674	-4.60952
H	2.20241	-1.99142	-3.37483
C	2.98607	-2.29361	2.43267
H	4.01357	-1.91455	2.29173
C	2.05460	-1.06530	2.56857
H	1.00584	-1.38444	2.71463
H	2.09297	-0.42604	1.66642
H	2.34135	-0.44530	3.43635
C	2.96758	-3.13360	3.72564
H	1.94833	-3.46271	3.99718
H	3.34795	-2.53494	4.57111
H	3.59947	-4.03283	3.63385
C	7.11456	-2.45948	-1.50677
H	7.03193	-1.46122	-1.96946
H	6.78070	-3.20465	-2.24716
H	8.18018	-2.64567	-1.28903
C	6.09895	-4.28875	0.81807
H	7.13680	-4.63694	0.95319
H	5.57901	-5.00346	0.15931
H	5.60071	-4.30706	1.80099
C	-4.19666	3.01639	-0.11031
C	-3.79961	3.59455	-1.36431
C	-3.01128	4.76454	-1.37569
H	-2.72366	5.20261	-2.33926
C	-2.59615	5.38431	-0.18831
H	-1.99227	6.29826	-0.21876
C	-2.99048	4.83048	1.03873
H	-2.68678	5.32166	1.97101
C	-3.78871	3.67020	1.10406
C	-4.22888	2.98779	-2.70032
H	-4.78414	2.06504	-2.46353
C	-5.17449	3.94163	-3.46641
H	-6.04973	4.22093	-2.85585
H	-5.53968	3.46798	-4.39488
H	-4.65797	4.87631	-3.74986
C	-3.02804	2.59556	-3.58895
H	-2.41719	3.47456	-3.86379
H	-3.37845	2.13346	-4.52883
H	-2.36412	1.86904	-3.08801
C	-4.20275	3.13296	2.47550
H	-4.96467	2.35588	2.29172
C	-4.83104	4.22034	3.37403
H	-4.09714	4.99380	3.66377
H	-5.21625	3.77044	4.30564
H	-5.66822	4.72876	2.86752
C	-3.01679	2.45302	3.19750
H	-2.62650	1.60462	2.60349
H	-3.32677	2.06130	4.18266
H	-2.18976	3.16815	3.36677
C	-7.45354	3.40535	0.42557
H	-8.54916	3.37824	0.29912
H	-7.06147	4.25060	-0.16477
H	-7.23833	3.60030	1.48852
C	-7.38481	1.29969	-1.84163
H	-6.91371	0.38093	-2.23016
H	-7.22731	2.10064	-2.58295
H	-8.47094	1.11833	-1.76485
C	-4.57343	-2.53229	0.38695
C	-3.85293	-3.22541	1.42166
C	-3.26807	-4.48062	1.14937
H	-2.73061	-5.00096	1.95138
C	-3.36727	-5.08314	-0.11296
H	-2.92271	-6.06748	-0.29813
C	-4.06960	-4.41480	-1.12671
H	-4.16521	-4.88484	-2.11288
C	-4.67851	-3.16240	-0.90381
C	-3.67923	-2.63111	2.82021
H	-4.30791	-1.72765	2.86002
C	-2.22133	-2.18171	3.07025
H	-1.51589	-3.02856	2.97268
H	-2.10679	-1.77010	4.08870
H	-1.92807	-1.38929	2.35639
C	-4.14251	-3.59945	3.93065
H	-5.17089	-3.95663	3.75463
H	-4.11724	-3.09794	4.91364
H	-3.49039	-4.48876	3.99920
C	-5.42757	-2.49484	-2.05819
H	-5.97704	-1.64493	-1.61906
C	-4.44730	-1.91535	-3.10371

H	-3.78525	-1.15508	-2.64604
H	-4.99384	-1.42893	-3.93096
H	-3.81625	-2.71090	-3.54387
C	-6.44812	-3.43568	-2.73361
H	-5.95536	-4.27356	-3.25871
H	-7.03639	-2.88222	-3.48622
H	-7.14923	-3.86466	-1.99919
C	-7.97315	-2.24342	0.54229
H	-8.94323	-2.15450	1.06066
H	-7.62167	-3.28331	0.65662
H	-8.14270	-2.05328	-0.52974
C	-6.84670	-1.13385	3.17521
H	-6.14519	-0.44010	3.66778
H	-6.65354	-2.15150	3.55219
H	-7.86901	-0.84994	3.48068
C	1.55321	-0.04057	-1.60816
C	0.73796	0.41047	-2.65197
C	0.85865	1.72025	-3.17973
C	1.77252	2.59856	-2.52950
C	2.76871	0.72056	-1.21721
C	2.59849	2.17454	-1.49180
H	-0.06679	-0.23944	-3.03502
H	0.22651	2.06157	-4.00386
H	1.77641	3.66461	-2.80323
H	3.77694	0.30950	-2.02206
H	3.25826	2.90067	-1.00428
H	1.45258	-1.06951	-1.23934

B-Cs_2**[II]$_2$**
SCF (BP86) Energy = SCF
Enthalpy 0K = -2850.287040
Enthalpy 298K = -2850.187070
Free Energy 298K = -2850.431603
Lowest Frequency = 9.0330 cm^{-1}
Second Frequency = 10.1166 cm^{-1}
SCF (BP86-D3BJ) Energy = -2852.2095971
SCF (C6H6) Energy = -2851.72676518
SCF (BS2) Energy = -4475.78380796

Al	-4.54798	0.31121	-0.79524
Al	3.80424	-0.22815	0.10175
Cs	0.48791	-2.37499	-0.03681
Cs	0.99343	2.48338	-0.67771
Si	-6.65965	-0.22575	1.50754
Si	-5.92257	2.70011	0.57220
Si	6.59601	-1.93689	0.00606
Si	6.80477	1.04630	0.85479
O	-6.88197	1.40776	1.09886
O	7.15538	-0.60903	0.89878
N	-5.53206	-0.91529	0.33000
N	-4.33833	2.00978	0.12889
N	4.82335	-1.88295	0.07211
N	5.11029	1.20483	0.32503
C	-5.65157	-2.30709	0.00104
C	-6.41478	-2.75239	-1.13430
C	-6.46453	-4.12632	-1.44438
H	-7.04263	-4.44677	-2.31927
C	-5.81311	-5.08945	-0.66687
H	-5.87671	-6.15245	-0.92424
C	-5.08915	-4.66729	0.45292
H	-4.58175	-5.41287	1.07811
C	-4.99561	-3.30530	0.79916
C	-7.18489	-1.79355	-2.04541
H	-7.09692	-0.78328	-1.61152
C	-8.68528	-2.15617	-2.13731
H	-8.84066	-3.12655	-2.64271
H	-9.22718	-1.39197	-2.72233
H	-9.15332	-2.22179	-1.14169
C	-6.56832	-1.74402	-3.46202
H	-5.51472	-1.42344	-3.42921
H	-7.11593	-1.02431	-4.09604
H	-6.61706	-2.73340	-3.95327
C	-4.14128	-2.93072	2.00942
H	-4.24730	-1.84191	2.14769
C	-2.64985	-3.21652	1.72212
H	-2.47651	-4.29519	1.55042
H	-2.01115	-2.89675	2.56749
H	-2.35155	-2.67000	0.81069
C	-4.58562	-3.64597	3.30267
H	-5.65445	-3.47352	3.51089
H	-4.00492	-3.28662	4.17135
H	-4.43777	-4.73883	3.23433
C	-8.36906	-1.04189	1.45142
H	-8.97408	-0.71290	2.31354
H	-8.29435	-2.14170	1.48341
H	-8.90268	-0.75811	0.53067
C	-6.09416	-0.24070	3.32780
H	-5.08921	0.19145	3.46109
H	-6.08849	-1.25793	3.75326
H	-6.80272	0.36496	3.91990
C	-3.18653	2.80822	0.32351
C	-2.84284	3.88300	-0.57616
C	-1.78162	4.75674	-0.25730
H	-1.57171	5.59926	-0.92863
C	-1.02477	4.60752	0.91449
H	-0.24487	5.33303	1.17495
C	-1.29730	3.51405	1.75274
H	-0.71013	3.37954	2.66986
C	-2.34117	2.61005	1.47345
C	-3.62202	4.13460	-1.86911
H	-4.44734	3.40331	-1.89266
C	-4.21770	5.56012	-1.91878
H	-4.80863	5.78872	-1.01666
H	-4.87510	5.67442	-2.79822
H	-3.42618	6.32777	-1.99805
C	-2.75104	3.88986	-3.12387
H	-1.87550	4.56675	-3.14437
H	-3.33574	4.07820	-4.04123
H	-2.39126	2.84858	-3.17246
C	-2.56611	1.43033	2.41429
H	-3.52570	0.97623	2.11256
C	-1.46230	0.36634	2.21241
H	-0.46342	0.77481	2.45991
H	-1.45784	0.02158	1.16199
H	-1.63821	-0.50964	2.86181
C	-2.66103	1.83735	3.89930
H	-1.70598	2.24181	4.28112
H	-2.91792	0.96329	4.52319
H	-3.43590	2.60568	4.05592
C	-6.95621	3.43468	-0.84015
H	-6.94541	2.74822	-1.70274
H	-6.60789	4.42502	-1.17260
H	-7.99996	3.53670	-0.49605
C	-5.72398	3.97256	1.96547
H	-6.71165	4.38102	2.23911
H	-5.07919	4.81369	1.65901
H	-5.28180	3.51476	2.86546
C	4.04948	-3.07544	0.14855
C	3.64716	-3.78027	-1.03793
C	2.80144	-4.90477	-0.93318
H	2.50993	-5.43846	-1.84618
C	2.33957	-5.36491	0.30907
H	1.69490	-6.24877	0.37173
C	2.74473	-4.69319	1.47260
H	2.40813	-5.06240	2.44882
C	3.59590	-3.56926	1.42220

