

Supporting information for

VCD spectroscopy reveals conformational changes of chiral crown ethers upon complexation of potassium and ammonium cations

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1. Additional figures

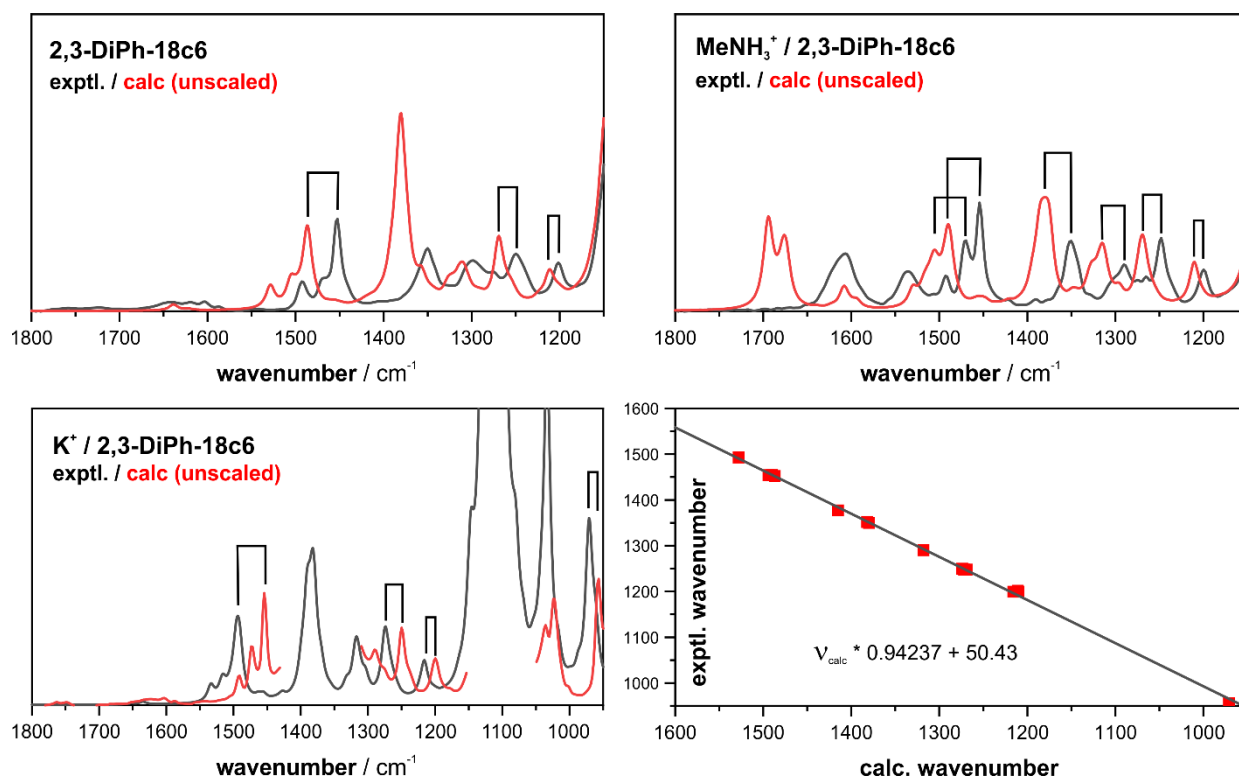


Fig. S1. Peak assignment for the determination of the frequency scaling factor.

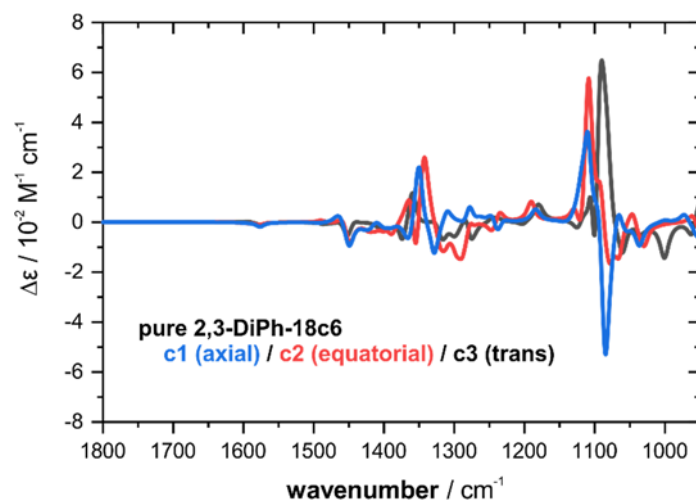


Fig. S2. Single conformer VCD spectra of the three lowest energy conformers of pure 2,3-DiPh-18c6.

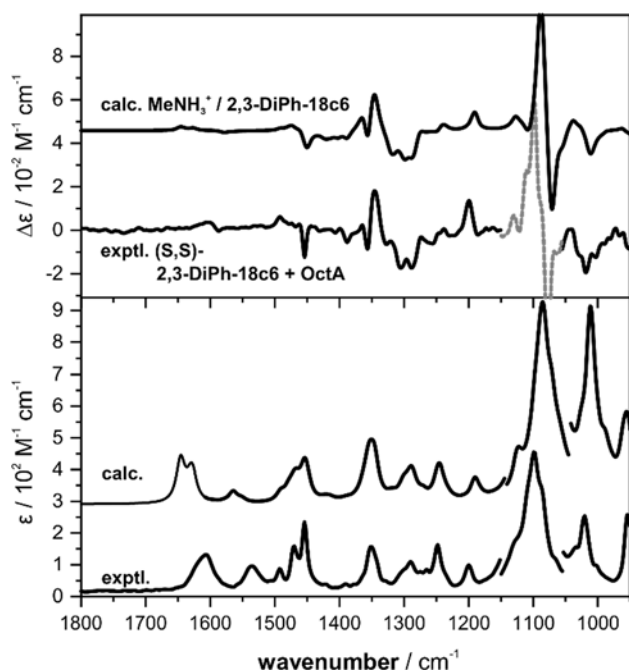


Fig. S3. Full range view of the comparison of the computed IR and VCD spectra of $\text{MeNH}_3^+ / 2,3\text{-DiPh-18c6}$ with the experimental ones.

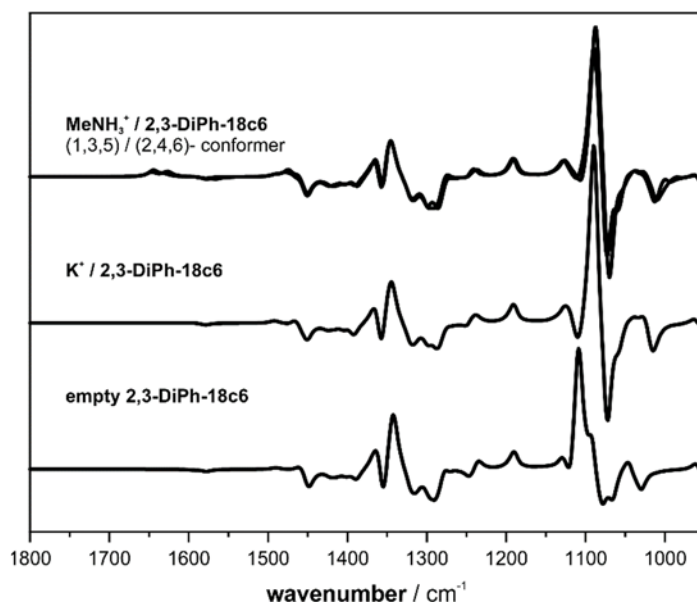


Fig. S4. Comparison of the computed VCD spectra of the two highly populated conformers of $\text{MeNH}_3^+ / 2,3\text{-DiPh-18c6}$ with empty equatorial conformer and the equatorial conformer of $\text{K}^+ / 2,3\text{-DiPh-18c6}$

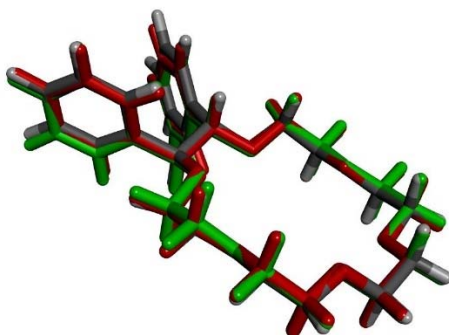


Figure S5. Overlap of the D_{3d} -symmetric crown ether structure of **2,3-DiPh-18c6**, its K^+ and $MeNH_3^+$ complexes.

2. X-ray structures of 2,3-DiPh-18c6 and 2-Ph-18c6

Note that the crystal structures were obtained for (R,R)-2,3-DiPh-18c6 and (R)-2-Ph-18c6. In order to avoid confusion as all calculations were carried out for the (S,S)- and (S)-isomers, the structures were mirrored for presentation in Figs. 4A and 7B of the main article.

Table S1. Crystal data and structure refinement for 2,3-DiPh-18c6.

CCDC-Nr	2157857
Empirical formula	C ₂₄ H ₃₂ K N O ₉
Formula weight [g/mol]	517.6
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁ (19)
Lattice parameters [Å]	
a	9.6493(4)
b	11.3747(5)
c	23.4471(9)
a	90
b	90
g	90
Density [g/cm ³]	1.333
Crystal size [mm ³]	0.296 x 0.221 x 0.071
Volume [Å ³]	2573.50(18)
Z	4
Temperature [K]	292.8(4)
Diffraction Device	SuperNova, Single source at offset/far, Atlas
Radiation Type	1.54184 Å (Cu K/ micro-focus sealed X-ray tube)
F(000)	1092
Absorption coefficient [mm ⁻¹]	2.252
Absorption correction	Gaussian
Measurement range	3.8 - 66.5
Index range	-11 < h < 11 -13 < k < 9 -26 < l < 27
Measured reflexes	8501
Independent	4539
Observed	3880
R(int)	0.0258
Completeness (%) / theta (°)	100.0 / 66.494
Transmission (min / max)	0.456 / 1.000
R1 (observed/all)	0.0397 / 0.0486
wR2 (observed/all)	0.0982 / 0.1046
GooF = S	1.01
Rest electron density max./min. [e-/Å ³]	-0.198 / 0.225

Table S2. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for **2,3-DiPh-18c6**

	x	y	z	U(eq)	S.O.F.
K(1)	0.62957(9)	0.53281(7)	0.52512(3)	0.0578(2)	1
O(1)	0.5007(3)	0.5594(2)	0.63931(10)	0.0510(6)	1
O(2)	0.4207(3)	0.3808(3)	0.55594(13)	0.0721(8)	1
O(3)	0.4441(4)	0.4142(3)	0.44015(13)	0.0761(9)	1
O(4)	0.6485(3)	0.5689(3)	0.40424(12)	0.0728(8)	1
O(5)	0.7118(3)	0.7465(3)	0.48274(11)	0.0642(7)	1
O(6)	0.6950(3)	0.7148(2)	0.60111(10)	0.0522(6)	1
O(7)	0.9153(4)	0.4947(4)	0.52133(18)	0.1002(11)	1
O(8)	0.8313(4)	0.4482(3)	0.60267(16)	0.0846(9)	1
O(9)	1.0418(4)	0.5052(6)	0.5962(2)	0.140(2)	1
N(1)	0.9308(4)	0.4825(4)	0.5734(2)	0.0779(11)	1
C(1)	0.5436(4)	0.6082(3)	0.73880(15)	0.0483(8)	1
C(2)	0.4203(4)	0.6667(3)	0.75045(17)	0.0567(9)	1
C(3)	0.3681(5)	0.6731(4)	0.80499(19)	0.0671(10)	1
C(4)	0.4388(5)	0.6198(4)	0.84900(19)	0.0703(11)	1
C(5)	0.5594(5)	0.5620(4)	0.83836(19)	0.0735(12)	1
C(6)	0.6121(4)	0.5557(4)	0.78384(17)	0.0605(9)	1
C(7)	0.6013(3)	0.6026(3)	0.67882(15)	0.0461(7)	1
C(8)	0.6506(4)	0.7240(3)	0.65928(14)	0.0454(7)	1
C(9)	0.7090(5)	0.8277(3)	0.57454(17)	0.0608(10)	1
C(10)	0.7897(5)	0.8136(4)	0.52142(19)	0.0713(11)	1
C(11)	0.7799(6)	0.7365(5)	0.4293(2)	0.0866(15)	1
C(12)	0.6820(7)	0.6857(5)	0.3882(2)	0.0878(16)	1
C(13)	0.5559(5)	0.5159(5)	0.36610(18)	0.0783(14)	1
C(14)	0.5169(6)	0.3987(5)	0.3884(2)	0.0848(15)	1
C(15)	0.3989(7)	0.3062(4)	0.4628(2)	0.0883(15)	1
C(16)	0.3265(6)	0.3273(5)	0.5172(2)	0.0854(15)	1
C(17)	0.3648(5)	0.3922(4)	0.61122(18)	0.0656(10)	1
C(18)	0.4751(5)	0.4369(3)	0.64942(17)	0.0604(10)	1
C(19)	0.7652(4)	0.7667(3)	0.69740(14)	0.0452(7)	1
C(20)	0.7513(4)	0.8691(3)	0.72866(15)	0.0533(8)	1
C(21)	0.8548(5)	0.9045(4)	0.76634(17)	0.0664(11)	1
C(22)	0.9722(5)	0.8386(4)	0.77274(18)	0.0653(10)	1
C(23)	0.9889(4)	0.7377(4)	0.74060(17)	0.0618(10)	1
C(24)	0.8872(4)	0.7018(3)	0.70313(16)	0.0534(8)	1
H(2)	0.372103	0.702297	0.720761	0.068	1
H(3)	0.285832	0.713069	0.812069	0.08	1
H(4)	0.404079	0.623337	0.885963	0.084	1
H(5)	0.606818	0.526347	0.868235	0.088	1
H(6)	0.694627	0.515661	0.777287	0.073	1
H(7)	0.680887	0.54898	0.678705	0.055	1
H(8)	0.572895	0.779295	0.661464	0.055	1
H(9A)	0.756157	0.881514	0.600086	0.073	1
H(9B)	0.618203	0.859715	0.565949	0.073	1
H(10A)	0.809867	0.890125	0.505119	0.086	1
H(10B)	0.876822	0.774537	0.529532	0.086	1
H(11A)	0.860776	0.686381	0.432899	0.104	1
H(11B)	0.810136	0.8134	0.416408	0.104	1
H(12A)	0.598342	0.732937	0.386935	0.105	1
H(12B)	0.723016	0.685836	0.35038	0.105	1
H(13A)	0.599035	0.507821	0.32894	0.094	1
H(13B)	0.473841	0.564473	0.361933	0.094	1
H(14A)	0.458873	0.358056	0.360967	0.102	1
H(14B)	0.599348	0.351835	0.394881	0.102	1
H(15A)	0.47775	0.254922	0.469084	0.106	1
H(15B)	0.336746	0.267952	0.436103	0.106	1
H(16A)	0.247396	0.3784	0.511043	0.102	1
H(16B)	0.293235	0.253495	0.532787	0.102	1
H(17A)	0.331828	0.316613	0.624684	0.079	1
H(17B)	0.287261	0.446535	0.610735	0.079	1
H(18A)	0.447538	0.425633	0.688824	0.072	1
H(18B)	0.559686	0.392719	0.643016	0.072	1
H(20)	0.67205	0.914837	0.724477	0.064	1
H(21)	0.844009	0.973342	0.787254	0.08	1
H(22)	1.040302	0.861428	0.798532	0.078	1
H(23)	1.069563	0.693639	0.744271	0.074	1
H(24)	0.899953	0.634068	0.681571	0.064	1

Table S3. Anisotropic displacement parameters [\AA^2] for **2,3-DiPh-18c6**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
K(1)	0.0617(4)	0.0559(4)	0.0558(4)	0.0003(3)	-0.0015(4)	-0.0055(4)
O(1)	0.0547(13)	0.0427(12)	0.0555(13)	0.0032(10)	-0.0070(12)	-0.0076(10)
O(2)	0.0774(19)	0.0751(19)	0.0638(17)	-0.0122(14)	-0.0019(15)	-0.0293(15)
O(3)	0.102(2)	0.0636(17)	0.0630(17)	-0.0145(13)	0.0054(16)	-0.0053(15)
O(4)	0.0732(18)	0.089(2)	0.0557(15)	-0.0060(14)	-0.0070(15)	0.0025(16)
O(5)	0.0741(17)	0.0700(16)	0.0487(14)	0.0093(13)	0.0086(13)	-0.0069(13)
O(6)	0.0672(15)	0.0431(12)	0.0463(13)	0.0034(10)	-0.0004(12)	-0.0086(11)
O(7)	0.094(2)	0.115(3)	0.092(3)	0.010(2)	0.002(2)	0.017(2)
O(8)	0.083(2)	0.079(2)	0.091(2)	-0.0016(18)	0.002(2)	0.0201(17)
O(9)	0.079(2)	0.177(5)	0.164(5)	0.021(4)	-0.045(3)	0.002(3)
N(1)	0.073(2)	0.069(2)	0.092(3)	0.000(2)	-0.017(2)	0.0193(19)
C(1)	0.0469(18)	0.0455(17)	0.0526(19)	0.0030(15)	-0.0015(16)	-0.0059(14)
C(2)	0.0510(19)	0.056(2)	0.063(2)	0.0042(17)	-0.0053(18)	0.0009(15)
C(3)	0.058(2)	0.067(2)	0.076(3)	-0.007(2)	0.013(2)	-0.006(2)
C(4)	0.079(3)	0.077(3)	0.055(2)	-0.003(2)	0.006(2)	-0.018(2)
C(5)	0.078(3)	0.086(3)	0.056(2)	0.014(2)	-0.006(2)	-0.008(2)
C(6)	0.054(2)	0.066(2)	0.062(2)	0.0142(17)	-0.0035(19)	0.0011(17)
C(7)	0.0412(17)	0.0460(17)	0.0512(18)	0.0050(14)	-0.0026(14)	-0.0008(13)
C(8)	0.0465(17)	0.0430(16)	0.0468(17)	0.0041(13)	-0.0002(15)	-0.0012(13)
C(9)	0.079(3)	0.0449(19)	0.059(2)	0.0090(16)	0.000(2)	-0.0159(18)
C(10)	0.078(3)	0.072(3)	0.064(2)	0.010(2)	-0.002(2)	-0.029(2)
C(11)	0.098(4)	0.101(4)	0.060(3)	0.005(3)	0.020(3)	-0.021(3)
C(12)	0.111(4)	0.096(4)	0.056(2)	0.008(2)	0.011(3)	-0.010(3)
C(13)	0.060(2)	0.123(4)	0.052(2)	-0.007(3)	0.000(2)	0.008(3)
C(14)	0.082(3)	0.105(4)	0.067(3)	-0.039(3)	-0.003(3)	0.005(3)
C(15)	0.120(4)	0.071(3)	0.074(3)	-0.016(2)	-0.013(3)	-0.020(3)
C(16)	0.099(4)	0.078(3)	0.079(3)	-0.007(3)	-0.013(3)	-0.039(3)
C(17)	0.069(2)	0.062(2)	0.067(2)	-0.0026(18)	0.005(2)	-0.023(2)
C(18)	0.070(2)	0.049(2)	0.062(2)	0.0077(16)	0.002(2)	-0.0141(17)
C(19)	0.0477(17)	0.0423(17)	0.0457(17)	0.0023(13)	0.0033(15)	-0.0047(14)
C(20)	0.059(2)	0.0474(19)	0.0537(19)	-0.0010(15)	0.0022(18)	-0.0007(15)
C(21)	0.084(3)	0.061(2)	0.054(2)	-0.0111(17)	0.003(2)	-0.015(2)
C(22)	0.068(2)	0.073(2)	0.055(2)	0.004(2)	-0.012(2)	-0.018(2)
C(23)	0.0505(19)	0.069(2)	0.065(2)	0.0068(19)	-0.0096(19)	-0.0023(17)
C(24)	0.0523(19)	0.0515(18)	0.0565(19)	-0.0011(15)	-0.0019(17)	-0.0006(16)

Table S4. Crystal data and structure refinement for **2-Ph-18c6**.

CCDC-Nr	2157856
Empirical formula	C ₁₈ H ₂₈ K N O ₉
Formula weight [g/mol]	441.51
Crystal system	Tetragonal
Space group	P4 ₃ (78)
Lattice parameters [Å]	
a	8.0124(7)
b	8.0124(7)
c	33.848(3)
α	90
β	90
γ	90
Density [g/cm ³]	1.35
Crystal size [mm ³]	0.601 x 0.488 x 0.439
Volume [Å ³]	2173.0(4)
Z	4
Temperature [K]	170(2)
Diffraction Device	XtaLAB Mini (ROW)
Radiation Type	0.71073 Å (Mo K/ fine-focus sealed X-ray tube)
F(000)	936
Absorption coefficient [mm ⁻¹]	0.292
Absorption correction	Analytical
Measurement range	2.5 - 26.5
Index range	-10 < h < 10 -10 < k < 10 -42 < l < 42
Measured reflexes	16269
Independent	4311
Observed	4084
R(int)	0.0481
Completeness (%) / theta (°)	100.0 / 25.242
Transmission (min / max)	0.878 / 0.908
R1 (observed/all)	0.0409 / 0.0439
wR2 (observed/all)	0.1000 / 0.1031
Goof = S	1.085
Rest electron density max./min. [e-/Å ³]	-0.169 / 0.294

Table S5. Atomic coordinates and equivalent isotropic displacement parameters [\AA^2] for **2-Ph-18c6**

	x	y	z	U(eq)	S.O.F.
K(1)	0.57645(9)	1.05642(9)	0.51826(2)	0.03275(18)	1
O(1)	0.5181(3)	0.7946(3)	0.45972(8)	0.0394(6)	1
O(2)	0.2629(3)	0.9054(3)	0.50959(8)	0.0406(6)	1
O(3)	0.3144(3)	1.1475(3)	0.56810(9)	0.0409(6)	1
O(5)	0.8328(4)	1.2792(3)	0.50373(9)	0.0436(6)	1
O(6)	0.7685(3)	1.0396(3)	0.44656(8)	0.0395(6)	1
O(8)	0.7392(4)	1.0215(4)	0.59254(9)	0.0459(7)	1
O(7)	0.7660(5)	0.8175(4)	0.55241(10)	0.0601(9)	1
O(9)	0.8898(4)	0.8095(4)	0.60880(10)	0.0569(8)	1
O(4)	0.5748(3)	1.3763(3)	0.55471(8)	0.0410(6)	1
N(1)	0.7981(4)	0.8824(4)	0.58510(10)	0.0390(7)	1
C(1)	0.3495(5)	0.7439(4)	0.45419(12)	0.0359(8)	1
C(2)	0.2706(5)	0.7407(5)	0.49441(12)	0.0430(9)	1
C(3)	0.1717(6)	0.9077(7)	0.54538(13)	0.0569(13)	1
C(4)	0.1552(5)	1.0836(6)	0.55953(16)	0.0552(12)	1
C(5)	0.3095(5)	1.3137(6)	0.58131(16)	0.0512(11)	1
C(6)	0.4834(6)	1.3683(6)	0.59034(13)	0.0464(10)	1
C(7)	0.7435(5)	1.4188(5)	0.56152(12)	0.0387(8)	1
C(8)	0.8299(5)	1.4368(5)	0.52290(13)	0.0433(9)	1
C(9)	0.9137(6)	1.2833(6)	0.46672(14)	0.0520(11)	1
C(10)	0.9300(5)	1.1072(6)	0.45214(14)	0.0483(10)	1
C(11)	0.7770(6)	0.8758(6)	0.43164(15)	0.0487(10)	1
C(12)	0.6024(6)	0.8154(5)	0.42350(12)	0.0450(10)	1
C(13)	0.3346(5)	0.5723(4)	0.43557(10)	0.0326(7)	1
C(14)	0.4404(5)	0.4429(5)	0.44580(13)	0.0447(9)	1
C(15)	0.4216(6)	0.2871(5)	0.42889(13)	0.0459(10)	1
C(16)	0.2951(5)	0.2612(5)	0.40161(12)	0.0428(9)	1
C(17)	0.1902(5)	0.3877(5)	0.39192(12)	0.0434(9)	1
C(18)	0.2101(5)	0.5421(5)	0.40889(11)	0.0371(8)	1
H(1)	0.290626	0.827587	0.437267	0.043	1
H(2A)	0.156792	0.693309	0.492619	0.052	1
H(2AB)	0.337291	0.669384	0.512346	0.052	1
H(3A)	0.230137	0.839858	0.565533	0.068	1
H(3AB)	0.059588	0.858913	0.541113	0.068	1
H(4A)	0.101145	1.152597	0.538908	0.066	1
H(4AB)	0.084603	1.086995	0.583525	0.066	1
H(5A)	0.23939	1.322212	0.605307	0.061	1
H(5AB)	0.260692	1.386199	0.56064	0.061	1
H(6A)	0.481786	1.47931	0.60317	0.056	1
H(6AB)	0.53672	1.28806	0.608661	0.056	1
H(7A)	0.798272	1.330604	0.57739	0.046	1
H(7AB)	0.750001	1.524955	0.576411	0.046	1
H(8A)	0.770434	1.519171	0.506269	0.052	1
H(8AB)	0.945393	1.477064	0.527102	0.052	1
H(9A)	1.02546	1.334742	0.469419	0.062	1
H(9AB)	0.847827	1.350363	0.447745	0.062	1
H(10A)	0.992243	1.105586	0.426886	0.058	1
H(10B)	0.992332	1.039458	0.471643	0.058	1
H(11A)	0.831779	0.801715	0.451123	0.058	1
H(11B)	0.843438	0.874086	0.406986	0.058	1
H(12A)	0.542487	0.897515	0.40688	0.054	1
H(12B)	0.606274	0.707862	0.409112	0.054	1
H(14)	0.52656	0.461315	0.464576	0.054	1
H(15)	0.494662	0.198544	0.435891	0.055	1
H(16)	0.281889	0.154733	0.389674	0.051	1
H(17)	0.103041	0.369452	0.373399	0.052	1
H(18)	0.135783	0.629701	0.401949	0.045	1

Table S6. Anisotropic displacement parameters [\AA^2] for **2-Ph-18c6**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
K(1)	0.0344(4)	0.0328(4)	0.0311(3)	-0.0023(3)	0.0037(3)	-0.0053(3)
O(1)	0.0398(14)	0.0424(14)	0.0360(14)	-0.0104(12)	0.0060(12)	-0.0114(11)
O(2)	0.0408(14)	0.0431(14)	0.0379(15)	-0.0109(12)	0.0096(12)	-0.0092(11)
O(3)	0.0361(13)	0.0461(15)	0.0407(14)	-0.0094(13)	-0.0005(12)	-0.0003(11)
O(5)	0.0490(15)	0.0395(14)	0.0423(15)	-0.0048(12)	0.0085(13)	-0.0136(12)
O(6)	0.0370(14)	0.0380(14)	0.0437(15)	-0.0094(12)	0.0093(12)	-0.0088(11)
O(8)	0.0612(18)	0.0348(14)	0.0416(15)	-0.0016(12)	-0.0013(14)	0.0022(13)
O(7)	0.085(2)	0.0411(16)	0.0542(19)	-0.0091(15)	-0.0140(18)	0.0113(16)
O(9)	0.0400(15)	0.074(2)	0.0563(19)	0.0188(17)	0.0000(14)	0.0115(15)
O(4)	0.0434(15)	0.0414(14)	0.0382(14)	-0.0061(12)	-0.0021(12)	-0.0032(12)
N(1)	0.0355(16)	0.0430(18)	0.0384(17)	0.0086(15)	0.0021(14)	-0.0019(14)
C(1)	0.0367(18)	0.0323(18)	0.0387(19)	-0.0036(16)	0.0016(16)	-0.0069(15)
C(2)	0.044(2)	0.041(2)	0.044(2)	-0.0076(18)	0.0079(18)	-0.0119(17)
C(3)	0.055(3)	0.075(3)	0.041(2)	-0.020(2)	0.018(2)	-0.025(2)
C(4)	0.035(2)	0.072(3)	0.058(3)	-0.026(2)	0.010(2)	-0.008(2)
C(5)	0.044(2)	0.051(2)	0.058(3)	-0.020(2)	0.003(2)	0.0063(19)
C(6)	0.050(2)	0.046(2)	0.043(2)	-0.0188(19)	0.0045(19)	0.0012(19)
C(7)	0.048(2)	0.0318(18)	0.0362(19)	-0.0037(16)	-0.0074(17)	-0.0085(16)
C(8)	0.051(2)	0.0330(18)	0.046(2)	-0.0028(18)	-0.003(2)	-0.0136(16)
C(9)	0.052(2)	0.055(3)	0.048(2)	-0.004(2)	0.013(2)	-0.025(2)
C(10)	0.041(2)	0.058(2)	0.046(2)	-0.011(2)	0.0137(19)	-0.0146(19)
C(11)	0.044(2)	0.045(2)	0.057(3)	-0.013(2)	0.019(2)	-0.0030(18)
C(12)	0.054(2)	0.045(2)	0.036(2)	-0.0159(18)	0.0129(19)	-0.0163(19)
C(13)	0.0383(19)	0.0315(17)	0.0281(16)	-0.0003(14)	0.0023(15)	-0.0052(15)
C(14)	0.047(2)	0.042(2)	0.045(2)	-0.0010(18)	-0.0112(19)	-0.0027(17)
C(15)	0.055(2)	0.037(2)	0.046(2)	0.0047(18)	-0.001(2)	0.0027(18)
C(16)	0.055(2)	0.035(2)	0.039(2)	-0.0067(17)	0.0071(19)	-0.0150(18)
C(17)	0.042(2)	0.050(2)	0.039(2)	-0.0043(18)	-0.0012(18)	-0.0135(18)
C(18)	0.0385(19)	0.041(2)	0.0316(18)	0.0044(16)	0.0002(16)	0.0002(16)

3. Conformational analysis of 2,3-DiPh-18c6 and its complexes

Table S7. Relative energies and corresponding Boltzmann populations χ of the 15 lowest energy conformers ($\Sigma\chi > 97\%$) of **2,3-DiPh-18c6** at B3LYP/6-311G++(2d,p)/IEFPCM(CHCl₃). XYZ-coordinates for the first 10 structures can be found below.

Conformer	ΔE_{ZPC} [kcal / mol]	ΔG_{298K} [kcal / mol]	$\chi(\Delta E_{ZPC})$ [%]	$\chi(\Delta G_{298K})$ [%]
2,3-DiPh-18c6_c1	0.00	0.00	39.29	47.93
2,3-DiPh-18c6_c2	0.27	0.56	25.01	18.55
2,3-DiPh-18c6_c3	0.46	0.77	18.09	12.98
2,3-DiPh-18c6_c4	1.10	1.25	6.10	5.81
2,3-DiPh-18c6_c5	1.65	2.18	2.43	1.21
2,3-DiPh-18c6_c6	1.91	1.54	1.57	3.59
2,3-DiPh-18c6_c7	2.09	1.23	1.15	5.98
2,3-DiPh-18c6_c8	2.14	2.99	1.05	0.31
2,3-DiPh-18c6_c9	2.17	3.81	1.01	0.08
2,3-DiPh-18c6_c10	2.47	2.57	0.60	0.63
2,3-DiPh-18c6_c11	2.56	3.26	0.52	0.19
2,3-DiPh-18c6_c12	2.77	4.09	0.37	0.05
2,3-DiPh-18c6_c13	2.78	3.04	0.36	0.28
2,3-DiPh-18c6_c14	2.82	4.48	0.34	0.02
2,3-DiPh-18c6_c15	2.93	3.33	0.28	0.17

ΔE_{ZPC} referenced to -1384.992584 hartree / ΔG_{298K} referenced to -1385.055856 hartree

Table S8. Relative energies and corresponding Boltzmann populations χ of the 8 lowest energy conformers ($\Sigma\chi > 97\%$) of **K⁺/2,3-DiPh-18c6** at B3LYP/6-311G++(2d,p)/IEFPCM(CHCl₃). XYZ-coordinates for the structures can be found below.

Conformer	ΔE_{ZPC} [kcal / mol]	ΔG_{298K} [kcal / mol]	$\chi(\Delta E_{ZPC})$ [%]	$\chi(\Delta G_{298K})$ [%]
K ⁺ / 2,3-DiPh-18c6_c1	0.00	0.00	84.15	85.94
K ⁺ / 2,3-DiPh-18c6_c2	1.38	1.48	8.18	7.11
K ⁺ / 2,3-DiPh-18c6_c3	2.55	2.72	1.14	0.88
K ⁺ / 2,3-DiPh-18c6_c4	2.43	2.11	1.40	2.44
K ⁺ / 2,3-DiPh-18c6_c5	2.71	2.91	0.86	0.63
K ⁺ / 2,3-DiPh-18c6_c6	2.94	3.40	0.59	0.27
K ⁺ / 2,3-DiPh-18c6_c7	2.89	3.43	0.64	0.26
K ⁺ / 2,3-DiPh-18c6_c8	2.94	3.52	0.59	0.23

ΔE_{ZPC} referenced to -1984.89502 hartree / ΔG_{298K} referenced to -1984.958781 hartree

Table S9. Relative energies and corresponding Boltzmann populations χ of the 11 lowest energy conformers ($\Sigma\chi > 97\%$) of $\text{CH}_3\text{NH}_3^+/\text{2,3-DiPh-18c6}$ at B3LYP/6-311G++(2d,p)/IEFPCM(CHCl_3). XYZ-coordinates for the structures can be found below.

Conformer	ΔE_{ZPC} [kcal / mol]	$\Delta G_{298\text{K}}$ [kcal / mol]	$\chi(\Delta E_{\text{ZPC}})$ [%]	$\chi(\Delta G_{298\text{K}})$ [%]
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c1}$ (2,4,6)	0.00	0.00	49.93	54.77
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c2}$ (1,3,5)	0.27	0.94	31.66	11.15
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c3}$ (1,3,5)	1.53	0.84	3.78	13.27
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c4}$ (1,3,5)	1.66	1.67	3.01	3.28
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c5}$ (1,3,5)	1.68	1.48	2.95	4.49
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c6}$ (1,3,5)	2.11	1.68	1.41	3.23
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c7}$ (1,3,5)	2.14	1.54	1.36	4.08
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c8}$ (1,3,5)	2.29	2.12	1.05	1.53
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c9}$ (2,4,6)	2.47	2.96	0.77	0.37
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c10}$ (2,4,6)	2.51	2.93	0.72	0.39
$\text{MeNH}_3^+ / \text{2,3-DiPh-18c6_c11}$ (2,4,6)	2.52	3.04	0.70	0.32

ΔE_{ZPC} referenced to -1481.289975 hartree / $\Delta G_{298\text{K}}$ referenced to -1481.355318 hartree

3.1 Cartesian coordinates of 2,3-DiPh-18c6

2,3-DiPh-18c6_c1

O	0.11597500	0.87584600	3.03782600	H	1.46340900	-0.52961100	1.42235800
O	-1.17435700	-1.02007600	1.30639100	C	-1.08204500	-3.30293300	0.06099900
O	-0.82270900	-0.41122900	-1.55290900	H	-1.06185500	-4.33878800	0.43029700
O	1.61291800	1.00633800	-2.37929300	H	-1.00442300	-3.33411600	-1.03388000
O	2.79405000	3.01598100	-0.58500300	C	0.10653400	-2.56977800	0.63592300
O	2.23120400	2.47201600	2.18333400	H	0.97298600	-3.24031600	0.59939800
C	2.23051600	0.30827000	4.14607000	C	-0.08616700	-2.31765400	1.68660000
C	2.69665700	-0.47271800	3.08700100	C	-4.68781100	-2.68179300	0.47773300
H	2.23313200	-0.37473100	2.11407600	H	-4.61126600	-2.53336600	1.56300700
C	3.74229700	-1.36923200	3.28147000	H	-5.55051100	-3.33596700	0.28357800
H	4.09325600	-1.975208400	2.45181200	C	-3.43719100	-3.35822600	-0.02995300
C	4.33988900	-1.49399000	4.53385200	H	-3.43842000	-3.69030000	-1.12808400
H	5.15426000	-2.19346300	4.68242500	H	-3.43398100	-4.40118800	0.31936800
C	3.87891700	-0.72129600	5.59494800	C	-5.94400800	0.68197300	-0.32386600
H	4.33025200	-0.81749100	6.57566800	H	-6.89588000	1.18649600	-0.10273200
C	2.82647800	0.16953000	5.39973000	H	-5.86189600	0.57235000	-1.47722900
H	2.46243300	0.75911700	6.23527100	C	-5.94400200	-0.68196900	0.32391400
C	1.10638500	1.31387600	3.94976000	H	-6.89588300	-1.18648700	0.10280700
H	0.64430400	1.50540800	4.92898800	C	-5.86186000	-0.57234600	1.41327500
C	1.63205500	2.68125900	3.44859900	H	-4.68781000	2.68179300	-0.47772500
H	2.39967100	2.99473400	4.17075600	H	-4.61127900	2.53335600	-1.56299900
C	3.06824400	3.53014900	1.73975500	C	-5.55050800	3.33596300	-0.28356300
H	3.83864500	3.74356700	2.49391800	C	-3.43718500	3.35822800	0.02994000
H	2.48677700	4.44500700	1.57719800	H	-3.43840200	3.36904600	1.12807100
C	3.74996500	3.11645100	0.45683000	H	-3.43397800	4.40118600	-0.31939400
H	4.51440900	3.86669900	0.20623500	O	0.37177900	1.38499800	0.10921000
H	4.25328700	2.15165300	0.60042900	O	-2.29185900	2.67885000	-0.45627600
C	3.34813100	2.55024000	-1.80415300	O	0.43742300	1.43761800	0.17745100
H	3.95868100	1.65523200	-1.62763800	O	0.37177900	-1.38499400	-0.10923700
C	3.99515300	3.32124900	-2.24702300	O	-2.29186000	-2.67885500	0.45626000
H	2.24013600	2.21493500	-2.77484500	O	-4.85543500	-1.43761800	-0.17743400
H	2.66903100	2.10691200	-3.78174000	C	2.80214000	1.47907700	-0.03783800
C	0.53821400	0.63627200	-3.22601900	C	3.77111000	1.67958200	-1.01944600
H	0.90041500	0.48524700	-4.25351500	C	3.00952600	2.02367800	1.23160200
H	-0.22206100	1.42843400	-3.24745900	C	4.93189400	2.39613700	-0.73991400
C	-0.08157200	-0.65169900	-2.73663500	H	3.61919500	1.27072500	-2.01254400
H	-0.74115100	-1.04759200	-3.52277700	C	4.16608600	2.74191600	1.51455400
H	0.70628700	-1.39354400	-2.54998200	H	2.25339300	1.89564300	1.99716700
C	-1.39971300	-1.58814100	-1.01161200	C	5.13328500	2.92802800	0.52941300
H	-0.62374400	-2.34079300	-0.81867200	H	5.67493400	2.54227400	-1.51513600
H	-2.12084100	-2.01783100	-1.72213600	H	4.31287900	3.15879300	2.50421800
C	-2.11829000	-1.25463500	0.27444700	H	6.03415400	3.48872100	0.74917900
H	-2.74347400	-0.36534200	0.12144600	C	2.80213700	-1.47907500	0.03783900
H	-2.77806200	-2.09133900	0.54617900	C	3.77109200	-1.67958600	1.01946100
C	-1.76233400	-0.48568200	2.48074000	C	3.00953900	-2.02367400	-1.23159900
H	-2.47772800	-1.20121700	2.91224500	C	4.93187800	-2.39614300	0.73994300
H	-2.30521800	0.43799700	2.24265600	H	3.61916500	-1.27073200	2.01226800
C	-0.69033900	-0.19567800	3.50435400	C	4.16610100	-2.74191400	-1.51453700
H	-1.17338500	0.07935200	4.45254800	H	2.25341700	-1.89563600	-1.99717400
H	-0.08484000	-1.09279000	3.67687100	C	5.13328600	-2.92803100	-0.52938300
C	0.54141200	3.74102800	3.42724400	H	5.67490800	-2.54228400	1.51517500
C	0.34408700	4.55885100	4.54003900	H	4.31290600	-3.15879000	-2.50420000
H	0.99080700	4.45332900	5.40547300	H	6.03415700	-3.48872600	-0.74913800
C	-0.66866400	5.51451900	4.55181000				
H	-0.80797700	6.14320300	5.42365600				
C	-1.49082000	5.66856300	3.43994500				
C	-1.29280100	4.86266500	2.32094100				
C	-0.28517800	3.90369800	2.31468100				
H	-0.12852900	3.27739000	1.44636800				
H	-2.27595000	6.41562300	3.44206900				
H	-1.92639400	4.98098800	1.44945000				
H	1.50981400	3.03443800	-2.80314500				