C	4.12605	-3.34892	-2.42406
H	4.78194	-2.47683	-2.27200
C	4.94686	-4.46158	-3.11391
H	5.79180	-4.78827	-2.48463
H	5.35339	-4.10445	-4.07641
H	4.32856	-5.35240	-3.32528
C	2.96071	-2.89151	-3.32782
H	2.22436	-3.70112	-3.48569
H	3.33418	-2.58615	-4.32118
H	2.43552	-2.02393	-2.88935
C	4.02224	-2.90957	2.73538
H	4.79709	-2.16686	2.47823
C	4.63354	-3.92169	3.72932
H	3.88569	-4.65153	4.08800
H	5.02811	-3.39521	4.61565
H	5.46034	-4.48918	3.27130
C	2.85118	-2.14607	3.39520
H	2.47397	-1.34756	2.72845
H	3.17326	-1.67102	4.33862
H	2.01303	-2.82741	3.63489
C	7.29484	-3.49636	0.81967
H	8.38720	-3.54245	0.67245
H	6.85308	-4.41017	0.38797
H	7.09800	-3.49718	1.90369
C	7.31599	-1.76868	-1.74666
H	6.87061	-0.91675	-2.28828
H	7.15580	-2.67697	-2.35127
H	8.40433	-1.59686	-1.67990
C	4.59497	2.50031	0.01083
C	4.03489	3.34877	1.02965
C	3.47624	4.59505	0.67510
H	3.06491	5.23637	1.46342
C	3.44348	5.03766	-0.65544
H	3.02231	6.01742	-0.90705
C	3.97898	4.21275	-1.65474
H	3.96631	4.55517	-2.69645
C	4.55756	2.96167	-1.35283
C	3.98990	2.92160	2.49801
H	4.63586	2.03496	2.58996
C	2.56491	2.48701	2.91063
H	1.84096	3.31348	2.78178
H	2.53829	2.18440	3.97242
H	2.22789	1.62128	2.30979
C	4.51462	4.01254	3.45618
H	5.51063	4.37646	3.15425
H	4.59254	3.61434	4.48250
H	3.83959	4.88619	3.49669
C	5.11977	2.12439	-2.50376
H	5.65462	1.27734	-2.04116
C	3.98804	1.53556	-3.37759
H	3.32613	0.88050	-2.77917
H	4.40246	0.92987	-4.20278
H	3.37416	2.33744	-3.82992
C	6.11931	2.91101	-3.37966
H	5.62805	3.73543	-3.92671
H	6.57206	2.24439	-4.13432
H	6.93236	3.34530	-2.77606
C	8.00326	1.93590	-0.31913
H	9.03228	1.86040	0.07228
H	7.75219	3.00747	-0.40197
H	7.99126	1.49998	-1.33087
C	7.20155	1.63421	2.61538
H	6.58857	1.11617	3.37094
H	7.07098	2.72116	2.74232
H	8.25976	1.39722	2.82333
C	-1.72797	0.28782	-1.96493
C	-0.70206	-0.20817	-2.79537
C	-0.71224	-1.55743	-3.19595
C	-1.74205	-2.39583	-2.73008
C	-2.80557	-0.51353	-1.50034
C	-2.75618	-1.88030	-1.89742
H	0.08231	0.45765	-3.18136
H	0.05479	-1.93937	-3.87833
H	-1.77698	-3.44623	-3.04638
H	-5.36590	0.68846	-2.14875
H	-3.55984	-2.55819	-1.58571
H	-1.73286	1.35844	-1.71498

Rb**[II]**·C_6H_6

SCF (BP86) Energy = -1545.89395147

Enthalpy 0K = -1545.130572

Enthalpy 298K = -1545.076843

Free Energy 298K = -1545.226084

Lowest Frequency = 4.4373 cm^{-1}

Second Frequency = 8.2072 cm^{-1}

SCF (BP86-D3) Energy = -1546.12735248

SCF (C6H6) Energy = -1545.90446101

SCF (BS2) Energy = -2357.95838263

Rb	3.00115	0.69356	-0.16349
Al	-0.50061	0.16920	-0.13475
N	-0.22984	-1.77697	0.08396
N	-2.37289	0.40617	0.22022
C	1.13545	-2.14646	0.17342
C	-2.95752	1.62858	-0.25939
C	1.92013	-2.41928	-1.00318
C	1.80948	-2.14141	1.44724
C	4.29394	3.87656	-1.09797
C	5.14717	3.02644	-1.82594
C	6.10040	2.24040	-1.15184
C	1.28285	-2.48853	-2.39144
C	-3.56469	1.66587	-1.55765
C	-2.91101	2.83331	0.51251
C	3.96241	-2.60087	0.35392
C	5.34999	3.15771	0.97824
C	4.39593	3.94263	0.30423
C	3.30983	-2.63791	-0.88756
C	6.20148	2.30558	0.25046
C	3.20208	-2.35597	1.50829
C	-3.59355	0.42450	-2.44932
C	1.43637	-3.89581	-3.01150
C	-3.46680	4.01654	-0.01430
C	-2.44203	0.47308	-3.48006
C	1.83413	-1.40836	-3.34906
C	-4.10257	2.87336	-2.03979
C	1.04193	-1.89818	2.74756
C	-4.06342	4.04792	-1.27843
C	-2.25284	2.88985	1.89132
C	1.34091	-0.49885	3.33210
C	-0.98743	3.77746	1.87502
C	-4.94719	0.20282	-3.15527
C	-3.23420	3.36192	2.98707
C	1.30494	-2.99536	3.80167
H	3.55738	4.49393	-1.62232
H	5.07818	2.98730	-2.91821
H	6.77571	1.59160	-1.71982
H	0.20868	-2.28461	-2.25347
H	5.03969	-2.78988	0.42470
H	5.43992	3.22164	2.06787
H	3.73974	4.61308	0.86869
H	3.89008	-2.85481	-1.79343
H	6.95538	1.70751	0.77345
H	3.69862	-2.35045	2.48649
H	-3.40670	-0.44135	-1.79068
H	2.49631	-4.14265	-3.20367
H	0.90063	-3.95654	-3.97512