2,3-DiPh-18c6_c2

C	-1.08204000	3.30293900	-0.06104600
H	-1.06185600	4.33878500	-0.43036900
H	-1.00440400	3.33414900	1.03383200
C	0.10653300	2.56977100	-0.63596700
H	0.97298600	3.24030800	-0.59945800
H	-0.08617600	2.31763100	-1.68663800
C	1.53339300	0.69266300	-0.33872400
H	1.46342600	0.52961400	-1.42237100
C	1.53338800	-0.69266000	0.33871100

2,3-DiPh-18c6_c3

C	-0.45256400	3.46343300	-0.07996700
H	-0.38529400	4.36588900	-0.70426100
H	-0.31581100	3.76324900	0.96707400
C	0.63926800	2.49757700	-0.47642100
H	1.58138600	3.04325100	-0.60557500
H	0.38173300	2.02858600	-1.43364700
C	-0.37333400	-3.64456700	0.69017700
H	-0.51510800	-4.69930900	0.97039500
H	-0.36038900	-3.58556900	-0.40637800
C	0.95910000	-3.18387400	1.24993700
H	1.69579800	-3.96461800	1.04660900
H	0.88377200	-3.06615000	2.33546200
C	-3.81325700	-2.55748000	1.47896300
H	-3.58519100	-2.41337000	2.54338500
H	-4.75103600	-3.12726100	1.40751400
C	-2.71258700	-3.36083400	0.82792900
H	-2.82242100	-3.32503000	-0.26387000
H	-2.81109200	-4.40883500	1.14446400

C	-5.16040800	0.76228100	0.61603100
H	-6.10567400	1.24100900	0.91056400
H	-5.21417400	0.53716900	-0.45825700
C	-5.00118600	-0.52219000	1.39361400
H	-5.95069400	-1.07538500	1.35525300
H	-4.78222500	-0.29748300	2.44595200
C	-4.07438800	2.79442400	0.08108300
H	-4.16559700	2.52606300	-0.97961800
H	-4.92803700	3.43552800	0.34465700
C	-2.79338500	3.56430800	0.29826400
H	-2.63149300	3.72754500	1.37202300
H	-2.88493200	4.54758700	-0.18556800
O	-1.71199500	2.83609200	-0.25578800
O	-4.06832700	1.62483500	0.88225600
O	-1.43931700	-2.86496000	1.21544000
O	-3.96063500	-1.30519400	0.82949000
C	5.01692800	1.52797400	0.43565400
C	3.65079300	1.38089100	0.65524400
C	2.90019500	0.48167400	-0.10433000
C	3.54630300	-0.26153800	-1.09359700
C	4.91388500	-0.12312500	-1.31072200
C	5.65429600	0.77343000	-0.54540000
H	5.58484600	2.23233000	1.03254500
H	3.15810200	1.97060100	1.41786400
H	2.97353300	-0.95540600	-1.69802900
H	5.39932800	-0.70963800	-2.08221000
H	6.71827500	0.88802200	-0.71672700
C	1.40925200	0.30894200	0.12618500
H	0.95688900	-0.03833300	-0.81100600
C	1.02207500	-0.76273800	1.18351300
H	-0.07004700	-0.75386600	1.21734600
O	1.48212900	-2.00363500	0.64528200
O	0.76817500	1.50736800	0.53774200
C	1.54983600	-0.49827400	2.58158000
C	2.81306500	-0.93855100	2.98137400
C	0.76176300	0.19900600	3.49904100
C	3.28048100	-0.68116500	4.26645100
H	3.42738400	-1.49180500	2.28245200
C	1.22980500	0.46603900	4.78211300
H	-0.22591200	0.53382000	3.20442800
C	2.49217700	0.02589500	5.17026500
H	4.26250700	-1.03232000	4.56202000
H	0.60470800	1.00929500	5.48141600
H	2.85590300	0.22590700	6.17145600

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C	3.95029700	3.69264400	0.80664700
C	4.28594200	3.00503100	-0.35520900
C	3.44500100	2.00819700	-0.84265600
C	2.26467000	1.68138100	-0.17617500
C	1.93128700	2.38309700	0.98411500
C	2.76802000	3.38028700	1.47349400
H	2.49509900	3.91809400	2.37409400
H	1.00233400	2.15677800	1.49286900
C	1.34819600	0.58770100	-0.70049700
H	1.61881000	0.36366200	-1.74090900
C	1.45184500	-0.73718400	0.08619000
C	2.88084700	-1.21645100	0.28212900
C	3.59133500	-1.78219800	-0.77900700
C	4.90080500	-2.21641800	-0.60362600
C	5.51940500	-2.09232900	0.63828200
C	4.81714800	-1.53709900	1.70292500
C	3.50532500	-1.10625100	1.52372100
H	2.96266600	-0.67776100	2.35913800
H	5.28732100	-1.44314000	2.67481700
H	6.53935400	-2.43162200	0.77548400
H	5.43949500	-2.65385600	-1.43625200
H	3.11000300	-1.89376100	-1.74341700
H	0.99386800	-0.56771900	1.06939600
O	0.67315500	-1.68200200	-0.64098100
C	0.33874500	-2.85074000	0.08822800
C	-0.60484300	-3.70126200	-0.74780800
H	-0.22451200	-3.74783400	-1.77040300
O	-1.92879100	-3.18672100	-0.83444900
C	-2.76826500	-3.59530400	0.23655600

C	-4.12456500	-2.94329300	0.10849400
H	-4.47099200	-3.00898400	-0.93142800
O	-4.05133900	-1.548934700	0.52488700
C	-5.30401300	-0.92755100	0.46265200
C	-5.17817100	0.46356200	1.03602100
H	-4.65684000	0.41492300	2.00081600
O	-4.47060700	1.30335000	0.13755500
C	-4.21144900	2.58828600	0.68301600
C	-3.45896800	3.44894500	-0.31270000
H	-3.99608700	3.47271400	-1.26911900
O	-2.10665300	3.06143400	-0.51185200
C	-1.91086800	2.10946000	-1.55730800
C	-0.43746200	1.81647600	-1.70134000
H	0.13148900	2.75447100	-1.70617300
H	0.27147600	1.30335000	-2.66021800
O	-0.01755100	0.97443600	-0.63605400
H	-2.45643800	1.18633700	-1.34639600
H	-2.28026600	2.52673200	-2.50426100
H	-3.43125100	4.46787600	0.08293600
H	-3.62311700	2.49364500	1.60521200
H	-5.15840000	3.09075300	0.93403400
H	-6.18489800	0.86832100	1.21341400
H	-5.66034700	-0.87462600	-0.57485800
H	-6.05096700	-1.48063100	1.05029200
H	-4.83978800	-3.48956100	0.74022800
H	-2.89422500	-4.68685600	0.21000500
H	-2.33155700	-3.32765000	1.20613600
H	-0.62228600	-4.72251800	-0.34584100
H	1.24023300	-3.44231400	0.30751300
H	-0.12588800	-2.58257700	1.04431700
H	3.71126100	1.47912200	-1.75108400
H	5.19894200	3.24760200	-0.88639500
H	4.60086400	4.47172900	1.18632100

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C	0.37327400	3.21614800	2.07078000
H	-0.50599200	3.85112800	1.90011600
C	1.24212300	3.34085200	0.79533400
H	1.63648000	4.36678300	0.78981400
C	3.37943400	3.21906100	0.00276600
H	2.99860500	2.82900700	-1.00225900
H	3.99321400	3.47101100	0.32566000
C	4.22735200	1.36944500	-0.03457000
H	4.45846700	1.05031400	0.99006600
H	5.17585700	1.58766700	-0.54635000
C	3.24581600	-1.95450900	-1.29521000
H	3.81105100	-2.89327900	-1.38909700
H	2.979981300	-1.61639100	-2.30557200
C	4.12476800	-0.92461100	-0.62521700
H	5.10668900	-0.92144300	-1.12093600
H	4.27648200	-1.19658400	0.42779400
C	-0.00766900	-3.31054900	-0.20673300
H	0.30424400	-3.38536600	0.84167000
H	-0.51216500	-4.24822800	-0.48003700
C	1.21653600	-3.14498000	-1.07687600
H	0.91223600	-2.85910900	-2.09252200
H	1.73893700	-4.11091400	-1.13784600
C	-1.93174700	-1.77325700	1.79437900
H	-1.06384000	-2.23299300	2.28483500
H	-2.82641300	-2.05743200	2.36916500
C	-2.08174900	-2.28690500	0.37344300
H	-2.82164700	-1.67593000	-0.14753000
H	-2.45347800	-3.31984800	0.40498700
C	-1.49271100	0.18482700	3.04548700
H	-2.33571600	0.03124700	3.73504600
H	-0.60979800	-0.30844900	3.47253400
C	-1.23083600	1.66682600	2.91863600
H	-1.15002200	2.09359500	3.92677400
H	-2.06715100	2.15674300	2.40328000
O	2.30898600	2.41591300	0.91609800
O	-0.02826800	1.86323700	2.18975600
O	-1.78900800	-0.36367200	1.77265200
O	3.51756400	0.35085700	-0.71971800
O	2.07598500	-2.16367800	-0.52180700
O	-0.89298400	-2.21732500	-0.40410000
C	1.08985100	3.72302900	3.31328500

C	0.97204700	5.06215500	3.68784500
C	1.88647600	2.87631000	4.08461000
C	1.64541200	5.55294600	4.80312100
H	0.34273100	5.72849500	3.10637600
C	2.55621400	3.36218700	5.20338700
H	1.97268700	1.83525000	3.80261100
C	2.44106400	4.70233500	5.56468200
H	1.54080300	6.59514500	5.08164700
H	3.17107800	2.69321300	5.79455700
C	2.96248200	5.07905000	6.43679700
C	0.42213300	3.14085000	-0.46994700
C	-0.07644200	4.25059600	-1.15370200
C	0.13288300	1.86275100	-0.95127500
C	-0.86235000	4.09326400	-2.29222800
H	0.15504400	5.24940200	-0.79678200
C	-0.64844900	1.70423700	-2.09129900
H	0.52367700	0.99653700	-0.43432800
C	-1.15077100	2.81615200	-2.76349400
H	-1.24006200	4.96547000	-2.81332900
H	-0.86809800	0.70624800	-2.45189200
H	-1.75870500	2.68799800	-3.65168700

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C	-0.63679600	3.79903000	0.83867000
H	-0.68075200	4.88695800	0.67811200
H	-0.88090700	3.60162000	1.89103000
C	0.77315700	3.33041700	0.53457600
H	1.46948000	4.00736800	1.03505500
H	0.95859200	3.39153800	-0.54205800
C	0.73674800	0.92709400	0.18978400
H	-0.31833000	0.99066100	-0.08673100
C	0.85381700	-0.32865500	1.10001600
H	0.20473900	-0.12204700	1.96028200
C	-0.80334000	-3.52775800	0.28618300
H	-0.76996400	-4.52761300	0.74062800
H	-0.37924000	-3.59830000	-0.72352000
C	0.02358300	-2.57475700	1.11739700
H	0.95312000	-3.07204300	1.41605400
H	-0.52738500	-2.30610000	2.02734200
C	-4.37598600	-3.24921100	-0.66219800
H	-4.76467800	-3.28393400	0.36297600
H	-4.99299700	-3.90537300	-1.28087400
C	-2.95368000	-3.77839300	-0.69437500
H	-2.54294700	-3.68025500	-1.70805800
H	-2.97511600	-4.84856600	-0.43797600
C	-4.37719600	0.43152200	-1.00144700
H	-5.41715500	0.63065700	-1.29302300
H	-3.76568400	0.40801200	-1.91241500
C	-4.25282200	-0.89323200	-0.27285800
H	-4.96428900	-0.94016900	0.56184000
H	-3.24248200	-0.98369700	0.12790000
C	-3.81705600	2.72547700	-0.67908500
H	-3.41682500	2.67090700	-1.69916100
H	-4.81224500	3.18820100	-0.72612800
C	-2.90379900	3.57512300	0.17288000
H	-3.19156100	3.48537100	1.22850800
H	-3.00625700	4.62911100	-0.12088900
O	1.08441000	2.02923000	1.03029600
O	-1.56398500	3.14351400	-0.01290500
O	-3.89830100	1.42780000	-0.11240500
O	0.30633400	-1.40747700	0.35120300
O	-2.14495300	-3.06605500	0.22966100
O	-4.52458300	-1.94094000	-1.20128400
C	1.56452000	0.87090700	-1.08112600
C	0.99496300	0.37813600	-2.25661600
C	2.89144400	1.30438800	-1.11063500
C	1.73676900	0.30279300	-3.43150800
H	-0.03842300	0.05159200	-2.25049500
C	3.63343100	1.23922600	-2.28591600
C	3.34031400	1.70144100	-0.20909500
C	3.06018700	0.73411200	-3.44966900
H	1.27829500	-0.08334000	-4.33457500
H	4.66154700	1.58258200	-2.29247100
H	3.63790500	0.68404500	-4.36526700
C	2.25110000	-0.61347100	1.62195500

C	2.64792500	-0.11219000	2.86266000
C	3.15987100	-1.37664800	0.88623100
C	3.92767600	-0.35340500	3.35336700
H	1.94910800	0.47376000	3.44860600
C	4.43724100	-1.62733800	1.37747300
H	2.86063800	-1.77990400	-0.07295500
C	4.82717100	-1.11325700	2.61114100
H	4.21920100	0.04543900	4.31809300
H	5.12969400	-2.22430100	0.79522600
H	5.82205300	-1.30877000	2.99385500

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C	-1.30720100	2.82758500	-0.15755300
H	-1.04454200	3.88545400	-0.02568200
H	-1.46185000	2.38682300	0.83484300
C	-0.19706000	2.07179000	-0.86649900
H	0.13058400	2.60974800	-1.76494800
H	-0.57174700	1.09008200	-1.15736100
C	1.92288300	1.04464400	-0.34834500
H	1.87797000	0.88829400	-1.43117900
C	1.70242100	-0.32719200	0.33882700
H	1.66352400	-0.14431900	1.42023500
C	-1.53691400	-2.08217500	0.14650500
H	-1.43424600	-2.45488600	-0.88044500
H	-2.14508800	-1.17436800	0.12133100
C	-0.16350500	-1.78432700	0.72306200
H	0.44394400	-2.69642700	0.74173800
H	-0.25776200	-1.41299500	1.75121000
C	-4.59549800	-2.85106400	0.80406400
H	-4.58752300	-2.58773400	1.87028300
H	-5.46890400	-3.49551300	0.62151900
C	-3.34272000	-3.63565600	0.46402600
H	-3.27231000	-3.77342400	-0.62188500
H	-3.43165600	-4.62168900	0.92651700
C	-5.87269200	0.33719400	-0.54733900
H	-6.86553000	0.80047500	-0.45525100
H	-5.71186600	0.08584000	-1.60410800
C	-5.85134500	-0.91804500	0.29193100
H	-6.74948300	-1.51027300	0.06595800
H	-5.88050100	-0.65049600	1.35644200
C	-4.85677200	2.46564200	-0.79505300
H	-4.81795700	2.29315800	-1.87854000
H	-5.76903500	3.07335800	-0.57264100
C	-3.64529600	3.25847700	-0.36234700
H	-3.57608500	3.23735000	0.73127100
H	-3.75401100	4.30409100	-0.67837100
O	0.88743900	1.94562600	0.05123000
O	-2.48047300	2.68791800	-0.94321300
O	-4.86897700	1.23017100	-0.09588400
O	0.43031700	-0.79158400	-0.10387400
O	-2.13609600	-3.07834200	0.96959500
O	-4.68558800	-1.67745200	0.00934900
C	3.26056600	1.66374300	0.00117300
C	4.29808100	1.68720100	-0.92972400
C	3.47486500	2.22756900	1.26128500
C	5.52931600	2.25354600	-0.61020900
H	4.14484800	1.25859600	-1.91374800
C	4.70236000	2.79618200	1.58266500
H	2.67221700	2.23501400	1.98862400
C	5.73526900	2.80859300	0.64823900
H	6.32445400	2.26377800	-1.34642500
H	4.85284100	3.23269400	2.56322100
H	6.69148400	3.25258200	0.89873700
C	2.80174900	-1.33285000	0.04333400
C	3.75056500	-1.65985100	1.01132600
C	2.87936800	-1.94768300	-1.20864200
C	4.76533200	-2.57204200	0.73486900
H	3.69748800	-1.19685900	1.99048900
C	3.88993000	-2.86126300	-1.48772600
H	2.13503400	-1.71968700	-1.96238500
C	4.83849500	-3.17436400	-0.51690200
H	5.49417300	-2.81540300	1.49904400
H	3.93653600	-3.33179700	-2.46299300
H	5.62506600	-3.88745700	-0.73369600

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C	2.28160300	3.26035800	0.49930200
H	2.23642600	4.29900900	0.14139200
C	2.98968800	2.45656600	-0.61904900
H	4.00254900	2.87660500	-0.69987600
C	3.97940800	0.30950700	-0.94555300
H	3.66768400	0.24302900	-1.99410600
H	4.98398300	0.75421800	-0.91420300
C	4.04368400	-1.07182700	-0.33849300
H	4.21971600	-0.98959900	0.74196700
H	4.89177600	-1.61394500	-0.78136500
C	1.44613800	-3.69653600	-0.15553100
H	1.50271800	-4.71247000	0.26258300
H	1.26299400	-3.77885700	-1.22822100
C	2.78924100	-3.02467000	0.07472600
H	3.56975100	-3.69423800	-0.31804100
H	2.98663400	-2.89214100	1.14643400
C	-1.06474100	-2.39985700	2.23383200
H	-1.11317900	-2.47183200	3.32995000
H	-1.88523600	-3.00054300	1.81706700
C	0.27003000	-2.94951200	1.78664100
H	0.39753100	-3.95360400	2.21700200
H	1.06639700	-2.30510100	2.17403800
C	-2.46411400	0.96242200	1.71843600
H	-3.39999900	1.42197100	2.06882100
H	-2.53754400	0.82546700	0.63221700
C	-2.30284300	-0.38588600	2.37990800
H	-3.22227000	-0.96428300	2.21032100
H	-2.17157000	-0.26862100	3.46472400
C	-1.31433100	2.98193600	1.25963200
H	-1.55405000	2.76398800	0.21173800
H	-2.05058300	3.70695700	1.63544200
C	0.06616100	3.59014500	1.33540800
H	0.37258000	3.70492100	2.38159100
H	0.04038200	4.58723400	0.87426700
O	3.07234200	1.10690000	-0.19733400
O	0.96907700	2.74893100	0.63166600
O	-1.35444500	1.78897200	2.02677100
O	2.83359500	-1.77196300	-0.58383900
O	0.31635500	-3.01571200	0.36945700
O	-1.18479600	-1.05126600	1.82036400
C	3.06699600	3.24287900	1.80191100
C	4.02122400	4.22965600	2.05138000
C	2.86422700	2.24412600	2.75493400
C	4.77227700	4.21504100	3.22368600
H	4.17695300	5.02213900	1.32607000
C	3.60787100	2.23144100	3.93062100
H	2.11673300	1.48406700	2.56939900
C	4.56679600	3.21363800	4.16768800
H	5.50882400	4.98971700	3.40291100
H	3.43850800	1.45212400	4.66478400
H	5.14430100	3.20228700	5.08466200
C	2.29954000	2.62295400	-1.96401400
C	2.72057700	3.62174200	-2.84221400
C	1.23307900	1.80252600	-2.33516400
C	2.08251000	3.81113000	-4.06539300
H	3.55918500	4.25590900	-2.57200200
C	0.59932200	1.98447400	-3.56000500
H	0.90835000	1.02142200	-1.66030300
C	1.01860100	2.99088400	-4.42740200
H	2.42260500	4.59080200	-4.73711300
H	-0.22536700	1.33851700	-3.83837800
H	0.52346400	3.12988200	-5.38136900

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C	-5.83153300	0.21754800	-1.52176400
C	-5.85523200	0.12520500	-0.13357800
C	-4.66649300	0.19402100	0.58799700
C	-3.44205500	0.34661600	-0.06366700
C	-3.42752100	0.44167200	-1.45588700
C	-4.61430400	0.37909900	-2.17945400
H	-4.58915700	0.45465500	-3.26049200
H	-2.48100300	0.56527200	-1.96525400
C	-2.15249600	0.38355800	0.74230800
H	-2.39655900	0.71183300	1.76129000

C	-1.50817800	-1.01618500	0.89063300
C	-0.42344500	-1.03173600	1.95663300
C	0.87569100	-0.60282600	1.67854200
C	1.84043400	-0.59965500	2.68113800
C	1.52231000	-1.01874500	3.97081000
C	0.23029500	-1.45070600	4.25385800
C	-0.73257500	-1.46047700	3.24839800
H	-1.73556100	-1.81083200	3.47130100
H	-0.02606800	-1.78789700	5.25156800
H	2.27769900	-1.01375100	4.74807800
H	2.84606500	-0.26666000	2.45336600
H	1.12882200	-0.27452500	0.67886400
H	-2.31172200	-1.69277200	1.21459400
O	-1.04156400	-1.41065700	-0.38827500
C	-0.70121100	-0.27829000	-2.49135800
C	-0.12855900	-3.04230800	-1.87349600
H	-0.83102500	-2.67613100	-2.62440500
O	1.09754500	-2.37367100	-2.13357900
C	2.24131800	-2.99446000	-1.56524000
C	3.47017700	-2.18289500	-1.90216200
H	3.45784800	-1.92756600	-2.96984700
O	3.50102500	-1.00352600	-1.11415500
C	4.54784300	-0.12876000	-1.48654800
C	4.51214600	1.11958700	-0.62938900
H	4.50572100	0.84359900	0.43371300
O	3.36490000	1.88802900	-0.94429000
C	3.30060800	3.11334800	-0.23172900
C	1.97992200	3.78949000	-0.51914500
H	1.78182000	3.74926300	-1.59765600
O	0.94766600	3.13237400	0.19760000
C	-0.35343300	3.44308600	-0.26898300
C	-1.37421900	2.62302100	0.48431100
H	-1.26835500	2.78424400	1.56513300
H	-2.37627500	2.95500800	0.18333300
O	-1.18371700	1.24934000	0.17863500
H	-0.42817800	3.22873200	-1.34289400
H	-0.57640500	4.50942500	-0.11692000
H	2.03743800	4.84626800	-0.22189800
H	3.39660700	2.93588900	0.84748600
H	4.12235300	3.77455600	-0.54246000
H	5.42633900	1.70007500	-0.82214600
H	4.44975100	0.15429900	-2.54443800
H	5.52377300	-0.61337800	-1.35352200
H	4.36571700	-2.79073100	-1.79052200
H	2.35916000	-4.00730000	-1.97619900
H	2.15068600	-3.07731800	-0.47616600
H	-0.01211900	-4.12623900	-2.01209900
H	-1.59691900	-3.40978900	-0.36022000
H	0.01495700	-3.06382600	0.28936900
H	-4.69391600	0.13409400	1.67142900
H	-6.79792500	0.00935900	0.38855900
H	-6.75489900	0.16990600	-2.08701700

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O	-0.89715600	-0.45909000	2.16654200
O	-0.99035800	0.71655400	-0.54658200
O	1.51964200	1.59247300	-1.69690700
O	3.36137300	2.79915100	0.25049300
C	3.84779800	2.65629200	2.59642200
H	4.58405200	2.24130300	3.29886700
H	3.92562700	3.74943100	2.62949600
C	4.18474600	2.15862600	1.21106400
H	5.24505000	2.37844900	1.01811400
H	4.04405500	1.07160800	1.15837200
C	3.66141700	2.42936300	-1.08739700
H	3.95413200	1.37375400	-1.13710400
H	4.49640700	3.03339400	-1.46834600
C	2.44097100	2.63899200	-1.95321100
H	2.73621000	2.63727100	-3.01247500
C	0.25067200	1.78620600	-2.29349000
H	0.34136000	1.82617900	-3.38886800
H	-0.19097800	2.73243100	-1.95374600
C	-0.65117400	0.63366300	-1.92069000
H	-1.55939200	0.67165700	-2.53970500
H	-0.13765900	-0.31419000	-2.12906700
C	-1.72259100	-0.40930200	-0.09434300

H	-1.14311100	-1.32886600	-0.25049500	H	-1.16912200	3.07307000	5.68703400
H	-2.66280400	-0.50106100	-0.65779800	H	-1.81523000	3.29754600	8.05808200
C	-2.05452000	-0.25651000	1.37033500	H	-0.50065600	2.14721600	9.81895100
H	-2.47051100	0.74372500	1.55105000	C	0.92053200	1.67224700	4.62243100
H	-2.82430100	-0.99577200	1.63532600	H	0.13456500	2.10500200	3.99435500
C	-1.17098600	-0.30003900	3.54764900	C	2.22436600	2.44664200	4.32529900
H	-1.94810900	-1.01300500	3.86316800	H	3.01831400	2.01434500	4.94988100
H	-1.56423000	0.70669900	3.74006800	O	2.54056200	2.23278000	2.95750000
C	0.06095300	-0.58405100	4.38774900	O	1.15467700	0.31827300	4.24365700
H	-0.25851600	-0.63520600	5.43554200	C	2.09056500	3.92662300	4.65471900
H	0.46712600	-1.55796800	4.10970800	C	1.33983200	4.76560600	3.82781000
H	1.98981900	3.61375600	-1.72652900	C	2.71765800	4.47237500	5.77362500
C	0.88307500	1.27646100	8.41891600	C	1.20992800	6.11826300	4.12308400
C	1.24576900	1.15386000	7.08228000	H	0.87196400	4.35850600	2.93932900
C	0.51562100	1.80248400	6.08310000	C	2.58795400	5.82591700	6.07392200
C	-0.58984200	2.56752700	6.45176900	H	3.31127000	3.83419200	6.41891200
C	-0.95450600	2.69635300	7.78954800	C	1.83120300	6.65239000	5.24977400
C	-0.21773000	2.05144000	8.77732600	H	0.62633000	6.75788600	3.47113000
H	1.45883600	0.76632000	9.18244100	H	3.08165300	6.23398400	6.94814800
H	2.09564500	0.53923300	6.80926800	H	1.73120100	7.70685800	5.47880000

3.2. Cartesian Coordinates of K⁺/2,3-DiPh-18c6

K⁺ / 2,3-DiPh-18c6_c1				H	5.51173800	-3.01421800	-2.35757400
C	-0.24690000	-3.26337900	-0.96285800	H	6.77142000	-3.60715200	-0.30626900
H	-0.35264200	-4.30643800	-0.64030600	C	3.57731600	1.44785300	0.13383500
H	0.05943800	-3.25929200	-2.01614300	C	4.76794100	1.69928700	-0.54567200
C	0.80638100	-2.60300000	-0.11074000	C	3.44842500	1.88539300	1.45419800
H	1.68830800	-3.24879900	-0.09604000	C	5.81830800	2.36262800	0.08267900
H	0.44559300	-2.49278200	0.91953100	H	4.87865100	1.37169900	-1.57327300
C	2.23530800	-0.69149500	0.04309000	C	4.49396700	2.55162400	2.08327600
H	1.96443200	-0.58065100	1.10031800	H	2.52162400	1.71609500	1.98977400
C	2.43306200	0.71561100	-0.54994500	C	5.68397300	2.78918200	1.39955700
H	2.66486900	0.60400800	-1.61605200	H	6.73823000	2.54891100	-0.45838800
C	0.00465500	3.50912600	-0.73912000	H	4.38084800	2.88619100	3.10767000
H	0.12966300	4.52305600	-1.13858000	H	6.49900200	3.30771500	1.88999000
H	-0.09114000	3.57980700	0.35127500	K	-1.31682300	0.17473800	-0.89893200
C	1.22160900	2.69769800	-1.10207600				
H	2.10832000	3.26665500	-0.80947400	K⁺ / 2,3-DiPh-18c6_c2			
H	1.26107800	2.53327600	-2.18601100	C	-2.21429100	-4.53287700	1.44771500
C	-3.51225100	3.01758600	-1.73686200	C	-3.46494400	-4.15720800	0.96707300
H	-3.30650100	2.99729200	-2.81410000	C	-3.61868700	-2.94672000	0.29884600
H	-4.40913400	3.62652600	-1.56913200	C	-2.53307300	-2.08931900	0.11086500
C	-2.35283800	3.63958600	-1.00079100	C	-1.28304400	-2.47814300	0.59081800
H	-2.53689400	3.63285500	0.08068300	C	-1.12289300	-3.69167100	1.25274000
H	-2.24762300	4.68205100	-1.32469100	H	-0.14365400	-3.98115100	1.61547500
C	-4.93246200	-0.36928800	-1.38326400	H	-0.42440100	-1.83897100	0.43584200
H	-5.80283700	-0.84368100	-1.85283600	C	-2.76136800	-0.75556900	-0.58382600
H	-5.10160200	-0.33796800	-0.29960900	H	-3.62443900	-0.86730400	-1.25038200
C	-4.78501500	1.02686400	-1.93276300	C	-3.12571100	0.37547800	0.40970300
H	-5.72624600	1.57014900	-1.78293900	C	-3.76588900	1.57174700	-0.27952200
H	-4.57799100	0.98810400	-3.00929200	C	-5.14286200	1.55807200	-0.51225000
C	-3.83846600	-2.47128700	-1.24612200	C	-5.76535400	2.61125100	-1.17387400
H	-4.03431800	-2.51564300	-0.16755900	C	-5.01741200	3.70355800	-1.60335100
H	-4.66024900	-2.97897900	-1.76594500	C	-3.64735500	3.73342700	-1.36332600
C	-2.54402100	-3.17499200	-1.56690100	C	-3.02733900	2.67354900	-0.70778300
H	-2.32311600	-3.10017300	-2.63877100	H	-1.96397200	2.71710500	-0.51484200
H	-2.64373100	-4.23647200	-1.30984000	H	-3.05909100	4.58479700	-1.68474500
O	1.14201400	-1.31782800	-0.64817900	H	-5.50006900	4.52869100	-2.11291600
O	-1.49072700	-2.58451900	-0.80916300	H	-6.83486400	2.58310600	-1.34456800
O	-3.75198800	-1.11410600	-1.67073100	H	-5.73800700	0.71829700	-0.16851900
O	1.19668300	1.43624000	-0.42259000	H	-3.86365500	-0.05705000	1.09958500
O	-1.16302100	2.91180000	-1.29751100	O	-1.94456000	0.69529800	1.13848500
O	-3.72087100	1.69211900	-1.25756100	C	-2.16529200	1.42074400	2.35011800
C	3.51040300	-1.51414600	-0.05501800	C	-0.90583200	1.38800000	3.18182400
C	4.21938800	-1.86243400	1.09310600	H	-0.63055300	0.35190900	3.41418300
C	3.98634100	-1.93990500	-1.29742400	O	0.15717700	2.02192500	2.47234400
C	5.39090000	-2.60945600	1.00586400	C	1.36097000	2.08799400	3.23473600
H	3.85598200	-1.54566200	2.06429900	C	2.45339100	2.71153600	2.40203600
C	5.15342000	-2.68977500	-1.38779900	H	3.33764100	2.86126000	3.03333200
H	3.43567600	-1.69507500	-2.19820000	O	2.77032900	1.84632400	1.31318600
C	5.86128100	-3.02377900	-0.23557400	C	3.81553100	2.35254700	0.48575200
H	5.93208100	-2.87021100	1.90745400	C	4.10527700	1.36440400	-0.61705600

H	4.34622000	0.38231200	-0.19220800	H	-0.16355400	4.31313900	-1.23847900
O	2.96770300	1.26043200	-1.47056400	H	0.30012000	2.81775500	-2.06708200
C	3.16810500	0.36252600	-2.56051700	H	-2.23082500	4.14629300	-2.50508000
C	1.91787600	0.31374800	-3.40368200	H	-4.31654600	2.99508700	-2.94569500
H	1.63563800	1.32589400	-3.71954900	H	-4.13245100	3.24607800	-1.19516600
O	0.86112800	-0.27591900	-2.64925900	H	-5.78357000	1.08826600	-2.53722400
C	-0.36674100	-0.362085300	-3.37209600	H	-6.24015800	-0.95749800	-1.34692300
C	-1.40487900	-1.05516300	-2.54106700	H	-4.69726400	-1.13755300	-2.21001800
H	-2.32908600	-1.13177700	-3.12547200	H	-5.49493800	-2.72417200	0.00800900
H	-1.06600800	-2.06610000	-2.29402000	H	-3.49770700	-3.01630200	-1.51374400
O	-1.64380100	-0.30741900	-1.34643000	H	-3.48917200	-4.08746300	-0.10168200
H	-0.22571200	-0.89528400	-4.30805500	H	-1.08180100	-3.08683900	-1.67869100
H	-0.70756700	0.67178900	-3.62098300	H	0.23019900	-2.58699600	1.04175800
H	2.11737000	-0.28257400	-4.30220200	H	1.05842400	-3.21660800	-0.39667800
H	4.00359900	0.70595200	-3.18249600	H	3.55185400	1.78217500	-2.30948100
H	3.40869200	-0.63879100	-2.18291900	H	5.76179800	2.76710800	-1.82912300
H	4.97395500	1.71513000	-1.18735700	H	6.55697300	2.95362800	0.51193900
H	4.72707800	2.50048200	1.07734500	K	-1.94219600	0.27698200	0.04062200
H	3.52183800	3.32002800	0.05997300				
H	2.13200200	3.68972900	2.02340100				
H	1.20410200	2.69912000	4.13190300	K⁺ / 2,3-DiPh-18c6_c4			
H	1.65882300	1.08136600	3.55277900	C	-4.80054400	1.24563400	1.66332900
H	-1.09606000	1.91344700	4.12581300	H	-5.37787100	0.50377300	1.09808500
H	-2.97332200	0.95377100	2.92447100	H	-5.36354100	1.50344800	2.56878800
H	-2.45191500	2.45331000	2.12783500	C	-4.60567500	2.49144600	0.83663500
H	-4.59464500	-2.66855600	-0.08534600	H	-3.97368500	3.20160800	1.38112000
H	-4.31895600	-4.80989300	1.10298400	H	-5.58114200	2.96089400	0.66223200
H	-2.08932200	-5.47764900	1.96277900	C	-3.77597000	3.23674500	-1.28612400
K	0.52579900	0.98758600	-0.13735000	H	-3.72935800	2.81650200	-2.29220500
				H	-4.61436700	3.94108700	-1.24778700
				C	-2.48609200	3.97370800	-0.98683600
				H	-2.47782300	4.37064800	0.03556700
				H	-2.39480900	4.82238400	-1.67659000
				C	0.97916800	2.71036800	-1.25177700
				H	1.92886200	3.25092500	-1.20494900
				H	0.85563700	2.32081100	-2.26974500
				C	-0.12690500	3.68163000	-0.92800700
				H	-0.00872800	4.56356600	-1.56942100
				H	-0.05638000	4.00645800	0.11740300
				C	1.93478100	-0.47630100	0.40629600
				H	1.88560900	-0.14887900	1.45004100
				C	2.12823200	0.77240400	-0.47559100
				H	2.17582600	0.44109200	-1.51997000
				C	-0.30485800	-1.93723900	2.13441600
				H	0.33805000	-1.82616800	2.73936400
				H	-0.43824700	-2.87835300	2.68300100
				C	0.32199400	-2.24458800	0.79027700
				H	-0.39875900	-2.78204700	0.17155800
				H	1.18934300	-2.89219700	0.93627400
				C	-2.23981500	-0.97007000	3.13110100
				H	-2.32478800	-1.84903900	3.78133200
				H	-1.67312700	-0.19885200	3.66722500
				C	-3.62537000	-0.47381200	2.80128500
				H	-4.16105100	-0.26469100	3.73543100
				H	-4.18044000	-1.24426100	2.25184900
				O	-4.01127400	2.13337100	-0.41054800
				O	-3.52697400	0.70940000	2.01348500
				O	-1.56931300	-1.31572100	1.92213800
				O	-1.39431900	3.07531600	-1.16788400
				O	0.98167300	1.62372300	-0.31794900
				O	0.68333000	-1.07870200	0.03550800
				C	3.41588500	1.50208700	-0.12559900
				C	4.50320100	1.48576000	-0.99739600
				C	3.52509600	2.20561800	1.07625200
				C	5.68400400	2.14801900	-0.67303400
				H	4.43023700	0.94878400	-1.93639900
				C	4.70157500	2.87129400	1.40146900
				H	2.68145600	2.24520200	1.75539300
				C	5.78621900	2.84150900	0.52817000
				H	6.52079100	2.12483100	-1.36078000
				H	4.77274100	3.41438400	2.33645100
				H	6.70303500	3.36011200	0.78153900
				C	3.09742400	-1.44255800	0.24726800
				C	4.00658200	-1.63514700	1.28600300
				C	3.27149300	-2.15350300	-0.94267700
				C	5.07851300	-2.51128700	1.13926700
				H	3.88085800	-1.09296900	2.21645300

K⁺ / 2,3-DiPh-18c6_c3							
C	5.58742800	2.51963500	0.29911400				
C	5.14161500	2.41438400	-1.01385800				
C	3.89360400	1.85930900	-1.28334700				
C	3.08191200	1.39650500	-0.24912200				
C	3.53533400	1.51138600	1.06739800				
C	4.77887100	2.06941200	1.34023000				
H	5.11811300	2.15365100	2.36581600				
H	2.90789700	1.17560500	1.88476400				
C	1.72576400	0.78019300	-0.54965800				
H	1.50391700	0.91075600	-1.61453700				
C	1.72074400	-0.73105600	-0.24907000				
C	2.78571000	-1.46319900	-1.04995600				
C	3.91795800	-1.98034100	-0.42278300				
C	4.89669200	-2.64380100	-1.15765600				
C	4.74785800	-2.80294800	-2.53127600				
C	3.61492300	-2.29832600	-3.16517600				
C	2.64100600	-1.63322700	-2.42890400				
H	1.75625300	-1.25537700	-2.92780300				
H	3.49025000	-2.42401200	-4.23421500				
H	5.50692100	-3.32097400	-3.10500800				
H	5.77175500	-3.03904700	-0.65588700				
H	4.03912100	-1.86192100	0.64818000				
H	1.92340800	-0.85992900	0.82073900				
O	0.40880800	-1.24382100	-0.53108700				
C	0.23419500	-2.58374400	-0.05507100				
C	-1.05074800	-3.16627600	-0.58507900				
H	-1.08425300	-4.22960500	-0.31772100				
O	-2.16701200	-2.48830900	-0.01413200				
C	-3.41730400	-3.03968500	-0.42019600				
C	-4.53306200	-2.25116800	0.23532400				
H	-4.39662500	-2.25978400	1.31809000				
O	-4.55121600	-0.87496900	-0.14498000				
C	-5.19973800	-0.61401700	-1.38920600				
C	-5.18271800	0.87187800	-1.64537700				
H	-5.62377900	1.40546300	-0.79452600				
O	-3.83742400	1.29979600	-1.84496500				
C	-3.73492400	2.70433400	-2.06221600				
C	-2.28980000	3.07329800	-2.28624700				
H	-1.88164500	2.52412100	-3.14372600				
O	-1.54144200	2.76793900	-1.11256100				
C	-0.19094200	3.21799400	-1.17189700				
C	0.52785300	2.79372500	0.09208300				
H	-0.04958300	3.11270900	0.96158300				
H	1.50074300	3.28887500	0.13305400				
O	0.67675200	1.37394700	0.23480700				