H	1.03145	-4.67531	-2.34437
H	-3.42544	4.93506	0.58396
H	-2.54527	1.34981	-4.14471
H	-2.43225	-0.43525	-4.11038
H	-1.46187	0.55447	-2.97340
H	1.61145	-0.39442	-2.96874
H	1.36563	-1.49531	-4.34504
H	2.92756	-1.50359	-3.48883
H	-4.56185	2.89393	-3.03484
H	-0.02922	-1.91938	2.48323
H	-4.49058	4.97804	-1.66931
H	-1.93200	1.86317	2.13589
H	2.41662	-0.38473	3.56753
H	0.77654	-0.33215	4.26669
H	1.05160	0.29588	2.61825
H	-0.26051	3.39868	1.13533
H	-0.50330	3.78760	2.86923
H	-1.23182	4.82177	1.60866
H	-5.78273	0.19469	-2.43497
H	-4.94608	-0.76336	-3.69020
H	-5.15931	0.98702	-3.90400
H	-3.56198	4.40333	2.81758
H	-2.75725	3.32346	3.98299
H	-4.14051	2.73336	3.01643
H	1.10535	-4.00055	3.39492
H	0.65361	-2.84509	4.68025
H	2.34941	-2.98165	4.16254
O	-2.87645	-2.29542	0.86833
Si	-1.53979	-2.97435	0.08439
Si	-3.35171	-0.69688	1.20308
C	-5.20126	-0.54309	0.81981
H	-5.55666	0.48870	0.97833
H	-5.41760	-0.82220	-0.22395
H	-5.77892	-1.21217	1.48033
C	-3.09211	-0.49566	3.07703
H	-2.01984	-0.54400	3.33282
H	-3.48800	0.46332	3.45074
H	-3.60662	-1.31047	3.61559
C	-1.05316	-4.55096	1.02238
H	-0.13153	-4.99657	0.61052
H	-0.88786	-4.34491	2.09221
H	-1.85898	-5.30060	0.94222
C	-2.14465	-3.46703	-1.65017
H	-2.36927	-2.57706	-2.26176
H	-1.40574	-4.08035	-2.19309
H	-3.07273	-4.05775	-1.55913

A-Rb**[II]**
SCF (BP86) Energy = -1545.85103542
Enthalpy 0K = -1545.088892
Enthalpy 298K = -1545.036768
Free Energy 298K = -1545.173295
Lowest Frequency = 14.1658 cm^{-1}
Second Frequency = 23.6632 cm^{-1}
SCF (BP86-D3) Energy = -1546.10247780
SCF (C6H6) Energy = -1545.86064673
SCF (BS2) Energy = -2357.92017561

Rb	-3.67919	2.08501	-0.35503
Al	0.40131	0.13199	-0.10312
N	2.14824	-0.39043	0.22904
N	-0.82712	-1.26142	0.13296
C	3.21445	0.44168	-0.30097
C	-2.19894	-1.02231	0.44897
C	3.66829	0.24362	-1.64453
C	3.80942	1.47201	0.49130
C	-0.04662	1.96289	-0.70823
C	-0.72077	2.82120	0.37702
C	-1.31793	4.02105	-0.00957
C	3.03828	-0.80210	-2.56504
C	-3.24047	-1.33452	-0.48957
C	-2.56347	-0.48237	1.73275
C	5.27406	2.07364	-1.38133
C	-1.54750	3.21622	-2.29246
C	-0.95435	2.00313	-1.94773
C	4.68745	1.06818	-2.15695
C	-1.67110	4.29216	-1.36377
C	4.82967	2.26573	-0.07030
C	-2.93841	-1.80157	-1.91582
C	4.07730	-1.64780	-3.33201
C	-3.92770	-0.33927	2.05839
C	-3.42685	-0.76739	-2.95762
C	2.05164	-0.13642	-3.55325
C	-4.58992	-1.17554	-0.10899
C	3.36106	1.78415	1.91972
C	-4.94519	-0.69573	1.15883
C	-1.50992	-0.08342	2.77112
C	2.66127	3.16113	2.00166
C	-1.90140	1.15831	3.59850
C	-3.53408	-3.19314	-2.22440
C	-1.15361	-1.26084	3.70771
C	4.53670	1.72701	2.92205
H	0.96031	2.40255	-0.96129
H	-0.49697	2.65298	1.43761
H	-1.60764	4.74174	0.77306
H	2.45885	-1.48661	-1.92165
H	6.06572	2.70550	-1.79787
H	-2.01572	3.31153	-3.28597
H	-0.90972	1.19841	-2.69294
H	5.02390	0.92024	-3.18915
H	-2.12435	5.24500	-1.65386
H	5.27716	3.06028	0.53765
H	-1.84145	-1.86382	-2.00636
H	4.64147	-1.04285	-4.06343
H	3.57395	-2.45199	-3.89735
H	4.80694	-2.11288	-2.64854
H	-4.20103	0.04171	3.04811
H	-2.94158	0.21285	-2.79766
H	-4.52485	-0.63940	-2.91492
H	-3.17530	-1.09905	-3.98020
H	1.27080	0.44612	-3.03181
H	1.55390	-0.89312	-4.18665
H	2.58166	0.56754	-4.21894
H	-5.37724	-1.44636	-0.82302
H	2.62619	1.01398	2.20911
H	-5.99823	-0.61156	1.44971
H	-0.58199	0.17743	2.21995
H	3.34963	3.97182	1.70353
H	2.33358	3.36682	3.03701
H	1.77670	3.21576	1.34545
H	-2.17568	2.00558	2.94700
H	-1.04813	1.47662	4.22093
H	-2.74072	0.95233	4.28639
H	-3.17502	-3.96170	-1.52005
H	-3.25933	-3.51180	-3.24525
H	-4.63730	-3.18247	-2.16882
H	-2.05702	-1.63456	4.22145
H	-0.43524	-0.93442	4.48020
H	-0.69559	-2.09456	3.15447
H	5.08841	0.77380	2.85790
H	4.17035	1.84449	3.95718
H	5.26270	2.53846	2.73706
O	1.23289	-2.89612	1.10362
Si	-0.19215	-2.93738	0.19119
Si	2.58853	-1.86859	1.13134
C	2.92934	-1.61131	2.97687

H 3.85396 -1.04044 3.15708
H 2.09625 -1.08490 3.47094
H 3.03937 -2.59859 3.45838
C 4.06987 -2.74557 0.34576
H 3.82467 -3.13695 -0.65430
H 4.92849 -2.06089 0.24562
H 4.37888 -3.59346 0.98047
C 0.24008 -3.63132 -1.52160
H -0.66289 -3.89881 -2.09508
H 0.82333 -2.91341 -2.12166
H 0.84771 -4.54487 -1.40250
C -1.39106 -4.10853 1.06715
H -1.56757 -3.81178 2.11245
H -2.36812 -4.15119 0.55938
H -0.96081 -5.12450 1.06749

TS(A-B)-Rb**[II]**
SCF (BP86) Energy = -1545.83471090
Enthalpy 0K = -1545.075865
Enthalpy 298K = -1545.025132
Free Energy 298K = -1545.157406
Lowest Frequency = -665.6442 cm^{-1}
Second Frequency = -4.7929 cm^{-1}
SCF (BP86-D3) Energy = -1546.08800989
SCF (C6H6) Energy = -1545.84856768
SCF (BS2) Energy = -2357.90492325

Rb 0.00369 4.48194 -0.53400
Al -0.00069 -0.32789 0.21188
N -1.58278 -1.23452 -0.18280
N 1.58087 -1.23406 -0.18685
C -2.85446 -0.56180 -0.06881
C 2.85340 -0.56445 -0.06138
C -3.60488 -0.60203 1.14908
C -3.37748 0.17246 -1.18311
C -0.00115 1.46103 0.97478
C -1.23061 2.27125 1.20773
C -1.21538 3.34555 2.10435
C -3.09717 -1.31834 2.40099
C 3.59677 -0.61414 1.16061
C 3.38426 0.17639 -1.16771
C -5.34613 0.79663 0.13462
C 1.20768 3.34453 2.11168
C 1.22754 2.27018 1.21528
C -4.83534 0.08103 1.22211
C -0.00519 3.87780 2.62318
C -4.61156 0.83868 -1.05622
C 3.07938 -1.33519 2.40589
C -4.12265 -2.33521 2.95077
C 4.61964 0.83802 -1.02970
C 2.67580 -0.32712 3.50726
C -2.70405 -0.30692 3.50296
C 4.82864 0.06507 1.24483
C -2.59941 0.31078 -2.49292
C 5.34764 0.78586 0.16472
C 2.61282 0.32851 -2.48003
C -1.93191 1.70505 -2.57393
C 1.94921 1.72521 -2.55111
C 4.10093 -2.35217 2.96270
C 3.47493 0.08135 -3.73547
C -3.45659 0.05372 -3.74977
H -0.00417 0.46081 1.91658
H -2.19362 1.92047 0.82126
H -2.17074 3.82905 2.35938
H -2.18540 -1.86770 2.11305
H -6.30648 1.31772 0.21366
H 2.16186 3.82720 2.37258
H 2.19267 1.91856 0.83488
H -5.40054 0.05432 2.16088
H -0.00699 4.70911 3.33475
H -5.00533 1.40132 -1.91087
H 2.17082 -1.88488 2.10837
H -5.02621 -1.83085 3.33760
H -3.68581 -2.90959 3.78648
H -4.45106 -3.05044 2.17765
H 5.01949 1.40555 -1.87825
H 3.55078 0.25474 3.84969
H 2.26180 -0.85786 4.38312
H 1.91645 0.38571 3.14527
H -1.94247 0.40560 3.14511
H -2.29686 -0.83486 4.38369
H -3.58231 0.27510 3.83664
H 5.38837 0.03107 2.18660
H -1.78955 -0.43843 -2.46841
H 6.30908 1.30356 0.25239
H 1.80078 -0.41850 -2.46626
H -2.70017 2.50071 -2.59058
H -1.31768 1.79850 -3.48829
H -1.28446 1.86389 -1.69223
H 1.29853 1.87695 -1.67058
H 1.33931 1.82845 -3.46733
H 2.71961 2.51896 -2.55689
H 4.43856 -3.06443 2.19093
H 3.65623 -2.92999 3.79185
H 4.99941 -1.84765 3.36097
H 4.26213 0.84732 -3.85323
H 2.84857 0.11575 -4.64455
H 3.96924 -0.90283 -3.69850
H -3.95387 -0.92870 -3.70504
H -2.82621 0.07744 -4.65640
H -4.24128 0.82052 -3.87844
O -0.00285 -3.19355 -1.34756
Si 1.56144 -2.92198 -0.75096
Si -1.55997 -2.92780 -0.72906
C 1.90959 -4.20829 0.60053
H 2.95807 -4.16161 0.93836
H 1.26338 -4.07423 1.48318
H 1.73045 -5.21955 0.19561
C 2.76638 -3.22612 -2.17782
H 2.42511 -2.73259 -3.10143
H 3.77574 -2.85454 -1.93486
H 2.83986 -4.30903 -2.37582
C -2.78598 -3.25241 -2.13300
H -3.79309 -2.88304 -1.87773
H -2.46149 -2.76557 -3.06619
H -2.85724 -4.33739 -2.32007
C -1.87265 -4.20176 0.64271
H -1.21632 -4.04574 1.51436
H -2.91681 -4.16524 0.99478
H -1.68416 -5.21586 0.24939

B-Rb**[II]**
SCF (BP86) Energy = -1545.91113597
Enthalpy 0K = -1545.149750
Enthalpy 298K = -1545.097945
Free Energy 298K = -1545.232678
Lowest Frequency = 23.4698 cm^{-1}
Second Frequency = 25.1071 cm^{-1}
SCF (BP86-D3) Energy = -1546.16163327
SCF (C6H6) Energy = -1545.92360572
SCF (BS2) Energy = -2357.97746986

Rb -3.18749 2.27799 0.34122
Al 0.33573 0.07083 -0.88008
N 2.08270 -0.55449 -0.40127
N -0.99563 -1.22256 -0.23063

C	3.05855	0.28307	0.23438
C	-2.37215	-0.93984	-0.07429
C	3.75157	1.30898	-0.49053
C	3.34736	0.13080	1.63195
C	-0.05546	1.95365	-0.16257
C	0.00264	2.40562	1.18331
C	-0.31094	3.72810	1.55891
C	3.59048	1.49460	-2.00053
C	-3.23546	-0.69258	-1.21002
C	-2.97941	-0.87966	1.23761
C	4.88995	2.03410	1.55840
C	-0.73286	4.27242	-0.76913
C	-0.41596	2.94285	-1.12051
C	4.64495	2.16158	0.18758
C	-0.69302	4.66731	0.58160
C	4.24442	1.01334	2.26389
C	-2.73513	-0.78135	-2.65367
C	4.91075	1.16950	-2.73848
C	-4.35285	-0.58517	1.37896
C	-2.77821	0.59310	-3.35846
C	3.11566	2.91486	-2.37881
C	-4.59949	-0.38638	-1.00968
C	2.71928	-0.98216	2.47008
C	-5.17371	-0.33140	0.26969
C	-2.17168	-1.13810	2.50951
C	1.74255	-0.43588	3.53413
C	-2.13040	0.10366	3.42975
C	-3.53155	-1.81771	-3.47974
C	-2.71788	-2.35189	3.29527
C	3.78537	-1.87120	3.14982
H	0.18999	0.25279	-2.49318
H	0.32930	1.71216	1.96684
H	-0.23294	4.03386	2.60946
H	2.81963	0.78129	-2.33934
H	5.58365	2.71247	2.06723
H	-0.98471	5.00449	-1.54673
H	-0.42690	2.65917	-2.18185
H	5.16270	2.94438	-0.38000
H	-0.91822	5.70203	0.86489
H	4.44410	0.89029	3.33558
H	-1.67849	-1.09476	-2.61321
H	5.70235	1.89320	-2.47207
H	4.77067	1.21408	-3.83341
H	5.28567	0.16492	-2.48037
H	-4.79086	-0.57375	2.38509
H	-3.81266	0.98285	-3.42238
H	-2.38960	0.51195	-4.38811
H	-2.14678	1.33121	-2.83571
H	2.17177	3.17138	-1.87228
H	2.95421	2.98965	-3.46931
H	3.86432	3.67934	-2.10230
H	-5.23536	-0.22271	-1.88860
H	2.13756	-1.60326	1.76875
H	-6.24406	-0.13229	0.39641
H	-1.14008	-1.35640	2.18670
H	2.25162	0.25483	4.23030
H	1.31219	-1.25917	4.13359
H	0.90702	0.11163	3.06742
H	-1.67451	0.97220	2.92158
H	-1.52493	-0.09745	4.33029
H	-3.14331	0.38836	3.77206
H	-3.54365	-2.80508	-2.99194
H	-3.07782	-1.93441	-4.47929
H	-4.58109	-1.50490	-3.62978
H	-3.72092	-2.14534	3.71099
H	-2.05261	-2.59908	4.14075
H	-2.80510	-3.24440	2.65462
H	4.50982	-2.26641	2.41996
H	3.30947	-2.72811	3.66041
H	4.35387	-1.30933	3.91254
O	0.96180	-2.88003	-1.29316
Si	-0.41433	-2.90406	-0.30657
Si	2.46559	-2.07092	-1.21764
C	2.96902	-1.95756	-3.04347
H	2.25260	-1.32840	-3.59650
H	3.97895	-1.53687	-3.17627
H	2.95845	-2.96690	-3.49082
C	3.75548	-3.11822	-0.30209
H	4.67253	-2.53231	-0.11781
H	3.37932	-3.47956	0.66780
H	4.03069	-3.99402	-0.91438
C	-1.66610	-4.05560	-1.14561
H	-2.68059	-3.93509	-0.72884
H	-1.70660	-3.85904	-2.22857
H	-1.36272	-5.10681	-1.00235
C	0.05892	-3.70877	1.35218
H	0.70508	-3.06550	1.97002
H	-0.82952	-3.97582	1.94803
H	0.60930	-4.64256	1.14109

Rb_2**[II]$_2$**$\cdot C_6H_6$ Adduct
SCF (BP86) Energy = -2859.57971847
Enthalpy 0K = -2858.150594
Enthalpy 298K = -2858.048503
Free Energy 298K = -2858.308573
Lowest Frequency = 3.6691 cm^{-1}
Second Frequency = 7.6130 cm^{-1}
SCF (BP86-D3) Energy = -2860.05396248
SCF (C6H6) Energy = -2859.58812210
SCF (BS2) Energy = -4483.64808917