C	4.33810600	-3.03260900	-1.09069100
H	2.56221500	-2.02966200	-1.75271000
C	5.24699100	-3.21149100	-0.05036200
H	5.77777600	-2.64850500	1.95529500
H	4.46086100	-3.57932400	-2.01809900
H	6.07857200	-3.89611100	-0.16625100
K	-1.66389300	0.51364600	-0.15597100

K⁺ / 2,3-DiPh-18c6_c5

C	-2.01394700	1.12108800	-3.66806400
H	-1.99895600	1.94913600	-4.38709800
H	-1.49501700	0.26550400	-4.11711300
C	-3.44809500	0.76407900	-3.36640000
H	-3.96043300	0.52942300	-4.30747500
H	-3.96076000	1.61443200	-2.89955300
C	-4.80166900	-0.79269700	-2.18878800
H	-5.35592600	0.01590500	-1.69614200
H	-5.33421900	-1.06181900	-3.10926800
C	-4.73589900	-2.00320200	-1.29152400
H	-4.14443300	-2.79498000	-1.76750300
H	-5.75248600	-2.38235400	-1.13078000
C	-3.39137700	-2.23877700	2.13992200
H	-3.38193300	-3.05075400	2.87580800
H	-3.96815300	-1.40968300	2.55284500
C	-4.04863700	-2.72721600	0.86441200
H	-5.04784300	-3.11071800	1.10748800
H	-3.47916000	-3.54587500	0.40785200
C	0.29714200	-2.07421600	1.79107200
H	1.05940600	-2.85675800	1.85519500
H	0.41665400	-1.40336100	2.65025100
C	-1.05908400	-2.73164300	1.83018500
H	-1.09715600	-3.39753300	2.70061700
H	-1.20620200	-3.33659600	0.92869600
C	1.76707700	0.24445400	-0.70622500
H	1.52774200	-0.28516100	-1.63507700
C	1.77517600	-0.78610100	0.44053100
H	2.02696100	-0.25288700	1.36454000
C	0.60186600	2.29283400	-1.32801800
H	-0.03255400	3.01767700	-0.81498100
H	1.57347600	2.76038000	-1.50414400
C	-0.01774500	1.93638200	-2.66395900
H	0.55256600	1.15317100	-3.17778700
H	-0.00101800	2.83019300	-3.30068000
O	-3.47790100	-0.36222100	-2.49418800
O	-1.36076400	1.50632000	-2.46116500
O	0.72653100	1.19412600	-0.41474600
O	-4.14544300	-1.63695800	-0.04725400
O	-2.07065100	-1.73110500	1.94514600
O	0.45355100	-1.33050200	0.57684500
C	2.80139200	-1.88147400	0.19954800
C	3.96119900	-1.95436700	0.96899600
C	2.59138600	-2.83767000	-0.79689400
C	4.90292900	-2.95424900	0.74179600
H	4.13368600	-1.22263500	1.75016200
C	3.52819800	-3.83948700	-1.02425500
H	1.68457000	-2.80625200	-1.38962100
C	4.68901500	-3.89845200	-0.25669600
H	5.80015700	-2.99675800	1.34754000
H	3.35288900	-4.57539400	-1.80010600
H	5.41926200	-4.67888400	-0.43386200
C	3.12821700	0.90319800	-0.85240600
C	3.91598900	0.65527200	-1.97501300
C	3.61151400	1.76662500	0.13412300
C	5.16920800	1.24669800	-2.10909400
H	3.55019100	-0.00960400	-2.74942600
C	4.85994900	2.36299700	0.00076700
H	3.00355000	1.98518800	1.00431000
C	5.64400100	2.10190500	-1.12065800
H	5.77103100	1.04175600	-2.98627400
H	5.22212800	3.03243300	0.77191500
H	6.61742000	2.56608000	-1.22363700
K	-1.87426900	0.07930700	-0.14610900

K⁺ / 2,3-DiPh-18c6_c6

C	5.58484800	-3.32932200	-0.29609200
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C	5.48220200	-2.64273400	0.90897300
C	4.40284000	-1.79375000	1.13772100
C	3.42030000	-1.61491900	0.16576300
C	3.52853400	-2.31193400	-1.04003500
C	4.60263300	-3.16405400	-1.26977400
H	4.67399600	-3.69990700	-2.20885000
H	2.76291200	-2.19873100	-1.79879700
C	2.24531000	-0.68137200	0.41368600
H	2.26723500	-0.35084800	1.45938500
C	2.33544500	0.56360800	-0.48835000
C	3.63391300	1.31900800	-0.24962700
C	4.63271200	1.33890800	-1.22135200
C	5.82422900	2.02454500	-1.00187500
C	6.02515800	2.70618300	0.19362900
C	5.02839200	-2.70051900	1.16648800
C	3.84140400	2.01110500	0.94591500
H	3.06635800	2.02293700	1.70338400
H	5.17632800	3.23421900	2.09784000
H	6.95041000	-1.29152400	0.36571800
H	6.59193300	2.02879300	-1.76627100
H	4.48137500	0.81164600	-2.15651800
H	2.30488000	0.22827200	-1.53202700
O	1.18838600	1.39365400	-0.24225100
C	1.11400800	2.50331000	-1.14721300
C	-0.00986400	3.42716800	-0.75350800
H	0.07159900	4.34560800	-1.34678300
O	-1.26356800	2.79828000	-1.01824700
C	-2.40265800	3.61680100	-0.74436200
C	-2.83664400	3.56519300	0.70612700
H	-2.02937400	3.88471500	1.37691400
O	-3.22433300	2.22920000	1.01230600
C	-3.66477000	2.06644900	2.35747500
C	-4.11127500	0.64047900	2.56083300
H	-4.90151800	0.38660600	1.84365500
O	-2.99756500	-0.23090300	2.38527800
C	-3.33912200	-1.60371900	2.55729400
C	-2.10862100	-2.44955200	2.34806500
H	-1.31405100	-2.12216600	3.02757000
O	-1.69160600	-2.33509100	0.98726000
C	-0.54588200	-3.12322200	0.65877200
C	0.77338900	-2.46858900	1.01079900
H	1.56975600	-3.20386300	0.86275400
H	0.79693400	-2.15832000	2.06255800
O	0.98669500	-1.32973800	0.16768700
H	-0.59295200	-3.29227300	-0.41855100
H	-0.60476300	-4.09642000	1.15851100
H	-2.34872400	-3.49464400	2.57606300
H	-3.72136600	-1.77122900	3.57122900
H	-4.12021200	-1.88864500	1.84186800
H	-4.51910900	0.53465100	3.57363400
H	-4.50919700	2.73538800	2.56379500
H	-2.85238400	-0.31489600	3.05178400
H	-3.68297000	4.24903800	0.84923000
H	-2.20346700	4.65491400	-1.03119200
H	-3.20606600	3.23541200	-1.37676600
H	0.07964500	3.69366400	0.30551300
H	0.96130300	2.13713000	-2.16978800
H	2.04748300	3.07210400	-1.12242600
H	4.32847900	-1.26263100	2.08002700
H	6.23941900	-2.76933500	1.67338600
H	6.42252000	-3.99247900	-0.47552700
K	-1.40473500	0.25261000	0.04828600

K⁺ / 2,3-DiPh-18c6_c7

C	5.89879200	2.75929600	1.02541700
C	5.74899400	2.37391300	-0.30243300
C	4.59220400	1.71575600	-0.71080900
C	3.57797300	1.42835600	0.20068600
C	3.73452100	1.82286900	1.53151200
C	4.88625600	2.48458700	1.94163600
H	4.99449500	2.78666700	2.97657400
H	2.94666700	1.62389900	2.24871800
C	2.31713100	0.70467600	-0.24589000
H	2.32696300	0.61458700	-1.33906000
C	2.25432300	-0.71261200	0.35417400

C	3.47304600	-1.53031500	-0.04513500	H	-4.85943700	-3.15316600	0.71985700
C	4.44029500	-1.87238700	0.89816100	H	-2.71835800	-1.93861000	0.84500200
C	5.55967000	-2.61429800	0.53119500	C	-1.66891600	-0.16635500	-0.94974700
C	5.71846300	-3.02939200	-0.78664700	H	-1.48469000	0.33554900	-1.90772200
C	4.75198300	-2.70080100	-1.73424800	C	-1.72388800	0.90668400	0.15416600
C	3.63749800	-1.95603900	-1.36536800	C	-2.84804300	1.89737700	-0.10782100
H	2.88475900	-1.71494700	-2.10689800	C	-3.97821500	1.92297900	0.70726600
H	4.86724000	-3.02543200	-2.76162100	C	-5.01095000	2.82367600	0.46184400
H	6.58733800	-3.60905300	-1.07427100	C	-4.91903100	3.71557200	-0.60129000
H	6.30379800	-2.87054400	1.27571200	C	-3.78882100	3.70403400	-1.41527700
H	4.32163500	-1.55418600	1.92781100	C	-2.76101700	2.80066200	-1.16975400
H	2.22986100	-0.61688800	1.44636100	H	-1.88001400	2.80665400	-1.80093300
O	1.03471500	-1.33884500	-0.07701400	H	-3.70887000	4.39963800	-2.24228500
C	0.81080800	-2.60243200	0.56246700	H	-5.72059900	4.41861200	-0.79339600
C	-0.38277900	-3.29312100	-0.04661200	H	-5.88413400	2.82965600	-1.10312800
H	-0.41981600	-4.32200700	0.33050600	H	-4.05613400	1.23089500	1.53817000
O	-1.57802000	-2.60672200	0.32466000	H	-1.90872000	0.40110300	1.10956700
C	-2.77936300	-3.21777200	-0.15096500	O	-0.44687800	1.56226900	0.22557400
C	-3.14209900	-2.79773700	-1.56074400	C	-0.36520400	-2.80066800	1.32381400
H	-2.34035000	-3.04112700	-2.26916800	C	0.93457600	3.24222000	1.27662100
O	-3.38498600	-1.39405400	-1.56260100	H	0.88784500	4.05437900	2.01185500
C	-3.73211500	-0.88405800	-2.84675000	O	2.01757200	2.36980800	1.59842000
C	-4.03423900	0.58872400	-2.72739900	C	3.29235900	3.01310800	1.66005700
H	-4.83025500	0.75110300	-1.99045500	C	3.95223400	3.16258900	0.30407900
O	-2.85431000	1.28188000	-2.32893800	H	3.32703400	3.74434300	-0.38465100
C	-3.06564300	2.68181500	-2.16457100	O	4.18286500	1.86197600	-0.22851300
C	-1.77198000	3.33287300	-1.74459600	C	4.78598600	1.88033800	-1.51893100
H	-0.98813900	3.10911100	-2.47684800	C	5.05751500	0.46305400	-1.95703400
O	-1.40906200	2.85293200	-0.44951300	H	5.68588600	-0.04625200	-1.21603400
C	-0.20335100	3.41978100	0.06764100	O	3.82154800	-0.23119900	-2.10488900
C	1.05577800	2.73123100	-0.41593500	C	3.99745900	-1.58810800	-2.50405300
H	1.91617800	3.32570500	-0.09526400	C	2.64775000	-2.64979800	-2.62484900
H	1.08075600	2.67087500	-1.51080900	H	2.01877900	-1.68602700	-3.32262600
O	1.12809600	1.41303100	0.14195500	O	2.04321500	-2.31213800	-1.33281200
H	-0.27037100	3.33705200	1.15390400	C	0.76505300	-2.95073700	-1.31327300
H	-0.14880300	4.48317000	-0.18961100	C	-0.38337900	-2.03974300	-1.69295300
H	-1.91268100	4.41963300	-1.71145900	H	-1.28556500	-2.65043000	-1.79272900
H	-3.39863600	3.12839700	-3.10951800	H	-0.20222100	-1.55107200	-2.65801900
H	-3.84015000	2.85764900	-1.40800400	O	-0.56633400	-1.04599600	-0.67684600
H	-4.38278900	0.96194600	-3.69828900	H	0.62261600	-3.31203900	-0.29314300
H	-4.62157100	-1.39782500	-3.23133600	H	0.76814700	-3.81743600	-1.98326900
H	-2.90811900	-1.04943200	-3.55204800	H	2.78092500	-3.26299700	-3.02199000
H	-4.04336400	-3.34014900	-1.87397400	H	4.50474500	-1.63412100	-3.47559800
H	-2.69555300	-4.30876300	-0.10285800	H	4.61390600	-2.11835900	-1.76783900
H	-3.56836500	-2.90460900	0.53481300	H	5.59781100	0.48166700	-2.91148400
H	-0.27445100	-3.33063000	-1.13630300	H	5.73530800	2.42874100	-1.48638000
H	0.65347800	-2.45038200	1.63721700	H	4.12377300	2.38187100	-2.23570300
H	1.68215400	-3.24987000	0.43117900	H	4.90262000	3.69746200	0.42781000
H	4.48108700	1.42028300	-1.74810700	H	3.19894900	3.99649200	2.13341900
H	6.52959800	2.58813000	-1.02250200	H	3.91453600	2.38396400	2.29868500
H	6.79668900	3.27426700	1.34519400	H	1.06997800	3.68600300	0.28416500
K	-1.39997400	0.10852400	-0.17141500	H	-0.44907100	1.93360300	2.27081700
				H	-1.18459700	3.20275300	1.27171100
				H	-3.53848000	-0.09980400	-2.93861900
				H	-5.67893100	-1.31980300	-3.06905900
				H	-6.35098900	-2.84996100	-1.23737000
				K	1.97975500	0.06678600	0.07409200
K⁺ / 2,3-DiPh-18c6_c8							
C	-5.41228900	-2.31208700	-1.18081800				
C	-5.03536400	-1.45340400	-2.20782500				
C	-3.82672600	-0.76648400	-2.13370300				
C	-2.98630800	-0.92245900	-1.03315400				
C	-3.37017800	-1.79056900	-0.00819100				
C	-4.57432200	-2.48151700	-0.08119500				

3.3 Cartesian coordinates of CH₃NH₃⁺ / 2,3-DiPh18c6

CH₃NH₃⁺ / 2,3-DiPh-18c6_c1				C	2.41526400	0.74471700	-0.42404300
C	-0.23989700	-3.26480300	-0.80426700	H	2.57289900	0.64056900	-1.50447100
H	-0.29101900	-4.32240800	-0.51501900	C	-0.05676600	3.50932300	-0.57520800
H	0.06396500	-3.21287700	-1.85684600	H	0.05747500	4.52569300	-0.96851700
C	0.79056000	-2.58362100	0.06143000	H	-0.19798800	3.57411100	0.51011700
H	1.69400400	-3.19722400	0.05852100	C	1.19279200	2.73044500	-0.90132400
H	0.43392700	-2.50421100	1.09511100	C	2.05489900	3.33522300	-0.60375300
C	2.24176900	-0.66884000	0.16436100	H	1.25392000	2.55566900	-1.98249300
H	2.05369000	-0.57485100	1.24065100	C	-3.49070900	3.00922500	-1.85469000

H	-3.16369400	2.90912400	-2.89679300
H	-4.37880300	3.65364800	-1.83326300
C	-2.39822400	3.65194700	-1.03638500
H	-2.68463500	3.69926800	0.02102100
H	-2.23607800	4.67325500	-1.39827500
C	-4.90249200	-0.38363500	-1.52003900
H	-5.69658100	-0.89767000	-2.07364100
H	-5.20509000	-0.31428900	-0.46830600
C	-4.71492100	0.99302700	-2.10797600
H	-5.68713700	1.50179300	-2.13337500
H	-4.34309400	0.91206100	-3.13681800
C	-3.81874200	-2.48713700	-1.23133800
H	-4.09485900	-2.54196400	-0.17146200
H	-4.60743300	-2.97018300	-1.81951600
C	-2.51485800	-3.20619200	-1.47310600
H	-2.21867900	-3.10573700	-2.52468700
H	-2.65210000	-4.27305900	-1.25511300
O	1.08768100	-1.27429700	-0.45285500
O	-1.51222000	-2.65323300	-0.62889600
O	-3.68386200	-1.12205800	-1.63171500
O	1.20428000	1.48002800	-0.20659200
O	-1.19435200	2.89280500	-1.18440900
O	-3.79247900	1.72896600	-1.31332200
C	-1.83838900	0.26853600	1.19991200
H	-1.92599600	-0.74548000	1.58116800
N	-1.46570100	0.21492500	-0.23750000
H	-0.55191300	-0.24617300	-0.36245100
H	-2.17728900	-0.30317400	-0.77447000
H	-1.39771200	1.16925100	-0.62958100
C	3.49411400	-1.50335400	-0.05021600
C	4.29721100	-1.86694800	1.02914200
C	3.85820500	-1.91918600	-1.33326400
C	5.45126800	-2.62063100	0.83396600
H	4.02294300	-1.55566300	2.03072100
C	5.00706400	-2.67654500	-1.53076800
H	3.23399700	-1.66159600	-2.18094100
C	5.80907300	-3.02666400	-0.44709700
H	6.06679400	-2.89293100	1.68288400
H	5.27739300	-2.99416300	-2.53082400
H	6.70501700	-3.61583800	-0.60135300
C	3.61505300	1.45371800	0.18622800
C	4.76212600	1.69018200	-0.56910000
C	3.57930000	1.88814200	1.51333600
C	5.86106000	2.33590000	-0.00931400
H	4.80025900	1.36450400	-1.60250700
C	4.67374400	2.53647000	2.07450200
H	2.68665200	1.73086100	2.10753300
C	5.81971200	2.75932500	1.31480900
H	6.74611500	2.51096100	-0.60912500
H	4.63306300	2.86895800	3.10500700
H	6.67263000	3.26435500	1.75204600
H	-1.06713400	0.80615700	1.74598000
H	-2.78985600	0.78489500	1.29683700

CH₃NH₃⁺ / 2,3-DiPh-18c6_c2

C	-0.24753100	-3.22969400	-1.09370600
H	-0.32552300	-4.30054700	-0.87274300
H	-0.01318500	-3.11198100	-2.15780200
C	0.85522500	-2.64323800	-0.24912000
H	1.72667800	-3.30007300	-0.32394500
H	0.54717000	-2.60916400	0.80396800
C	2.25130600	-0.71796900	0.01750300
H	1.95893100	-0.63187900	1.07191200
C	2.44709800	0.70132800	-0.54662800
H	2.69371100	0.60637100	-1.61005800
C	0.01842700	3.49569300	-0.83057800
H	0.16556100	4.49337800	-1.26390300
H	-0.07301500	3.60873200	0.25735400
C	1.22168600	2.65318900	-1.16877100
H	2.11894400	3.22208200	-0.91115600
H	1.24331900	2.43571600	-2.24265200
C	-3.49723000	3.00887700	-1.81420000
H	-3.28539400	2.90268400	-2.88438100
H	-4.38602300	3.64012800	-1.69675800
C	-2.33064000	3.66481500	-1.12029000