Al	-3.05702	-0.17225	0.04108
Al	2.83151	-0.92518	0.04485
Rb	-0.41862	-2.93788	-0.12847
Rb	0.19853	1.87702	0.21268
Si	-6.09433	-1.03720	0.96987
Si	-5.77930	1.40887	-0.95150
Si	5.56750	-2.37458	-1.07612
Si	5.85257	-0.22176	1.17229
O	-6.58949	0.24872	-0.01747
O	6.35757	-1.40671	0.06966
N	-4.42802	-1.46182	0.53241
N	-4.06809	1.40566	-0.48020
N	3.84330	-2.42943	-0.66072
N	4.20002	0.26568	0.74613
C	-3.95181	-2.80309	0.58775
C	-3.95340	-3.61804	-0.59769
C	-3.37183	-4.90192	-0.56602
H	-3.38341	-5.51510	-1.47504
C	-2.80227	-5.42279	0.60567
H	-2.37425	-6.43121	0.61630
C	-2.81746	-4.64221	1.77030
H	-2.39470	-5.05096	2.69643
C	-3.37984	-3.34788	1.78842
C	-4.57264	-3.11503	-1.90259
H	-5.13758	-2.20215	-1.64679
C	-5.55306	-4.13064	-2.52756
H	-5.03793	-5.04252	-2.87949
H	-6.05914	-3.68476	-3.40150
H	-6.32629	-4.44145	-1.80539
C	-3.48513	-2.70976	-2.92360
H	-2.83836	-1.90875	-2.51713
H	-3.93924	-2.33437	-3.85793
H	-2.84456	-3.57255	-3.18648
C	-3.37713	-2.56783	3.10324
H	-3.85327	-1.59603	2.89408

C	-1.94791	-2.27936	3.61331
H	-1.38512	-3.21147	3.80508
H	-1.97986	-1.71347	4.56101
H	-1.38142	-1.67325	2.88349
C	-4.20631	-3.29122	4.18874
H	-5.23516	-3.49055	3.84429
H	-4.26356	-2.68003	5.10670
H	-3.75588	-4.26201	4.46338
C	-7.28489	-2.48562	0.69087
H	-8.29927	-2.21159	1.02748
H	-6.96762	-3.37874	1.25559
H	-7.34209	-2.75639	-0.37577
C	-6.29277	-0.40844	2.75324
H	-5.56492	0.39048	2.97486
H	-6.15920	-1.20994	3.49882
H	-7.30553	0.01080	2.88356
C	-3.27171	2.58715	-0.53421
C	-2.56240	2.96087	-1.72689
C	-1.69537	4.07439	-1.70505
H	-1.16760	4.35449	-2.62518
C	-1.50197	4.83769	-0.54480
H	-0.83305	5.70517	-0.55211
C	-2.20207	4.48428	0.61868
H	-2.07161	5.08705	1.52548
C	-3.08711	3.38712	0.64690
C	-2.72265	2.18690	-3.03558
H	-3.44357	1.37719	-2.83761
C	-3.29363	3.08268	-4.15809
H	-4.24302	3.55499	-3.85402
H	-3.48133	2.49035	-5.07095
H	-2.59261	3.89333	-4.42692
C	-1.40171	1.52541	-3.48777
H	-0.60808	2.27518	-3.66265
H	-1.54581	0.97161	-4.43224
H	-1.04133	0.80476	-2.73125
C	-3.82890	3.06637	1.94528
H	-4.59347	2.31308	1.68866
C	-2.88637	2.42629	2.98989
H	-2.06226	3.11428	3.25676
H	-2.44328	1.48929	2.60198
H	-3.43181	2.18235	3.91894
C	-4.54462	4.29743	2.54167
H	-3.82940	5.06382	2.89063
H	-5.15451	4.00033	3.41264
H	-5.21068	4.77353	1.80301
C	-6.09966	0.89937	-2.75517
H	-5.59069	-0.04894	-2.99744
H	-5.76316	1.66352	-3.47540
H	-7.18315	0.74845	-2.90287
C	-6.59071	3.09434	-0.64127
H	-7.63306	3.08446	-1.00300
H	-6.05359	3.89989	-1.17036
H	-6.60570	3.33942	0.43295
C	3.04708	-3.58667	-0.89636
C	2.37070	-3.79085	-2.14816
C	1.50184	-4.89234	-2.30202
H	1.00117	-5.04373	-3.26636
C	1.27744	-5.80485	-1.26143
H	0.61048	-6.66186	-1.40599
C	1.94517	-5.61838	-0.04167
H	1.79142	-6.33999	0.76953
C	2.82991	-4.53933	0.15945
C	2.57899	-2.85323	-3.33774
H	3.27844	-2.06978	-3.00344
C	3.21713	-3.59623	-4.53368
H	4.15857	-4.09302	-4.24429
H	3.43821	-2.89309	-5.35600
H	2.54258	-4.37438	-4.93401
C	1.27354	-2.14982	-3.77054
H	0.49904	-2.87611	-4.07866
H	1.45864	-1.48211	-4.63036
H	0.86521	-1.53044	-2.95165
C	3.53873	-4.40203	1.50775
H	4.31587	-3.63013	1.37370
C	4.22819	-5.70902	1.95455
H	3.49845	-6.50700	2.18147
H	4.81693	-5.53574	2.87220
H	4.91018	-6.09119	1.17683
C	2.57339	-3.89349	2.60266
H	2.15216	-2.90663	2.33120
H	3.09477	-3.78287	3.57013
H	1.73463	-4.59887	2.75358
C	6.35626	-4.09772	-1.03379
H	7.40691	-4.04085	-1.36585
H	5.82496	-4.79773	-1.70082
H	6.34402	-4.51799	-0.01524
C	5.93772	-1.56970	-2.75861
H	5.43768	-0.59060	-2.85001
H	5.61555	-2.19921	-3.60479
H	7.02499	-1.40446	-2.85375
C	3.72483	1.59004	0.97811
C	3.12212	1.96350	2.22824
C	2.56132	3.25023	2.37757
H	2.11329	3.52544	3.34057
C	2.57682	4.18703	1.33448
H	2.15043	5.18696	1.46880
C	3.17641	3.83270	0.11655
H	3.20782	4.57049	-0.69379
C	3.75791	2.56350	-0.08029
C	3.07403	1.00385	3.41736
H	3.57843	0.07797	3.09691
C	1.62649	0.62657	3.80293
H	1.03607	1.51505	4.09384
H	1.61914	-0.06952	4.66020
H	1.11399	0.12528	2.96192
C	3.83237	1.57241	4.63793
H	4.87194	1.83644	4.38001
H	3.85891	0.83326	5.45791
H	3.34715	2.48455	5.02949
C	4.40708	2.24555	-1.42799
H	4.96359	1.30257	-1.29078
C	3.34252	1.99436	-2.52020
H	2.68398	1.14890	-2.24322
H	3.81663	1.74969	-3.48747
H	2.71091	2.88952	-2.67357
C	5.40472	3.33296	-1.88074
H	4.89980	4.28879	-2.10870
H	5.92793	3.01340	-2.79889
H	6.16333	3.53169	-1.10544
C	7.06184	1.23561	1.07658
H	8.06406	0.91769	1.41110
H	6.73510	2.06879	1.72185
H	7.15158	1.61433	0.04572
C	6.01665	-1.03921	2.88130
H	5.28220	-1.85293	3.00629
H	5.87767	-0.32143	3.70682
H	7.02537	-1.47680	2.97921
C	2.75640	7.90132	-1.34521
C	2.96130	8.00644	0.04143
C	1.88977	8.34389	0.88622
C	0.61378	8.57564	0.34463
C	1.48063	8.13256	-1.88679
C	0.40901	8.47015	-1.04214
H	3.95648	7.83030	0.46288
H	2.05155	8.43426	1.96575
H	-0.21981	8.84583	1.00166

H	1.32235	8.05648	-2.96790
H	-0.58369	8.65824	-1.46478
H	3.59345	7.64678	-2.00411

A-Rb_2**[II]$_2$**
SCF (BP86) Energy = SCF
Enthalpy 0K = -2858.095703
Enthalpy 298K = -2857.995079
Free Energy 298K = -2858.243514
Lowest Frequency = 4.4924 cm^{-1}
Second Frequency = 8.3559 cm^{-1}
SCF (BP86-D3BJ) Energy = -2860.0166952
SCF (C6H6) Energy = -2859.53305189
SCF (BS2) Energy = -4483.59578147

Al	4.08861	-0.07350	-0.28200
Al	-3.79221	0.16906	0.09870
Rb	-0.61767	2.25911	-0.54345
Rb	-1.09289	-2.28227	-0.67665
Si	6.49477	0.24238	1.81146
Si	6.03906	-2.46755	0.29533
Si	-6.62419	1.77688	-0.01171
Si	-6.67438	-1.07017	1.25212
O	6.67992	-1.40333	1.44644
O	-7.10535	0.55600	1.06527
N	5.32957	0.94158	0.64204
N	4.38868	-1.89994	-0.09045
N	-4.85272	1.78371	-0.02644
N	-5.03972	-1.25942	0.57584
C	5.39619	2.37124	0.40367
C	6.16257	2.88421	-0.69075
C	6.20844	4.27560	-0.90370
H	6.78915	4.66423	-1.74774
C	5.52726	5.16930	-0.07078
H	5.58015	6.24799	-0.25278
C	4.77119	4.66579	0.99275
H	4.22429	5.36085	1.64018
C	4.68829	3.28288	1.24846
C	6.88860	1.97265	-1.68138
H	6.86776	0.95251	-1.25801
C	8.36777	2.36510	-1.89129
H	8.46111	3.34967	-2.38263
H	8.87063	1.62845	-2.54227
H	8.91886	2.41476	-0.93787
C	6.14712	1.94393	-3.03993
H	5.08176	1.68145	-2.92658
H	6.61669	1.21852	-3.72810
H	6.18461	2.93680	-3.52266
C	3.78087	2.80437	2.38281
H	3.97031	1.72738	2.51991
C	2.29286	2.96133	1.98748
H	2.03246	4.02871	1.86395
H	1.63237	2.53500	2.76514
H	2.09456	2.45514	1.02440
C	4.06058	3.51677	3.72320
H	5.12307	3.44365	4.01052
H	3.45478	3.07231	4.53238
H	3.80601	4.59039	3.67627
C	8.18055	1.08889	1.69328
H	8.83638	0.71685	2.49871
H	8.09194	2.18261	1.79876
H	8.66670	0.87212	0.72908
C	5.91755	0.26818	3.61833
H	4.92043	-0.18837	3.73520
H	5.88142	1.28758	4.03505
H	6.63027	-0.31997	4.22226
C	3.31811	-2.85294	-0.16835
C	3.03183	-3.55288	-1.38258
C	1.97929	-4.49158	-1.40349
H	1.77530	-5.03723	-2.33250
C	1.21035	-4.76059	-0.26312
H	0.42326	-5.52358	-0.29017
C	1.48595	-4.06693	0.92693
H	0.90461	-4.29309	1.82819
C	2.52615	-3.11937	0.99783
C	3.83274	-3.31810	-2.66250
H	4.56689	-2.52585	-2.43793
C	4.60782	-4.58746	-3.08492
H	5.27198	-4.95142	-2.28225
H	5.22680	-4.38413	-3.97640
H	3.91829	-5.41165	-3.34173
C	2.93913	-2.81428	-3.81840
H	2.20303	-3.58228	-4.12085
H	3.55403	-2.58364	-4.70561
H	2.38917	-1.90261	-3.53031
C	2.78820	-2.36669	2.30232
H	3.84153	-2.03795	2.27046
C	1.91476	-1.09157	2.37687
H	0.84322	-1.35457	2.44969
H	2.03094	-0.45396	1.47823
H	2.17153	-0.48167	3.26084
C	2.60042	-3.22172	3.57113
H	1.54363	-3.49678	3.73887
H	2.93003	-2.65727	4.46018
H	3.18802	-4.15378	3.52206
C	7.20082	-2.41904	-1.20192
H	7.19864	-1.42344	-1.67754
H	6.91858	-3.16124	-1.96660
H	8.23410	-2.63525	-0.88016
C	5.99832	-4.19826	1.05179
H	7.02477	-4.51390	1.30377
H	5.57469	-4.93663	0.35107
H	5.39706	-4.21969	1.97490
C	-4.09180	2.98674	-0.09924
C	-3.74686	3.57769	-1.36289
C	-2.90447	4.70899	-1.39827
H	-2.65801	5.15808	-2.36801
C	-2.38308	5.27576	-0.22624
H	-1.73585	6.15860	-0.27482
C	-2.72989	4.71271	1.01060
H	-2.34687	5.16641	1.93263
C	-3.58231	3.59284	1.10144
C	-4.29235	3.02795	-2.68089
H	-4.84346	2.10561	-2.43302
C	-5.28037	4.02693	-3.32715
H	-6.09835	4.29268	-2.63628
H	-5.72765	3.59940	-4.24207
H	-4.77060	4.96506	-3.61136
C	-3.17804	2.65394	-3.68266
H	-2.58888	3.53689	-3.98969
H	-3.61456	2.21863	-4.59877
H	-2.47515	1.91229	-3.26397
C	-3.95525	3.06067	2.48690
H	-4.73945	2.29969	2.33195
C	-4.53120	4.16490	3.40100
H	-3.77331	4.92766	3.65475
H	-4.88772	3.72852	4.35041
H	-5.37845	4.68371	2.92256
C	-2.76044	2.36001	3.17286
H	-2.40577	1.50340	2.56910
H	-3.04729	1.97767	4.16857
H	-1.91400	3.05790	3.31357
C	-7.33683	3.40690	0.63598
H	-8.43685	3.40170	0.55239
H	-6.95409	4.26905	0.06418
H	-7.07640	3.55555	1.69630

C	-7.41098	1.36247	-1.69284
H	-6.96610	0.45261	-2.13058
H	-7.29060	2.18176	-2.42077
H	-8.49211	1.18270	-1.56122
C	-4.48547	-2.55366	0.34301
C	-3.75928	-3.25248	1.37003
C	-3.12703	-4.47840	1.07210
H	-2.58654	-5.00435	1.86837
C	-3.18422	-5.04592	-0.20903
H	-2.70368	-6.00898	-0.41482
C	-3.89433	-4.37358	-1.21408
H	-3.95871	-4.81788	-2.21466
C	-4.55120	-3.14994	-0.96615
C	-3.62612	-2.69094	2.78653
H	-4.29292	-1.81656	2.84365
C	-2.19218	-2.18552	3.06590
H	-1.45067	-2.99962	2.95599
H	-2.10615	-1.79510	4.09530
H	-1.92472	-1.36453	2.37433
C	-4.05768	-3.70826	3.86533
H	-5.06655	-4.10690	3.66719
H	-4.06691	-3.23213	4.86113
H	-3.36643	-4.56848	3.91985
C	-5.31255	-2.48481	-2.11452
H	-5.86415	-1.63800	-1.67198
C	-4.34896	-1.90408	-3.17470
H	-3.68343	-1.14068	-2.72912
H	-4.90988	-1.42274	-3.99507
H	-3.72003	-2.69675	-3.62217
C	-6.33326	-3.43662	-2.77582
H	-5.83774	-4.27780	-3.29276
H	-6.92680	-2.89394	-3.53224
H	-7.03004	-3.86074	-2.03467
C	-7.94071	-2.18296	0.37714
H	-8.92255	-2.09571	0.87335
H	-7.63317	-3.24215	0.42067
H	-8.06875	-1.90525	-0.68137
C	-6.84764	-1.36903	3.11991
H	-6.16594	-0.72581	3.70052
H	-6.66490	-2.41851	3.40326
H	-7.88065	-1.11587	3.41652
C	1.43755	-0.18747	-1.65934
C	0.57538	0.19037	-2.69692
C	0.69351	1.45332	-3.33772
C	1.57163	2.41075	-2.73254
C	2.77031	0.56067	-1.59739
C	2.45807	2.05046	-1.72659
H	-0.27558	-0.45626	-2.97810
H	0.02197	1.73700	-4.15316
H	1.47319	3.47360	-3.00792
H	3.36642	0.25693	-2.52776
H	3.07487	2.80614	-1.22871
H	1.37882	-1.18661	-1.21034