H	-2.51731500	3.73670300	-0.04086800
H	-2.21520700	4.68247100	-1.51422000
C	-4.95635700	-0.34716200	-1.29227200
H	-5.85181000	-0.81698300	-1.71862200
H	-5.08849200	-0.28770500	-0.20384900
C	-4.80921600	1.03289300	-1.88189300
H	-5.74426700	1.58736900	-1.73800700
H	-4.61151900	0.95917400	-2.95748100
C	-3.86532000	-2.45350800	-1.15247500
H	-4.01077200	-2.48140400	-0.06461900
H	-4.70842800	-2.97560700	-1.62264700
C	-2.58679900	-3.16001300	-1.52733000
H	-2.40305800	-3.06173100	-2.60316900
H	-2.67931300	-4.22494000	-1.28512000
O	1.18082800	-1.38086600	-0.71201600
O	-1.49469800	-2.59704800	-0.79588900
O	-3.79840600	-1.10904700	-1.60763200
O	1.20397600	1.42011500	-0.43174300
O	-1.15624500	2.90155500	-1.36808700
O	-3.73522800	1.72294300	-1.24065700
C	-1.70316600	0.27008400	1.30472600
H	-0.94697600	-0.30288200	1.83552300
N	-1.43980100	0.19406400	-0.15678800
H	-0.50253300	0.56657000	-0.37820000
H	-1.48128900	-0.78582600	-0.48542700
H	-2.14296800	0.73741400	-0.67966700
C	3.53829000	-1.52397700	-0.06884000
C	4.22593900	-1.88779500	1.08734300
C	4.04572700	-1.91927400	-1.30889000
C	5.40767200	-2.61982300	1.01092900
H	3.83806800	-1.59495700	2.05666500
C	5.22308600	-2.65413800	-1.38852000
H	3.51146500	-1.66256300	-2.21626700
C	5.90969800	-3.00340600	-0.22797000
H	5.93221100	-2.89277800	1.91874700
H	5.60588500	-2.95504600	-2.35651400
H	6.82791900	-3.57495600	-0.29034200
C	3.56905500	1.43911700	0.16557500
C	4.77207400	1.70439300	-0.48630900
C	3.40747600	1.86805800	1.48509200
C	5.80254900	2.37318100	0.16861600
H	4.90781500	1.38353400	-1.51296400
C	4.43315400	2.53949500	2.14074000
H	2.47074100	1.68734300	1.99909100
C	5.63570000	2.79110800	1.48454400
H	6.73233400	2.57065600	-0.35119100
H	4.29481400	2.86729700	3.16424500
H	6.43518800	3.31397300	1.99553800
H	-1.66532600	1.30904200	1.62184000
H	-2.68745400	-0.14216200	1.51148400

CH₃NH₃⁺ / 2,3-DiPh-18c6_c3

C	-2.03656800	1.12136400	-3.67034900
H	-2.02842600	1.89726400	-4.44658800
H	-1.53074700	0.23263400	-4.06772900
C	-3.46779200	0.79298300	-3.32633700
H	-3.99713600	0.50968400	-4.24343500
H	-3.96877900	1.66813200	-2.89507200
C	-4.82015000	-0.75011500	-2.12247000
H	-5.39076500	0.03630100	-1.61421200
H	-5.32931000	-0.99216700	-3.06250000
C	-4.75970800	-1.99253500	-1.26991300
H	-4.12814500	-2.74789400	-1.75377400
H	-5.77259700	-2.40361800	-1.17177000
C	-3.40447000	-2.34159300	2.13999500
H	-3.34821100	-3.18313000	2.83833200
H	-3.99758400	-1.55097100	2.60149200
C	-4.06797500	-2.79286000	0.85473400
H	-5.04171500	-3.23753200	1.09977400
H	-3.47139500	-3.55961900	0.34533400
C	0.28453000	-2.06272900	1.75632000
H	1.05604300	-2.84627300	1.82403800
H	0.37835000	-1.40666900	2.63054000
C	-1.05886700	-2.74739900	1.76210700
H	-1.08166500	-3.46117100	2.59307000
H	-1.20084200	-3.29831200	0.82705200

C	1.78504100	0.25281900	-0.72191600
H	1.55100000	-0.28511600	-1.64625700
C	1.77592100	-0.76423000	0.43605900
H	2.02216900	-0.22414000	1.35818800
C	0.63943500	2.29259400	-1.41021200
H	0.03148300	3.05102500	-0.91523900
H	1.62333900	2.72302200	-1.60626400
C	-0.00433600	1.90804000	-2.72631500
H	0.51383600	1.06272900	-3.19544000
H	0.07351200	2.76395000	-3.41001600
O	-3.49464000	-0.29224200	-2.39745500
O	-1.36933400	1.58058700	-2.50210300
O	0.74671900	1.21901400	-0.45945000
O	-4.23300100	-1.66288100	0.00887000
O	-2.09998100	-1.78210100	1.94766200
O	0.45318200	-1.30129100	0.55774500
C	-2.70225600	1.59023900	0.66750900
H	-2.63749700	2.40721400	-0.04638700
N	-2.01951900	0.39807900	0.10028400
H	-2.46017300	0.12230800	-0.79042700
H	-1.02030500	0.58477200	-0.08296000
H	-2.07718200	-0.40862700	0.74572300
C	2.80418500	-1.86254900	0.21125200
C	3.95700600	-1.93317500	0.99120100
C	2.60098900	-2.82403800	-0.78153300
C	4.89886300	-2.93605700	0.77783400
H	4.12414200	-1.19723900	1.76958100
C	3.53801200	-3.82864900	-0.99526200
H	1.69898600	-2.79408200	-1.38158500
C	4.69203100	-3.88537900	-0.21732200
H	5.79072200	-2.97684300	1.39159900
H	3.36812700	-4.56847400	-1.76860900
H	5.42248100	-4.66796900	-0.38390700
C	3.14898500	0.90686400	-0.85873000
C	3.94927300	0.64546600	-1.96934100
C	3.62327300	1.77796300	0.12543900
C	5.20618600	1.23113200	-2.09360300
H	3.59016300	-0.02509600	-2.74194500
C	4.87539200	2.36858900	0.00170200
H	3.00555500	2.00694400	0.98601800
C	5.67207900	2.09391300	-1.10751500
H	5.81782100	1.01580200	-2.96144400
H	5.23067500	3.04396300	0.77087200
H	6.64845300	2.55348400	-1.20289900
H	-3.74444400	1.34365900	0.85522000
H	-2.21643000	1.87093000	1.59900200

CH₃NH₃⁺ / 2,3-DiPh-18c6_c4

C	-4.84568900	1.21003700	1.58295600
H	-5.45022400	0.52296100	0.97911900
H	-5.38691500	1.42116000	2.51263700
C	-4.62642600	2.50664900	0.84433400
H	-3.94672700	3.14390900	1.42077600
H	-5.58732000	3.02711800	0.74718800
C	-3.80151800	3.38179000	-1.22800900
H	-3.78607000	3.04642300	-2.26655100
H	-4.59672200	4.12916700	-1.12299900
C	-2.47289400	4.02499800	-0.88425400
H	-2.43253200	4.32504300	0.16901200
H	-2.34846000	4.92652700	-1.49637800
C	0.96505300	2.67878900	-1.24711900
H	1.91608900	3.21982500	-1.24137300
H	0.80600400	2.28026300	-2.25706200
C	-0.12312300	3.66050500	-0.89368400
H	0.01344100	4.56309200	-1.50040900
H	-0.05047900	3.94076300	0.16344700
C	1.96917600	-0.47187200	0.43754900
H	1.92815600	-0.12337400	1.47492400
C	2.14393800	0.75957800	-0.47183100
H	2.17163500	0.40860800	-1.51102500
C	-0.31388600	-1.90810600	2.19753400
H	0.25891200	-1.16685600	2.76905800
H	-0.37540100	-2.82208300	2.80319700
C	0.37150400	-2.24341500	0.88991500
H	-0.29996500	-2.84005300	0.27067600
H	1.26314400	-2.83985700	1.09083600

C	-2.33147700	-1.03208700	3.09516600
H	-2.43560600	-1.88549500	3.77739500
H	-1.79139700	-0.23503400	3.62136200
C	-3.70648900	-0.55509200	2.69990100
H	-4.27673600	-0.32149400	3.60644300
H	-4.23980500	-1.33882300	2.14871700
O	-4.09411500	2.22632400	-0.44696700
O	-3.58368000	0.61394400	1.88889700
O	-1.61982300	-1.41490100	1.92554700
O	-1.41366600	3.10594900	-1.16297400
O	1.00107200	1.60748200	-0.30059400
O	0.71425400	-1.09312500	0.09647300
C	-2.43101800	-0.42891800	-1.56573600
H	-3.39770900	0.01824000	-1.77926700
N	-1.78378800	1.36573300	-0.46928900
H	-1.66742000	1.33283000	-0.72677600
H	-2.35989700	0.31655600	0.38544100
H	-0.85270000	-0.04472800	-0.23935000
C	3.43902000	1.49514200	-0.16169800
C	4.50859100	1.46291000	-1.05466500
C	3.57184500	2.22070600	1.02458700
C	5.69552100	2.13083900	-0.76614800
H	4.41706100	0.90883000	-1.98203500
C	4.75463200	2.89160700	1.31421700
H	2.74160100	2.27276700	1.71916000
C	5.82168800	2.84568500	0.42017500
H	6.51837400	2.09516400	-1.46998400
H	4.84444200	3.45133600	2.23771100
H	6.74343300	3.36833700	0.64586700
C	3.13120700	-1.43837500	0.28097300
C	4.05700100	-1.60547400	1.30938400
C	3.28967200	-2.17365800	-0.89630000
C	5.12992200	-2.48069200	1.16450000
H	3.94308500	-1.04453800	2.23013500
C	4.35728100	-3.05182200	-1.04222800
H	2.56747900	-2.06989800	-1.69762300
C	5.28274600	-3.20534100	-0.01251700
H	5.84211600	-2.59817700	1.97235800
H	4.46788400	-3.61760900	-1.95966400
H	6.11499300	-3.88941900	-0.12675800
H	-1.79818300	-0.39051400	-2.44912100
H	-2.55954900	-1.46143700	-1.25051500

CH₃NH₃⁺ / 2,3-DiPh-18c6_c5

C	5.62261900	2.49240400	0.41611300
C	5.27190200	2.34053300	-0.92098700
C	4.03532400	1.79796300	-1.25966600
C	3.14050400	1.39420200	-0.27025000
C	3.49871700	1.55523200	1.07047100
C	4.73070800	2.10096900	1.41187500
H	4.99565300	2.22179100	2.45553700
H	2.80566500	1.26598800	1.85176100
C	1.79786200	0.78804300	-0.64334300
H	1.63888600	0.89997500	-1.72116300
C	1.75371100	-0.71574200	-0.31012500
C	2.85575500	-1.47409600	-1.03426400
C	3.94736900	-1.98322000	-0.33311700
C	4.96051600	-2.66982100	-0.99647300
C	4.88707500	-2.86051000	-2.37220400
C	3.79496800	-2.36392000	-3.07981900
C	2.78653700	-1.67547500	-2.41480100
H	1.93352200	-1.30414300	-2.97066900
H	3.72905400	-2.51401100	-4.15093300
H	5.67296700	-3.39665700	-2.89050200
H	5.80347800	-3.05827100	-0.43763500
H	4.01000600	-1.83927300	0.73966800
H	1.89779700	-0.82489100	0.77191900
O	0.45396600	-1.21148900	-0.65496700
C	0.23972400	-2.55248300	-0.20653700
C	-1.05327200	-3.09397200	-0.76155600
H	-1.07965100	-4.17599500	-0.58876400
O	-2.17492000	-2.48904800	-0.11246900
C	-3.42319100	-3.01177600	-0.57398900
C	-4.55550700	-2.35925700	0.19375200
H	-4.39339000	-2.49427300	1.26470100
O	-4.64766800	-0.95252200	-0.01533000

C	-5.32976700	-0.57827400	-1.20858600
C	-5.29343400	0.92270000	-1.35307700
H	-5.67032900	1.40440100	-0.44305100
O	-3.95425700	1.34746900	-1.61413500
C	-3.86477100	2.74199500	-1.90974200
C	-2.44392500	3.08084300	-2.28519900
H	-2.12119000	2.46953000	-3.13722500
O	-1.59989500	2.84423000	-1.16611600
C	-0.23719100	3.16987300	-1.41012600
C	0.57939000	2.83601700	-0.17981300
H	0.08715000	3.24381400	0.70442000
H	1.56405400	3.29986300	-0.26106700
O	0.71596600	1.42461300	0.06435700
H	-0.13801000	4.24421700	-1.61495900
H	0.12980200	2.62676400	-2.29012900
H	-2.39916200	4.13632100	-2.58260900
H	-4.52376500	2.98680100	-2.75083700
H	-4.18079600	3.33006500	-1.03983300
H	-5.94028000	1.21135500	-2.18970500
H	-6.37608700	-0.90456100	-1.15878900
H	-4.86723900	-1.04072300	-2.08735200
H	-5.49792500	-2.85172600	-0.07291000
H	-3.51769700	-2.84144500	-1.65261700
H	-3.45550000	-4.09400100	-0.39912400
H	-1.10537200	-2.91518100	-1.84163300
H	0.22569200	-2.58338500	0.89036400
H	1.04984500	-3.20063600	-0.55395300
H	3.76780900	1.68382100	-2.30412700
H	5.95749300	2.64747600	-1.70162200
H	6.58292900	2.91728400	0.68246900
C	-2.38389300	0.69647300	1.76877300
H	-2.30549300	1.77361700	1.89356800
H	-3.40909500	0.37602400	1.93161500
N	-1.98787900	0.33672500	0.38170700
H	-2.59939500	0.79968900	-0.30730700
H	-1.01267900	0.61396900	0.18476300
H	-2.07177800	-0.68066200	0.21955300
H	-1.72021300	0.19638200	2.46997900

CH₃NH₃⁺ / 2,3-DiPh-18c6_c6

C	5.33147900	2.78324700	-0.50761600
C	4.99529200	2.22894700	-1.73803100
C	3.79813400	1.53397700	-1.88546100
C	2.92859100	1.37806300	-0.80754700
C	3.27097100	1.94311000	0.42313100
C	4.46385000	2.64132800	0.57268300
H	4.71726400	3.07540300	1.53262100
H	2.59664200	1.84790100	1.26606300
C	1.62604500	0.61002700	-0.96743900
H	1.46379100	0.39348700	-2.02974400
C	1.67144000	-0.73169800	-0.21291100
C	2.84369800	-1.57988000	-0.68417900
C	3.93493400	-1.81134300	0.15104300
C	5.01077700	-2.58130600	-0.28238400
C	5.00117500	-3.13577500	-1.55779300
C	3.90993400	-2.91866800	-2.39571700
C	2.83916300	-2.14562200	-1.96136900
H	1.98821600	-1.99275500	-2.61496400
H	3.89355700	-3.35255500	-3.38849100
H	5.83607300	-3.73737400	-1.89648100
H	5.85299900	-2.75006300	0.37788900
H	3.94876600	-1.38368900	1.14728100
H	1.79330100	-0.52030700	0.85700300
O	0.41680400	-1.39668200	-0.41140600
C	0.31627900	-2.62419600	0.31616600
C	-0.99400400	-3.30658600	0.01378200
H	-0.94757600	-4.33389100	0.39120000
O	-2.06430700	-2.61877200	0.67006400
C	-3.34241100	-3.25704200	0.55672500
C	-4.08893900	-2.87690500	-0.70423600
H	-3.49502300	-3.10092800	-1.59921700
O	-4.38357100	-1.48737200	-0.64833200
C	-5.02573300	-1.00183300	-1.81978800
C	-5.26367000	0.48065900	-1.67935900
H	-5.83453400	0.69235300	-0.76743400
O	-4.00927300	1.16422500	-1.64121300

C	-4.15245500	2.58604600	-1.65630300
C	-2.79003300	3.22287200	-1.76722000
H	-2.27009800	2.82537500	-2.64595300
O	-2.05518200	2.95746600	-0.57640100
C	-0.72316300	3.46563200	-0.58499000
C	0.28450900	2.56330100	-1.26716600
H	1.22063200	3.11962400	-1.36624900
H	-0.04677000	2.27809200	-2.27247600
O	0.50692600	1.37881900	-0.48427100
H	-0.44008700	3.59895000	0.46086900
H	-0.69754900	4.44802900	-1.07034900
H	-2.91193600	4.30521300	-1.89925000
H	-4.75667600	2.88760500	-2.51974600
H	-4.65953700	2.92250300	-0.74428200
H	-5.84633000	0.82803900	-2.54027800
H	-5.99210400	-1.50246500	-1.96138600
H	-4.40378300	-1.20108100	-2.70155200
H	-5.01519300	-3.46421300	-0.75985500
H	-3.22029500	-4.32649000	0.60225900
H	-3.91451900	-2.93845000	1.42941100
H	-1.15800300	-3.34127200	-1.06830600
H	0.39955100	-2.43124000	1.39319000
H	1.12563100	-3.30137400	0.02858000
H	3.54078000	1.10690900	-2.84819600
H	5.66137300	2.34011500	-2.58519200
H	6.26132400	3.32677000	-0.39084100
C	-2.41405700	0.73727200	1.76061200
H	-2.42987500	1.82265000	1.72704000
H	-3.39190500	0.35932000	2.04929000
N	-2.07767100	0.21810600	0.40835500
H	-2.76232800	0.54334500	-0.29171600
H	-1.14489500	0.53464700	0.10117300
H	-2.08340100	-0.81658600	0.40828900
H	-1.66546000	0.39322800	2.47019800

CH₃NH₃⁺ / 2,3-DiPh-18c6_c7

C	5.84319900	2.77435100	1.17816600
C	5.80538600	2.34937500	-0.14554300
C	4.68675900	1.67709600	-0.62992800
C	3.459908400	1.41531600	0.20119800
C	3.64269300	1.85072300	1.52774600
C	4.75664200	2.52597500	2.01348800
H	4.77766800	2.85907400	3.04435600
H	2.79660900	1.67266800	2.18117800
C	2.38110600	0.67233000	-0.32488000
H	2.46459900	0.56738400	-1.41260700
C	2.28567200	-0.74026900	0.28049900
C	3.54305000	-1.54300700	-0.02034500
C	4.43404000	-1.87615300	0.99802100
C	5.58695100	-2.60641600	0.72301500
C	5.85619300	-3.01887700	-0.57757000
C	4.96646600	-2.69896100	-1.60036300
C	3.81838400	-1.96557000	-1.32313100
H	3.12533500	-1.73231100	-2.12320600
H	5.16750400	-3.02200000	-2.61495100
H	6.75106800	-3.59000400	-0.79367900
H	6.27092400	-2.85558000	1.52541600
H	4.22944400	-1.56010900	2.01475000
H	2.17923600	-0.64234000	1.36832900
O	1.10967400	-1.37201900	-0.24278100
C	0.88069300	-2.66913600	0.31518500
C	-0.33648300	-3.30206800	-0.31062800
H	-0.35128700	-4.36497000	-0.04598000
O	-1.52363000	-2.68160300	0.19509100
C	-2.74547500	-3.29990800	-0.22734900
C	-3.23845700	-2.79637700	-1.56737300
H	-2.48238500	-2.94131700	-2.34933300
O	-3.55128100	-1.41574300	-1.44027000
C	-3.96509400	-0.81902400	-2.66216200
C	-4.23856400	0.64595300	-2.43227500
H	-4.97640500	0.77753300	-1.63193400
O	-3.02084400	1.31009400	-2.08901500
C	-3.16624500	2.72964500	-2.01681200
C	-1.81364400	3.35865600	-1.79711300
H	-1.12269600	3.02473500	-2.57913800
O	-1.33629700	2.99471500	-0.50538100