TS(A-B)-Rb_2**[II]$_2$**
SCF (BP86) Energy = -2859.51812437
Enthalpy 0K = -2858.093563
Enthalpy 298K = -2857.993667
Free Energy 298K = -2858.238919
Lowest Frequency = -607.1464 cm^{-1}
Second Frequency = 6.0213 cm^{-1}
SCF (BP86-D3) Energy = -2860.01091303
SCF (C6H6) Energy = -2859.52832984
SCF (BS2) Energy = -4483.59061359

Al	4.07922	-0.06531	-0.26128
Al	-3.79409	0.17526	0.09585
Rb	-0.66080	2.27220	-0.49800
Rb	-1.05180	-2.26302	-0.65861
Si	6.62025	0.16195	1.66808
Si	5.98951	-2.50118	0.12223
Si	-6.63530	1.77241	0.00161
Si	-6.66943	-1.09483	1.22359
O	6.71614	-1.48258	1.26448
O	-7.10562	0.53246	1.06018
N	5.40287	0.91212	0.60178
N	4.32255	-1.91277	-0.13119
N	-4.86297	1.78435	-0.02019
N	-5.02661	-1.26412	0.55977
C	5.41852	2.34913	0.42701
C	6.13108	2.93657	-0.66775
C	6.10836	4.33544	-0.83067
H	6.64748	4.77905	-1.67542
C	5.41133	5.16842	0.05069
H	5.41015	6.25411	-0.09442
C	4.71278	4.59419	1.11788
H	4.15852	5.24097	1.80810
C	4.70067	3.20080	1.32655
C	6.87866	2.09918	-1.70731
H	6.89046	1.05879	-1.33753
C	8.34201	2.55667	-1.90061
H	8.39637	3.56684	-2.34391
H	8.86895	1.87176	-2.58826
H	8.89563	2.58021	-0.94789
C	6.13580	2.11119	-3.06453
H	5.10005	1.74394	-2.96441
H	6.65781	1.47086	-3.79813
H	6.09393	3.13388	-3.48047
C	3.86675	2.64826	2.48366
H	4.09209	1.57195	2.56077
C	2.35380	2.78202	2.18696
H	2.06420	3.84564	2.10235
H	1.75427	2.32861	2.99761
H	2.10285	2.28329	1.23384
C	4.20642	3.31186	3.83584
H	5.28575	3.25941	4.05611
H	3.66359	2.81555	4.65958
H	3.91954	4.37840	3.84991
C	8.32637	0.95034	1.45604
H	9.01583	0.55174	2.21967
H	8.27942	2.04564	1.57523
H	8.74821	0.72780	0.46343
C	6.18395	0.17208	3.51561
H	5.19207	-0.27118	3.70511
H	6.19573	1.18714	3.94466
H	6.93215	-0.43257	4.05733
C	3.23732	-2.84434	-0.15427
C	2.90079	-3.56182	-1.34892
C	1.84080	-4.49204	-1.32100
H	1.60493	-5.05337	-2.23337
C	1.10993	-4.74093	-0.15061
H	0.31553	-5.49657	-0.13962
C	1.43304	-4.03241	1.01837
H	0.88402	-4.24360	1.94342
C	2.48391	-3.09366	1.04214
C	3.67412	-3.36797	-2.65381
H	4.41057	-2.56746	-2.47046
C	4.43701	-4.65375	-3.04954
H	5.11443	-4.99528	-2.24867
H	5.04081	-4.48114	-3.95784
H	3.73941	-5.48243	-3.26776
C	2.76614	-2.90431	-3.81499
H	1.99791	-3.66218	-4.05741
H	3.36686	-2.74494	-4.72726
H	2.26088	-1.95509	-3.57268
C	2.80836	-2.34953	2.33695

H	3.85007	-1.99658	2.24055
C	1.91151	-1.09752	2.48606
H	0.84984	-1.38695	2.59711
H	1.99251	-0.43269	1.60500
H	2.19337	-0.51165	3.37864
C	2.72372	-3.23018	3.59987
H	1.68706	-3.53602	3.82935
H	3.09513	-2.67144	4.47605
H	3.33044	-4.14546	3.49720
C	7.06088	-2.40779	-1.43918
H	6.98610	-1.41072	-1.90579
H	6.76721	-3.15750	-2.19195
H	8.11865	-2.58109	-1.17693
C	5.97630	-4.24834	0.84395
H	7.01285	-4.58956	1.00451
H	5.47806	-4.96727	0.17300
H	5.45498	-4.27033	1.81475
C	-4.10877	2.99138	-0.09533
C	-3.76949	3.58191	-1.36056
C	-2.92783	4.71374	-1.40021
H	-2.68369	5.16113	-2.37138
C	-2.40504	5.28363	-0.23021
H	-1.75882	6.16699	-0.28168
C	-2.74958	4.72317	1.00868
H	-2.36613	5.17999	1.92895
C	-3.59976	3.60171	1.10358
C	-4.31464	3.02669	-2.67646
H	-4.89861	2.12745	-2.42057
C	-5.25904	4.04201	-3.36021
H	-6.07825	4.34893	-2.68815
H	-5.70625	3.60710	-4.27154
H	-4.71687	4.95701	-3.65917
C	-3.19484	2.59358	-3.64781
H	-2.55436	3.44467	-3.94164
H	-3.62653	2.17285	-4.57298
H	-2.54482	1.81998	-3.20239
C	-3.96987	3.07184	2.49070
H	-4.75345	2.30970	2.33847
C	-4.54491	4.17770	3.40343
H	-3.78671	4.94069	3.65538
H	-4.90030	3.74274	4.35385
H	-5.39263	4.69568	2.92506
C	-2.77368	2.37343	3.17660
H	-2.42024	1.51408	2.57593
H	-3.05879	1.99433	4.17394
H	-1.92691	3.07155	3.31406
C	-7.35019	3.38967	0.67745
H	-8.44999	3.38477	0.59107
H	-6.96732	4.26201	0.12144
H	-7.09272	3.51988	1.74083
C	-7.42851	1.38611	-1.68323
H	-6.98301	0.48672	-2.14159
H	-7.31630	2.22039	-2.39553
H	-8.50815	1.19966	-1.54874
C	-4.46140	-2.55411	0.32468
C	-3.74120	-3.25367	1.35509
C	-3.10235	-4.47618	1.05742
H	-2.56585	-5.00310	1.85557
C	-3.14719	-5.03858	-0.22640
H	-2.66167	-5.99913	-0.43199
C	-3.85038	-4.36448	-1.23497
H	-3.90445	-4.80494	-2.23781
C	-4.51376	-3.14424	-0.98756
C	-3.62040	-2.69606	2.77428
H	-4.29714	-1.82949	2.83211
C	-2.19326	-2.17542	3.06050
H	-1.44200	-2.98012	2.94916
H	-2.11493	-1.78862	4.09183
H	-1.93263	-1.34825	2.37372
C	-4.04392	-3.72160	3.84841
H	-5.04637	-4.13323	3.64449
H	-4.06440	-3.24768	4.84504
H	-3.34146	-4.57249	3.90500
C	-5.26670	-2.47642	-2.14000
H	-5.82756	-1.63490	-1.69893
C	-4.29395	-1.88456	-3.18556
H	-3.63783	-1.12086	-2.72652
H	-4.84740	-1.40092	-4.00962
H	-3.65579	-2.67159	-3.62997
C	-6.27492	-3.42923	-2.81871
H	-5.76936	-4.26456	-3.33535
H	-6.86279	-2.88481	-3.57830
H	-6.97775	-3.86158	-2.08818
C	-7.92148	-2.19791	0.31691
H	-8.90873	-2.12182	0.80409
H	-7.61059	-3.25654	0.34763
H	-8.03953	-1.90446	-0.73850
C	-6.86025	-1.42677	3.08356
H	-6.19147	-0.78753	3.68316
H	-6.67154	-2.47928	3.35113
H	-7.89899	-1.18793	3.37193
C	1.46293	-0.08996	-1.76035
C	0.69843	0.36154	-2.84491
C	0.80445	1.68681	-3.33138
C	1.63816	2.58199	-2.60107
C	2.62594	0.70497	-1.28168
C	2.41465	2.16048	-1.52367
H	-0.04261	-0.31463	-3.30187
H	0.21524	2.02680	-4.18755
H	1.62386	3.65357	-2.85211
H	3.68061	0.35816	-2.05424
H	3.02689	2.89471	-0.98876
H	1.40847	-1.14602	-1.46472