C	-0.03504700	3.49188400	-0.20194800	O	-0.59838500	0.66234100	1.04566100
C	1.09833100	2.64163700	-0.73810800	H	0.83944100	2.84905400	1.40016100
H	2.03029000	3.19613200	-0.59744500	H	1.01956500	2.69611500	3.16005000
H	0.98148700	2.44475800	-1.81012200	H	3.28347600	2.81340200	1.25349900
O	1.16829000	1.39255000	-0.03039000	H	4.42473000	0.32486800	2.61065200
H	0.02902500	3.53709200	0.88675200	H	5.39225800	1.66614400	1.95478000
H	0.07904700	4.51083700	-0.58962800	H	6.38413600	0.04508500	0.61738100
H	-1.91191100	4.44910400	-1.86695800	H	6.13044400	-2.34290700	0.51902800
H	-3.58438900	3.10585800	-2.95759900	H	4.99912700	-1.77457900	1.76007200
H	-3.84999100	2.99719800	-1.20247100	H	4.50956200	-4.28212000	0.52246900
H	-4.64719500	1.07830100	-3.35286600	H	2.24586600	-5.05866900	0.06912500
H	-4.88252800	-1.29623000	-3.03004900	H	2.94801600	-4.31966000	-1.38765100
H	-3.18541600	-0.94089300	-3.42453700	H	-0.10188900	-4.40469900	0.03394700
H	-4.13134900	-3.36779800	-1.85387900	H	-0.42488800	-2.12615100	-1.99221200
H	-2.61873900	-4.11843100	-0.26407600	H	-1.69427300	-3.21373300	-1.40959900
H	-3.48125000	-3.06583600	0.54363300	H	-4.10375500	0.26969400	2.63258200
H	-0.28528700	-3.21625500	-1.40091300	H	-5.87951800	1.98204000	2.57675200
H	0.74685000	-2.59340800	1.40148600	H	-5.78293100	3.81873700	0.91404200
H	1.73831300	-3.32013600	0.12290100	C	1.80531500	0.25491900	-1.79880200
H	4.66296100	1.35045000	-1.66346100	H	2.70140700	-0.09038600	-2.31109800
H	6.64384300	2.54370200	-0.80354600	H	0.92507800	-0.06635400	-2.35190300
C	6.71152300	3.30001500	1.55679400	N	1.77714300	-0.33810200	-0.43375000
C	-2.11040500	0.58240700	1.51893600	H	2.62448000	-0.05482100	0.08427400
H	-1.50634700	0.17403300	2.32527800	H	0.94985300	-0.02947400	0.10116600
H	-2.12415500	1.66693000	1.57120500	H	1.75856800	-1.37210000	-0.46478000
N	-1.52452300	0.17179600	0.21521400	H	1.81806000	1.33456700	-1.71985700
H	-2.06489000	0.56378000	-0.57173600				
H	-0.55113200	0.50062500	0.11914700				
H	-1.52649400	-0.85896700	0.12405000				
H	-3.12339600	0.19339600	1.58848500				

CH₃NH₃⁺ / 2,3-DiPh-18c6_c8

C	-5.00496800	3.06517900	0.93875700
C	-5.05955600	2.03421800	1.87060300
C	-4.05646900	1.06942700	1.90202100
C	-2.99381600	1.11847500	1.00127000
C	-2.94337000	2.16088200	0.07304400
C	-3.94179700	3.12780600	0.04104300
H	-3.89123700	3.93134400	-0.68415400
H	-2.11349400	2.22331000	-0.62081800
C	-1.90655300	0.05823900	1.02900000
H	-2.01800800	-0.55062900	1.93324800
C	-1.98397600	-0.89373100	-0.17853600
C	-3.35439900	-1.53936300	-0.30544200
C	-4.21867700	-1.17787200	-1.33726800
C	-5.47562800	-1.76574600	-1.44989500
C	-5.87778700	-2.73004100	-0.53188100
C	-5.01653700	-3.10475800	0.49663200
C	-3.76344500	-2.51310000	0.60871400
H	-3.09364700	-2.81902500	1.40380600
H	-5.32174500	-3.85939100	1.21182800
H	-6.85423800	-3.19118600	-0.61886300
H	-6.13715800	-1.47321900	-2.25647600
H	-3.91083700	-0.42826000	-2.05775000
H	-1.78084800	-0.31161900	-1.08746500
O	-0.95164900	-1.86843900	-0.00141000
C	-0.75953900	-2.71687300	-1.12923400
C	0.25402000	-3.78423500	-0.79577700
H	0.38228200	-4.42208800	-1.67791300
O	1.50011700	-3.18719800	-0.43445800
C	2.58476500	-4.11605600	-0.37405700
C	3.68657100	-3.55637100	0.49245900
H	3.32201600	-3.40856800	1.51698700
O	4.13183800	-2.31728400	-0.04346900
C	5.21748200	-1.75600600	0.68531900
C	5.44482400	-0.33770500	0.20568500
H	5.51825700	-0.32723600	-0.88291000
O	4.37075200	0.55070200	0.53750800
C	4.45253200	1.11241700	1.85047500
C	3.29486800	2.05795800	2.04937400
H	3.41716100	2.57362500	3.01015800
O	2.08200200	1.31384400	2.04018700
C	0.93136600	2.12973700	2.22396200
C	-0.30507300	1.27213600	2.31163400
H	-1.13923700	1.91178000	2.61400100
H	-0.17311700	0.49100700	3.06885300

CH₃NH₃⁺ / 2,3-DiPh-18c6_c9

C	5.62673600	-3.32214100	-0.26149500
C	5.51951100	-2.60856200	0.92741700
C	4.43107900	-1.76679900	1.13943900
C	3.44336700	-1.62259200	0.16691500
C	3.55573000	-2.34757000	-1.02178800
C	4.63944500	-3.19179000	-1.23531900
H	4.71420400	-3.74898000	-2.16166200
H	2.78562200	-2.26216800	-1.77958400
C	2.25412900	-0.70156400	0.39686700
H	2.26986100	-0.35091400	1.43621000
C	2.32387900	0.53239500	-0.52262700
C	3.61615600	1.30146000	-0.29887900
C	4.60287000	1.32866000	-1.28254000
C	5.79227500	2.02219800	-1.07711300
C	6.00268500	2.70502400	0.11602100
C	5.01788200	2.69194600	1.10096600
C	3.83336500	1.99398500	0.89490900
H	3.06778700	1.99980500	1.66201100
H	5.17334800	3.22636400	2.03064700
H	6.92616200	3.24807000	0.27710300
H	6.55078600	2.03159200	-1.85056900
H	4.44390900	0.80080600	-2.21608800
H	2.28775300	0.18874000	-1.56310300
O	1.16576200	1.35450000	-0.12729600
C	1.10685000	2.50698900	-1.13108800
C	0.02239500	3.45299500	-0.67806500
H	0.17061800	4.41585000	-1.18264800
O	-1.25483200	2.92647500	-1.02489100
C	-2.35612600	3.75828500	-0.66880200
C	-2.79235200	3.59587800	0.77292000
H	-1.97690400	3.82743700	1.46843700
O	-3.23384400	2.25313800	0.97875800
C	-3.71370200	2.03469300	2.30684400
C	-4.16962400	0.60579500	2.46152900
H	-4.90613300	0.35452900	1.68761200
O	-3.04402700	-0.25829500	2.36828500
C	-3.37454600	-1.62965200	2.54794900
C	-2.12503400	-2.45807400	2.38448700
H	-1.34707700	-2.09625700	3.06439300
O	-1.68539000	-2.37462600	1.02475300
C	-0.51619300	-3.14919600	0.73116100
C	0.78781800	-2.45729000	1.06727200
H	1.59322300	-3.19399100	0.98314200
H	0.78477700	-2.08273900	2.09826900
O	1.01096000	-1.37432300	0.15993700
H	-0.55392500	-3.35858000	-0.33907500
H	-0.56529000	-4.10217000	1.26768600
H	-2.34731800	-3.50193500	2.63114900

H	-3.78324100	-1.79616900	3.55270600	H	4.18807000	2.28642300	-2.25731900
H	-4.13029500	-1.93805000	1.81470100	H	4.82355100	3.80724400	0.22289600
H	-4.65307700	0.49741500	3.44085200	H	3.14771000	4.23660700	1.91700700
H	-4.56038300	2.70198800	2.50588800	H	3.93269400	2.68440000	2.25283300
H	-2.92020200	2.25712300	3.02995400	H	0.99639300	3.66541100	0.20628100
H	-3.61508900	4.29313700	0.97387900	H	-0.38303600	1.93360500	2.30546200
H	-2.11912900	4.81192400	-0.85649500	H	-1.21707300	3.13573600	1.30214900
H	-3.17575500	3.47074000	-1.32988500	H	-3.54911100	-0.01925900	-2.92275000
H	0.10416200	3.61653900	0.40223700	H	-5.70262200	-1.21072900	-3.09991500
H	0.92821000	2.19000800	-2.16518600	H	-6.39122800	-2.80302500	-1.32830600
H	2.05899700	3.04072500	-1.09526700	C	2.28156500	-0.69703000	1.74030700
H	4.35310300	-1.21477100	2.06932600	H	3.26004900	-1.17061500	1.76759300
H	6.28024700	-2.70851200	1.69230400	H	2.22948000	0.09664600	2.47953300
C	6.47162900	-3.97952100	-0.42795000	N	2.06513400	-0.11111700	0.39094600
C	-2.02888100	-0.12853000	-1.67565900	H	1.14126000	0.34606300	0.32428500
H	-1.93629500	0.78027800	-2.26274200	H	2.77904400	0.60026100	0.17289200
H	-1.41649200	-0.91789300	-2.10468300	H	2.10626400	-0.84772400	-0.33406300
N	-1.56162800	0.14646000	-0.29094500	H	1.51069600	-1.43995000	1.93053700
H	-0.57605400	0.45168100	-0.28391900				
H	-2.12141800	0.88987800	0.15275600				
H	-1.63049600	-0.70600400	0.29105100				
H	-3.06741900	-0.44907600	-1.64215600				

CH₃NH₃⁺ / 2,3-DiPh-18c6_c10

C	-5.44668000	-2.27802400	-1.25148900
C	-5.06054400	-1.38428600	-2.24469500
C	-3.84473400	-0.71362200	-2.14435200
C	-3.00588900	-0.92120700	-1.05106800
C	-3.39841200	-1.82505200	-0.06107000
C	-4.61025900	-2.49932900	-0.15994500
H	-4.90253700	-3.19863500	0.61444200
H	-2.74735700	-2.01329600	0.78470700
C	-1.67960600	-0.18370500	-0.93838500
H	-1.48312800	0.34212800	-1.88103600
C	-1.72528400	0.86346100	0.19058900
C	-2.84224500	1.86711900	-0.04746000
C	-3.96315400	1.88985600	0.78035700
C	-4.99185200	2.80121900	0.55855800
C	-4.90461100	3.70704800	-0.49306800
C	-3.78362700	3.69809300	-1.31981400
C	-2.76020700	2.78366300	-1.09851700
H	-1.88620800	2.79206600	-1.73933500
H	-3.70737200	4.40459600	-2.13785100
H	-5.70259200	4.41898700	-0.66636400
H	-5.85779500	2.80488500	1.20958300
H	-4.03651200	1.18763900	1.60313700
H	-1.90868000	0.34115800	1.13691000
O	-0.43875200	1.50982900	0.26830700
C	-0.35985400	2.46043300	1.34435400
C	0.89492000	3.29007000	1.23060500
H	0.80175100	4.15125400	1.90372200
O	2.02565200	2.51115900	1.60947200
C	3.26864300	3.20665900	1.56164000
C	3.89382700	3.22639900	0.18159600
H	3.23220900	3.70077300	-0.55294600
O	4.17752500	1.88551300	-0.22105000
C	4.82350700	1.82202700	-1.49402900
C	5.10363800	0.38578700	-1.85772300
H	5.66761500	-0.10746300	-1.05584700
O	3.87274100	-0.29070300	-2.08053600
C	4.04354300	-1.64864100	-2.46680100
C	2.68565300	-2.28258900	-2.63619700
H	2.08504300	-1.69494200	-3.33804100
O	2.04320600	-2.35431400	-1.35908800
C	0.74456700	-2.95927100	-1.38211300
C	-0.37628000	-2.00899200	-1.74716600
H	-1.27937400	-2.60196300	-1.92425200
H	-0.14849800	-1.46332300	-2.67110300
O	-0.59399600	-1.08240400	-0.67942800
H	0.57753400	-3.35450800	-0.37888300
H	0.74563200	-3.79923000	-2.08402200
H	2.80564100	-3.29378100	-3.04008900
H	4.58623600	-1.71036000	-3.41862800
H	4.62090900	-2.19009300	-1.70676500
H	5.71775900	0.36876500	-2.76715300
H	5.77186900	2.37029900	-1.45257200

CH₃NH₃⁺ / 2,3-DiPh-18c6_c11

C	-5.42626000	-2.32031900	-1.24821200
C	-5.05555600	-1.41301700	-2.23497600
C	-3.84643000	-0.73029800	-2.13520500
C	-2.99899800	-0.93924100	-1.04882100
C	-3.37603500	-1.85663900	-0.06528900
C	-4.58115300	-2.54295800	-0.16365200
H	-4.86141700	-3.25267000	0.60569500
H	-2.71815700	-2.04752000	0.77500000
C	-1.67996000	-0.18874700	-0.93671400
H	-1.49411000	0.34747300	-1.87564000
C	-1.72996700	0.84777200	0.20182000
C	-2.85903100	1.84143400	-0.02025300
C	-3.97387700	1.84587300	0.81601000
C	-5.01368700	2.74808700	0.60912300
C	-4.94377700	3.66308600	-0.43583200
C	-3.82894000	3.67251400	-1.27085300
C	-2.79440500	2.76714000	-1.06449700
H	-1.92527300	2.78997400	-1.71156900
H	-3.76618800	4.38636500	-2.08363600
H	-5.75043400	4.36794600	-0.59748400
H	-5.87469600	2.73751400	1.26658000
H	-4.03362900	1.13664600	1.63386500
H	-1.90198400	0.31504300	1.14448100
O	-0.44961900	1.50674800	0.27740200
C	-0.37507200	2.45208500	1.35840800
C	0.87407800	3.29050700	1.24717400
H	0.77587200	4.14786800	1.92445500
O	2.01036400	2.51737600	2.51214900
C	3.24810400	3.22252700	1.57926700
C	3.87374500	3.25722000	0.19976300
H	3.20901500	3.73212000	-0.53164500
O	4.16743800	1.92147600	-0.12159400
C	4.81500300	1.87219800	-1.48535300
C	5.10458300	0.44073900	-1.86022900
H	5.67164600	-0.05519800	-1.06218400
O	3.87821600	-0.24204800	-2.08864700
C	4.05834400	-1.59566400	-2.48555400
C	2.70500900	-2.23737500	-2.66161800
H	2.10106800	-1.64817700	-3.35931500
O	2.06153300	-2.32419500	-1.38594900
C	0.76703100	-2.93778000	-1.41622600
C	-0.36011900	-1.99079700	-1.77019200
H	-1.25929800	-2.58764300	-1.95404200
H	-0.13614600	-1.43266500	-2.68761200
O	-0.58376600	-1.07836500	-0.69157400
H	0.60243000	-3.34584100	-0.41774500
H	0.77381900	-3.76941700	-2.12793800
H	2.83251600	-3.24432700	-3.07369900
H	4.60240200	-1.64615200	-3.43725500
H	4.63856700	-2.13931500	-1.72928000
H	5.71899200	0.43493500	-2.76964200
H	5.75986300	2.42608700	-1.43864000
H	4.17736600	2.33862400	-2.24555600
H	4.79912600	3.84462200	0.24587300
H	3.11922300	4.24881300	1.94232300
H	3.91573800	2.70001600	2.26682900

H	0.97202600	3.67145300	0.22456600	H	3.27100600	-1.15495300	1.75233800
H	-0.39313100	1.92013500	2.31677000	H	2.22634900	0.09504200	2.47429300
H	-1.23676200	3.12194900	1.32124500	N	2.06739300	-0.09505400	0.38349300
H	-3.56290000	-0.02540300	-2.90862500	H	2.11388700	-0.82504500	-0.34782000
H	-5.70443100	-1.23822900	-3.08480300	H	1.14014800	0.35285100	0.32084600
H	-6.36555200	-2.85472200	-1.32464900	H	2.77611600	0.62332600	0.17170100
C	2.28776700	-0.69116400	1.72777500	H	1.52427100	-1.44373400	1.90961600

4. Conformational analysis of 2-Ph-18c6 and its K⁺complex

Table S10. Relative energies and corresponding Boltzmann populations χ of the 14 lowest energy conformers ($\Sigma\chi > 97\%$) of **2-Ph-18c6** at B3LYP/6-311G++(2d,p)/IEFPCM(CHCl₃). XYZ-coordinates for the first six structures can be found below.

Conformer	ΔE_{ZPC}	ΔG_{298K}	$\chi(\Delta E_{ZPC})$	$\chi(\Delta G_{298K})$
	[kcal / mol]	[kcal / mol]	[%]	[%]
2-Ph-18c6_c1	0.00	0.00	56.79	63.69
2-Ph-18c6_c2	1.01	0.95	10.37	12.87
2-Ph-18c6_c3	1.18	1.51	7.75	5.01
2-Ph-18c6_c4	1.20	1.61	7.52	4.22
2-Ph-18c6_c5	1.46	2.07	4.84	1.93
2-Ph-18c6_c6	1.58	1.99	3.92	2.20
2-Ph-18c6_c7	2.07	2.40	1.73	1.12
2-Ph-18c6_c8	2.50	2.46	0.83	1.01
2-Ph-18c6_c9	2.51	2.60	0.82	0.78
2-Ph-18c6_c10	2.65	2.36	0.64	1.17
2-Ph-18c6_c11	2.70	2.57	0.60	0.84
2-Ph-18c6_c12	2.76	1.98	0.54	2.25
2-Ph-18c6_c13	2.81	3.17	0.49	0.30
2-Ph-18c6_c14	2.97	3.22	0.38	0.28

ΔE_{ZPC} referenced to -1153.961968 hartree / ΔG_{298K} referenced to -1154.018677 hartree

Table S11. Relative energies and corresponding Boltzmann populations χ of the 14 lowest energy conformers ($\Sigma\chi > 97\%$) of **K⁺/2-Ph-18c6** at B3LYP/6-311G++(2d,p)/IEFPCM(CHCl₃). XYZ-coordinates for the first six structures can be found below.