B-Rb_2**[II]$_2$**

SCF (BP86) Energy = SCF
Enthalpy 0K = -2858.148615
Enthalpy 298K = -2858.048830
Free Energy 298K = -2858.292336
Lowest Frequency = 5.1117 cm^{-1}
Second Frequency = 11.5607 cm^{-1}
SCF (BP86-D3BJ) Energy = -2860.0714795
SCF (C6H6) Energy = -2859.58937175
SCF (BS2) Energy = -4483.64517553

Al	4.51572	-0.02908	-0.80063
Al	-3.73346	0.10391	0.09079
Rb	-0.81313	2.46059	-0.38158
Rb	-0.79741	-2.31838	-0.43506
Si	6.32983	0.52549	1.73702
Si	6.19832	-2.32502	0.39562
Si	-6.67197	1.51960	-0.10380
Si	-6.56818	-1.36400	1.06571
O	6.88517	-0.96103	1.13096
O	-7.08620	0.24174	0.92978
N	5.17088	1.16736	0.56706
N	4.56432	-1.84391	-0.11184
N	-4.90121	1.64532	-0.06869
N	-4.87902	-1.41439	0.49649
C	4.97913	2.58093	0.44766
C	5.70270	3.36250	-0.51984
C	5.42516	4.73855	-0.64952
H	5.97763	5.31809	-1.39878
C	4.47987	5.38643	0.15338
H	4.29201	6.45986	0.03978
C	3.79451	4.63897	1.11780

H	3.06532	5.13927	1.76816
C	4.02546	3.25925	1.27984
C	6.77559	2.76441	-1.43401
H	6.89451	1.70482	-1.15082
C	8.13858	3.47531	-1.26401
H	8.09609	4.52378	-1.61066
H	8.91334	2.96371	-1.86232
H	8.46840	3.48573	-0.21267
C	6.34791	2.80133	-2.91893
H	5.41967	2.23110	-3.08271
H	7.13046	2.35100	-3.55511
H	6.18894	3.83948	-3.26478
C	3.20864	2.50726	2.32923
H	3.60189	1.47805	2.35836
C	1.72788	2.41210	1.89722
H	1.28915	3.42461	1.79906
H	1.12833	1.84573	2.63357
H	1.67775	1.89544	0.92183
C	3.32267	3.12547	3.73808
H	4.37581	3.21320	4.05258
H	2.79317	2.50557	4.48364
H	2.88327	4.13868	3.77830
C	7.85443	1.62995	1.95243
H	8.45464	1.28473	2.81160
H	7.56988	2.68022	2.13307
H	8.48982	1.59238	1.05372
C	5.64630	0.18234	3.48431
H	4.72922	-0.42939	3.46767
H	5.42281	1.11598	4.02784
H	6.40953	-0.36625	4.06390
C	3.54454	-2.81876	-0.25407
C	3.34378	-3.53920	-1.48432
C	2.30352	-4.48706	-1.58023
H	2.17140	-5.03294	-2.52258
C	1.47043	-4.78599	-0.49303
H	0.70531	-5.56762	-0.57412
C	1.67315	-4.10440	0.71962
H	1.05672	-4.36084	1.59153
C	2.67849	-3.12635	0.85538
C	4.26545	-3.34662	-2.69012
H	5.01148	-2.58600	-2.40437
C	5.00649	-4.66088	-3.03184
H	5.52481	-5.07925	-2.15293
H	5.75705	-4.48681	-3.82249
H	4.30766	-5.43339	-3.40159
C	3.52235	-2.82182	-3.93897
H	2.73505	-3.52538	-4.26891
H	4.22888	-2.69975	-4.77839
H	3.05432	-1.84231	-3.75138
C	2.83046	-2.38212	2.17869
H	3.82796	-1.91334	2.14544
C	1.80450	-1.23139	2.27412
H	0.77008	-1.62527	2.32403
H	1.89183	-0.55576	1.40590
H	1.96473	-0.63040	3.18682
C	2.74924	-3.28990	3.42140
H	1.73843	-3.71488	3.56435
H	2.98646	-2.71242	4.33197
H	3.45967	-4.13024	3.35470
C	7.41314	-2.73017	-1.00387
H	7.38445	-1.93579	-1.76769
H	7.19851	-3.69452	-1.49216
H	8.43668	-2.77591	-0.59301
C	6.15015	-3.77784	1.61770
H	7.17781	-4.12415	1.82134
H	5.58064	-4.62936	1.20743
H	5.69293	-3.48801	2.57744
C	-4.23664	2.90393	-0.09657
C	-3.92218	3.55429	-1.33949
C	-3.16034	4.74233	-1.33576
H	-2.93717	5.23472	-2.29032
C	-2.69777	5.31614	-0.14181
H	-2.11731	6.24531	-0.15812
C	-3.02462	4.70058	1.07604
H	-2.69402	5.16128	2.01465
C	-3.79513	3.51941	1.12749
C	-4.41089	2.99890	-2.67715
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C	-5.38308	3.97935	-3.37157
H	-6.23253	4.23662	-2.71665
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H	-4.87915	4.92352	-3.64533
C	-3.24760	2.62704	-3.62171
H	-2.62429	3.50544	-3.87084
H	-3.63299	2.21689	-4.57152
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C	-4.16273	2.93862	2.49485
H	-4.87452	2.11632	2.30658
C	-4.85883	3.98132	3.39828
H	-4.17477	4.79982	3.68549
H	-5.20982	3.50516	4.33020
H	-5.72906	4.43513	2.89604
C	-2.93636	2.33514	3.21636
H	-2.48998	1.51539	2.62247
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C	-7.50678	3.08016	0.56567
H	-8.60085	3.00588	0.44548
H	-7.16480	3.98220	0.03090
H	-7.29078	3.21307	1.63787
C	-7.38989	1.10376	-1.81514
H	-6.86549	0.25176	-2.28040
H	-7.33178	1.95870	-2.50927
H	-8.45374	0.82966	-1.70795
C	-4.23390	-2.67351	0.29027
C	-3.56211	-3.35285	1.36632
C	-2.86452	-4.55266	1.10995
H	-2.36805	-5.06680	1.94136
C	-2.80118	-5.10902	-0.17589
H	-2.27031	-6.05133	-0.34993
C	-3.44988	-4.45028	-1.22980
H	-3.41615	-4.88551	-2.23569
C	-4.16971	-3.25367	-1.02598
C	-3.55024	-2.79477	2.79073
H	-4.27687	-1.96816	2.81364
C	-2.17147	-2.19570	3.15119
H	-1.37324	-2.95928	3.08915
H	-2.17069	-1.80208	4.18282
H	-1.91508	-1.35679	2.47724
C	-3.96780	-3.84481	3.84324
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H	-4.07793	-3.37121	4.83396
H	-3.21472	-4.64635	3.94707
C	-4.86122	-2.60833	-2.22928
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C	-3.83819	-1.99529	-3.21346
H	-3.23588	-1.20835	-2.72101
H	-4.35054	-1.53528	-4.07673
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C	-5.79409	-3.59162	-2.97048
H	-5.23016	-4.41111	-3.45059
H	-6.34688	-3.06559	-3.76835
H	-6.52974	-4.04521	-2.28704
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H  -7.75001 -2.18832 -1.00980
C  -6.85838 -1.77032  2.89654
H  -6.27695 -1.11033  3.56097
H  -6.62133 -2.81712  3.14629
H  -7.92819 -1.60704  3.11577
C   1.66927 -0.31597 -1.98172
C   0.60825  0.09224 -2.81746
C   0.51922  1.43085 -3.24091
C   1.48355  2.35104 -2.78654
C   2.68506  0.56986 -1.53001
C   2.52998  1.92442 -1.94428
H  -0.12051 -0.63827 -3.19497
H  -0.26604  1.74140 -3.93913
H   1.44729  3.39474 -3.12571
H   5.47056 -0.00849 -2.11678
H   3.27764  2.66732 -1.64077
H   1.76103 -1.38356 -1.73584
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