Conformer	ΔE_{ZPC} [kcal / mol]	ΔG_{298K} [kcal / mol]	$\chi(\Delta E_{ZPC})$ [%]	$\chi(\Delta G_{298K})$ [%]
K ⁺ / 2-Ph-18c6_c1	0.00	0.00	79.97	92.82
K ⁺ / 2-Ph-18c6_c2	2.08	2.57	2.37	1.20
K ⁺ / 2-Ph-18c6_c3	2.10	2.85	2.32	0.75
K ⁺ / 2-Ph-18c6_c4	2.12	2.87	2.23	0.73
K ⁺ / 2-Ph-18c6_c5	2.20	3.38	1.94	0.31
K ⁺ / 2-Ph-18c6_c6	2.27	3.48	1.74	0.26
K ⁺ / 2-Ph-18c6_c7	2.74	3.44	0.79	0.28
K ⁺ / 2-Ph-18c6_c8	2.78	3.34	0.74	0.33
K ⁺ / 2-Ph-18c6_c9	2.79	3.19	0.72	0.43
K ⁺ / 2-Ph-18c6_c10	2.83	3.45	0.67	0.27
K ⁺ / 2-Ph-18c6_c11	2.83	3.32	0.67	0.34
K ⁺ / 2-Ph-18c6_c12	2.86	3.47	0.64	0.27
K ⁺ / 2-Ph-18c6_c13	2.86	3.54	0.64	0.24
K ⁺ / 2-Ph-18c6_c14	2.87	3.36	0.63	0.32
K ⁺ / 2-Ph-18c6_c15	2.87	3.40	0.62	0.30
K ⁺ / 2-Ph-18c6_c16	2.90	3.59	0.60	0.22

ΔE_{ZPC} referenced to -1153.961968 hartree / ΔG_{298K} referenced to -1154.018677 hartree

4.1 Cartesian Coordinates of 2-Ph-18c6

2-Ph-18c6_c1				C	1.83865800	3.97724500	-0.80511400
O	-2.19304800	0.88368000	0.17444400	H	2.30871600	4.96991600	-0.86421200
O	-0.85663900	-1.50055600	1.08296500	H	2.07705100	3.43333100	-1.72868200
O	1.85194600	-1.30814700	2.23633300	C	0.34309300	4.15374100	-0.69250900
O	2.32625600	3.26939500	0.32129500	H	0.01759400	4.88531200	-1.44662700
O	-0.30742600	2.91219100	-0.90452200	H	0.08906300	4.55310000	0.29846100
O	3.61251800	0.80387400	1.20657600	C	-1.71937000	3.01492700	-0.82823000
C	-2.76520300	-0.41638500	0.09022800	H	-2.08945700	3.68425900	-1.61862400
H	-2.43219900	-0.90020400	-0.83740700	H	-2.02079200	3.43650000	0.13990900
C	-2.23463000	-1.23299000	1.26146900	C	-2.35430400	1.65646300	-1.00903900
H	-2.79833100	-2.17392400	1.32027400	H	-1.89276700	1.14105500	-1.86102900
H	-2.40223500	-0.67823800	2.19474200	H	-3.41951100	1.79719000	-1.23046500
C	-0.32460200	-2.30274900	2.12585300	C	-4.28707200	-0.39143100	0.11475800
H	-0.50035600	-1.82749500	3.09990100	C	-4.97067600	0.44005100	1.00429500
H	-0.81842800	-3.28519200	2.13324700	H	-4.40899000	1.10380900	1.65072800
C	1.15792800	-2.50308100	1.92166900	C	-6.36103900	0.43206600	1.05374300
H	1.49660900	-3.32128900	2.57400300	H	-6.87886500	1.08389000	1.74777700
H	1.35303400	-2.79542700	0.88136700	C	-7.08713200	-0.40918900	0.21431000
C	3.25148100	-1.41235100	2.03532100	H	-8.17006200	-0.41372000	0.25170400
H	3.46672400	-1.74279800	1.01065700	C	-6.41421700	-1.23883900	-0.67735600
H	3.67973800	-2.15150600	2.72800000	H	-6.97142600	-1.89088000	-1.33980100
C	3.90312400	-0.07237100	2.28192400	C	-5.02282200	-1.22615100	-0.72630800
H	4.98985400	-0.21532200	2.37243300	H	-4.50389000	-1.86982000	-1.42894800
H	3.53599700	0.34798000	3.22748400	2-Ph-18c6_c2			
C	4.11975700	2.11239400	1.40390900	O	-2.04289200	0.83676800	-0.30412100
H	5.21761600	2.09019400	1.46645700	O	-0.89078000	-2.46788300	0.48746400
H	3.73441700	2.53352400	2.34196000	O	1.63814600	-1.65348900	1.99244500
C	3.71374800	2.99144000	0.24507000	O	1.88021600	3.34323700	0.49833800
H	4.29268600	3.92576300	0.28388600				
H	3.94939400	2.48491800	-0.70014600				

O	-0.46458200	3.08467600	-1.19164000	C	-2.54364300	-1.36367500	2.37949100
O	3.15058600	0.84286600	1.43567600	H	-3.58482000	-1.70173200	2.27886400
C	-1.92005300	-0.536215200	-0.53602200	H	-2.03744600	-2.01375200	3.09019700
H	-1.26433800	-0.73163300	-1.39964800	C	-1.74680600	-2.69551600	0.58693900
C	-1.20368900	-1.09773000	0.70465800	H	-2.73127500	-3.16009000	0.43595900
H	-1.85191100	-0.99306700	1.58458300	H	-1.17536600	-3.32775600	1.28134800
H	-0.29946300	-0.50810300	0.86636700	C	-1.00204800	-2.61836900	-0.72406100
C	-0.24706000	-3.11128400	1.57956800	H	-0.11430500	-1.99315000	-0.60432500
H	-0.66543700	-2.76066000	2.53088500	H	-0.68453100	-3.62968000	-1.01407200
H	-0.47757800	-4.17493000	1.47974500	C	-1.24992200	-1.87879400	-2.99341400
C	1.26267300	-2.96370600	1.59191000	H	-2.05047100	-1.96512900	-3.73269800
H	1.67903600	-3.70288900	2.29330400	H	-0.51621900	-2.66836100	-3.19830900
H	1.66177500	-3.18391900	0.59272300	C	-0.60894800	-0.51485600	-3.16728500
C	3.04687300	-1.48368900	2.03793200	H	-0.42909000	-0.34850700	-4.23803900
H	3.48639600	-1.67934900	1.05100700	H	-1.29906600	0.26136600	-2.81181500
H	3.48443500	-2.19634000	2.75154300	C	1.86032200	1.16449800	-3.81685000
C	3.39518300	-0.08312800	2.48239500	C	1.74776100	2.44194000	-4.36576900
H	4.45896700	-0.06110100	2.75997300	H	1.17093800	3.19911600	-3.84506600
H	2.80807500	0.18120400	3.37196200	C	2.36320200	2.75320200	-5.75486600
C	3.52488700	2.16578500	1.78804200	H	2.26376200	3.75028700	-5.98936300
H	4.59522800	2.19695600	2.03788800	C	3.09655200	1.78524200	-6.25321900
H	2.96166900	2.50044200	2.66916500	C	3.57285600	2.02386600	-7.19678800
C	3.27103900	3.10635100	0.63400000	H	3.20896600	0.50531500	-5.71607500
H	3.79864300	4.05157900	0.82808900	H	3.77493100	-0.25514000	-6.24149800
H	3.67709400	2.67526100	-0.29069400	C	2.59560100	0.19786000	-4.50566200
C	1.56767400	4.18773400	-0.59725100	H	2.67562900	-0.80205200	-4.09611300
H	1.99852700	5.18750000	-0.44225900				
H	1.98661800	3.77739700	-1.52556900				
C	0.06814000	4.31248500	-0.72779300				
H	-0.16356900	5.12462400	-1.43204100				
H	-0.36674700	4.57231900	0.24614900				
C	-1.88163700	3.03965200	-1.19858200				
H	-2.28490000	3.69656500	-1.98260800				
H	-2.27856400	3.37849900	-0.23279800				
C	-2.32374700	1.61862000	-1.45807300				
H	-1.78330700	1.22105300	-2.32534700				
H	-3.39646600	1.60349200	-1.68654600				
C	-3.25608900	-1.23303300	-0.80365800				
C	-4.36447800	-0.95241900	-0.00112100				
H	-4.27026400	-0.23425900	0.80517500				
C	-5.58537300	-1.57497300	-0.23600300				
H	-6.43760000	-1.34549200	0.39326700				
C	-5.71540500	-2.49104000	-1.27797100				
H	-6.66699100	-2.97604000	-1.46135700				
C	-4.61798400	-2.77504000	-2.08394500				
H	-4.71085100	-3.48280300	-2.89951400				
C	-3.39813300	-2.14555500	-1.84779600				
H	-2.54673400	-2.36745300	-2.48194200				

2-Ph-18c6_c3

O	0.61526000	-0.44220200	-2.44296400
O	1.61450000	0.87925200	-0.10665300
O	1.21398800	2.04922300	2.57796600
O	-1.88984700	-1.39087800	1.12350300
O	-1.86253200	-2.08167900	-1.72634000
O	-1.21114900	0.40421300	3.28644300
C	1.22442300	0.84644500	-2.47239600
H	0.46606900	1.60720000	-2.24794700
C	2.26620300	0.88780100	-1.36120800
H	2.87363100	1.79575900	-1.47142300
H	2.93345600	0.01954800	-1.45857200
C	2.51455800	0.80712200	0.98871100
H	3.19071000	1.67327600	0.98789100
H	3.12700800	-0.10214400	0.90965500
C	1.73649300	0.75475500	2.28101200
H	2.41173900	0.43923800	3.08857900
H	0.92774800	0.02563800	2.19499200
C	0.42188400	2.11093400	3.75741400
H	0.83626400	1.45406600	4.53263600
H	0.49078300	3.14090300	4.11672100
C	-1.04439600	1.79174300	3.53486200
H	-1.41844400	2.37327400	2.68255200
H	-1.61255500	2.09167700	4.42884500
C	-2.53335100	0.05122200	2.90825400
H	-3.20939900	0.12296600	3.77182000
H	-2.89860800	0.73272000	2.13013500

2-Ph-18c6_c4

O	1.35257700	-0.23254700	-2.50322300
O	1.46730000	1.10997800	0.05566800
O	0.96098100	1.30373600	2.93360800
O	-1.78509900	-1.40592200	1.22935600
O	-0.82826000	-2.04511600	-1.43493200
O	-1.37458700	-0.32539300	3.92785500
C	0.45424500	0.80723600	-2.10505700
H	-0.371110800	0.371110800	-1.53065900
C	1.23099000	1.74342200	-1.18823300
H	0.64696900	2.66047100	-1.03687300
H	2.17908600	2.02026700	-1.67133300
C	2.17800400	1.93225600	0.96641100
H	1.68601800	2.90970200	1.06397700
H	3.20193400	2.10311300	0.60509000
C	2.23891700	1.25765000	2.31610200
H	2.98010400	1.77445100	2.91828000
H	2.56280900	0.21644500	2.19297700
C	0.90521000	0.57158100	4.14870700
H	1.26231300	-0.45364900	3.98713100
H	1.55103500	1.04255300	4.90579400
C	-0.51667400	0.52849500	4.67470600
H	-0.93116000	1.54250600	4.72874600
H	-0.48707500	0.12375900	5.68982300
C	-2.06662700	0.31385600	2.85618200
H	-2.82152200	1.00068800	3.26331800
H	-1.37064800	0.88199000	2.23529400
C	-2.75402700	-0.72955700	2.00972500
H	-3.48338100	-0.23120300	1.35531800
H	-3.29998300	-1.43727800	2.64916500
C	-2.33617700	-2.40719200	0.38948900
H	-3.11868100	-1.97988700	-0.25300000
H	-2.79073900	-3.20740300	0.99082700
C	-1.23770800	-2.99558400	-0.46303600
H	-0.38969000	-3.27327400	0.17554300
H	-1.60799700	-3.90554700	-0.95609500
C	0.32901700	-2.44858800	-2.15155400
H	0.12147900	-3.36856300	-2.71954400
H	1.15020000	-2.65751200	-1.45378700
C	0.74922700	-1.36529800	-3.12484700
H	1.580964500	-1.78445900	-3.78840400
H	-0.10353000	-1.06302100	-3.74166800
C	-0.10084400	1.57667000	-3.29433300
C	0.70854400	1.89254500	-4.38731400
H	1.73396700	1.54355200	-4.40755200
C	0.20381500	2.63345400	-5.45154600
H	0.84293500	2.86917500	-6.29463700
C	-1.11838700	3.07018100	-5.43665400
H	-1.51196100	3.64478100	-6.26681400

C	-1.93343500	2.75725000	-4.35288000	H	-5.14085400	0.03754200	-0.48815500
H	-2.96634700	3.08501900	-4.33695300				
C	-1.42617400	2.01294300	-3.29149700				
H	-2.06850200	1.76368100	-2.45356500				

2-Ph-18c6_c5

O	-1.38955900	1.02042400	-1.33437100
O	-1.17966400	-1.80882200	-0.93443900
O	1.52708600	-2.87388800	-0.60105600
O	3.19870600	1.78783600	0.11650400
O	0.51913100	2.92830500	-0.33306400
O	3.42326200	-1.07315200	0.71155300
C	-2.52836800	0.17531400	-1.23050700
H	-3.31721100	0.55002200	-1.90026200
C	-2.12665700	-1.19112400	-1.78106000
H	-3.02776400	-1.81476500	-1.87020500
H	-1.70600800	-1.04933300	-2.78529500
C	-0.71358800	-3.05077900	-1.43298700
H	-0.27758500	-2.92208100	-2.43272100
H	-1.54626400	-3.76447600	-1.51375100
C	0.32376800	-3.61565400	-0.49113300
H	-0.05603100	-3.57602500	0.53805700
H	0.50259100	-4.67015100	-0.74739500
C	2.50305000	-3.25657700	0.35260900
H	2.80664700	-4.30109500	0.18945700
H	2.09388200	-3.17680600	1.36843000
C	3.71941400	-2.37049600	0.22332100
H	4.54415300	-2.81423700	0.80004600
H	4.03005400	-2.32003600	-0.82867800
C	4.50529900	-0.16917400	0.56760800
H	4.81973400	-0.11475000	-0.48310900
H	5.36567600	-0.50925500	1.16249300
C	4.09465800	1.20316100	1.04605500
H	3.62260300	1.12524900	2.03440700
H	4.99548200	1.82593200	1.14800800
C	2.75639000	3.07647700	0.51024700
H	3.60857100	3.76970400	0.56148000
H	2.29240200	3.03469100	1.50462200
C	1.75821800	3.59813800	-0.49624700
H	1.62744900	4.67988400	-0.34831400
H	2.14726300	3.43844200	-1.51026900
C	-0.39655400	3.19190700	-1.38209100
H	0.04844000	2.91890300	-2.34804200
H	-0.64851800	4.26224100	-1.41260600
C	-1.66476000	2.40264300	-1.16128400
H	-2.05511500	2.59963100	-0.15653200
H	-2.41761000	2.73255900	-1.89145200
C	-3.09807000	0.10331100	0.17780600
C	-2.25833100	0.09695300	1.29253000
H	-1.18861000	0.16787600	1.14502900
C	-2.79095000	0.00370000	2.57385000
H	-2.12858600	0.00176400	3.43182200
C	-4.16888700	-0.08972200	2.75809500
H	-4.58176600	-0.16212600	3.75750100
C	-5.01236700	-0.08213100	1.65180500
H	-6.08614700	-0.14589800	1.78482600
C	-4.47679400	0.01951000	0.37024100

2-Ph-18c6_c6

O	0.63756900	2.76469000	-0.33278700
O	0.38672700	0.72795600	-2.43322300
O	0.04436100	-1.97231300	-1.41092500
O	-0.52259700	-1.73336000	2.86003700
O	0.37478100	0.83902900	1.85951400
O	-0.76973800	-3.83396100	0.71949200
C	0.70163200	3.01470100	-1.73589100
H	1.73622000	2.90079900	-2.08090000
C	-0.17274300	2.02787100	-2.51149000
H	-0.24484700	2.34787900	-3.56043300
H	-1.18253400	2.03717400	-2.08064500
C	-0.44273600	-0.26907600	-3.01276300
H	-0.54037300	-0.09865700	-4.09420200
H	-1.44508300	-0.23101900	-2.56824800
C	0.16300500	-1.63320900	-2.78041100
H	1.21918200	-1.62731100	-3.08398800
H	-0.36460000	-2.36794000	-3.40533100
C	0.68989700	-3.18835600	-1.07179500
H	0.25013200	-4.02703600	-1.62956400
H	1.75710500	-3.13183300	-1.32931400
C	0.56312500	-3.42634100	0.41344200
H	0.81721600	-2.51104300	0.95307600
H	1.26564400	-4.21811400	0.70861500
C	-1.04389800	-3.96384500	2.10895200
H	-1.82151800	-4.72694300	2.19907400
H	-0.15648400	-4.32207600	2.64513300
C	-1.56387400	-2.69172800	2.75035700
H	-1.96529500	-2.93458000	3.74634500
H	-2.38356500	-2.28786100	2.14241200
C	-0.97346900	-0.47177400	3.33003800
H	-1.29236800	-0.54920400	4.37915400
H	-1.83128800	-0.13196200	2.73620900
C	0.14365200	0.53876500	3.22419800
H	-0.14385300	1.44660300	3.77360000
H	1.05538800	0.13709200	3.68798700
C	1.46901700	1.71737400	1.65641900
H	2.38563500	1.28114500	2.07854600
H	1.28882000	2.67862600	2.15752500
C	1.67819700	1.93311200	0.17693700
H	2.64971800	2.42335000	0.02627300
H	1.68451900	0.97013400	-0.33829600
C	0.24988000	4.43587300	-2.01390200
C	-0.74712900	5.03812600	-1.24500000
H	-1.17483000	4.49768400	-0.41028100
C	-1.17869500	6.32924700	-1.53491000
H	-1.95144700	6.78601300	-0.92750600
C	-0.62107600	7.03436700	-2.59777400
H	-0.95599500	8.04053900	-2.82053300
C	0.37446500	6.44112900	-3.36842100
H	0.82091400	6.98448000	-4.19300200
C	0.80570000	5.15068800	-3.07592500
H	1.58753500	4.69809500	-3.67687400

4.2 Cartesian Coordinates of K+/2-Ph-18c6

K+/2-Ph-18c6_c1

C	-2.66437600	-0.32336500	-0.63578500	H	-3.34419400	1.61556500	-0.04820900
H	-3.56333000	-0.56798900	-1.21235800	O	-1.87245900	0.93303800	1.23325900
C	-3.04216200	0.68148000	0.44160400	C	-2.03549200	2.01570700	2.15407600
C	-4.20667900	0.15106800	1.26109900	C	-0.82195100	2.11490900	3.04304300
C	-5.49068300	0.66011400	1.06935400	H	-0.62709200	1.14907600	3.52502300
C	-6.57046300	0.14986400	1.78469500	O	0.31070100	2.51542100	2.27473200
C	-6.37349300	-0.87310800	2.70653000	C	1.49914600	2.61215200	3.05699200
C	-5.09332800	-1.38253900	2.90928600	C	2.62312300	3.13831000	2.20037100
C	-4.01709800	-0.87528000	2.18929300	H	3.50698400	3.29296800	2.83141600
H	-3.02242900	-1.27059600	2.35828900	O	2.91353600	2.19742900	1.16998700
H	-4.93340300	-2.17676100	3.62880600	C	3.98028800	2.61782100	0.32318100
H	-7.21136700	-1.26877800	3.26778500	C	4.21730100	1.57496200	-0.74004200
H	-7.56222900	0.55622600	1.62659200	H	4.41602500	0.59926900	-0.27945400
H	-5.64909300	1.46370100	0.35814200	O	3.07044700	1.49303700	-1.58243700
				C	3.23740300	0.57451700	-2.65932200

C	1.98843100	0.56687400	-3.50459100	H	-4.22701900	-2.67270900	0.28726800
H	1.75780900	1.58224800	-3.84968400	H	2.60419400	-0.78762100	-0.36892400
O	0.90431200	0.05324500	-2.73481300	K	-1.93137700	0.23941100	-0.74177600
C	-0.31815000	-0.00762800	-3.46495300				
C	-1.38332900	-0.63279300	-2.60020900	K⁺ / 2-Ph-18c6_c3			
H	-2.28767200	-0.78392900	-3.20189200	O	2.03394500	-0.92595500	-1.15786600
H	-1.04536300	-1.61075200	-2.23602700	O	1.63595200	1.77237600	-0.63032100
O	-1.67054200	0.22510500	-1.49593300	O	-0.76053300	2.56598300	0.70501900
H	-0.18987600	-0.62117300	-4.36500700	O	-1.85823700	-2.14001100	1.48477500
H	-0.62181500	0.99959400	-3.77622300	O	0.55154200	-2.92179900	0.15318600
H	2.15826300	-0.06489800	-4.38495800	O	-2.14882100	0.59512100	2.22719800
H	4.08792800	0.87501100	-3.28324400	C	3.04469600	0.01905000	-1.51925700
H	3.43583900	-0.43118100	-2.26866200	H	3.48532500	-0.28807600	-2.47694500
H	5.09756100	1.86298200	-1.32775600	C	2.33138800	1.33961700	-1.79239200
H	4.89928200	2.74440800	0.90841100	H	3.07494400	2.08663600	-2.09307800
H	3.73271800	3.57998200	-0.14166100	H	1.62533500	1.20185400	-2.62108200
H	2.34300500	4.10281800	1.75902800	C	1.04812800	3.06194000	-0.78680400
H	1.34285800	3.30111100	3.89593800	H	0.34092800	3.05393100	-1.62580300
H	1.75995800	1.62749500	3.46484300	H	1.82492100	3.80618000	-0.99980500
H	-1.02046300	2.85585600	3.82713300	C	0.34022200	3.44662700	0.48832400
H	-2.91301400	1.84734400	2.78582700	H	1.03421800	3.39558500	1.33592500
H	-2.18261000	2.95285800	1.60314500	H	-0.01675600	4.47980600	0.39769800
H	-2.29495200	-1.24690000	-0.17242400	C	-1.48743800	2.87176400	1.89297800
K	0.61869300	1.21033300	-0.17784500	H	-1.87634800	3.89610200	1.84403400
				H	-0.82778900	2.79611800	2.76611200
				C	-2.64681500	1.91678200	2.03266100
K⁺ / 2-Ph-18c6_c2				H	-3.25453800	2.22132800	2.89353100
O	0.42799800	1.71434200	-0.56893600	H	-3.27850200	1.95236200	1.13638200
O	-2.01327400	3.08081000	-0.82133200	C	-3.18374000	-0.36929600	2.40439400
O	-4.42333200	1.55006200	-0.67232000	H	-3.82607200	-0.39909400	1.51543900
O	-4.27819800	-1.24469000	-1.21773600	H	-3.80480600	-0.10175800	3.26783300
O	-1.80559600	-2.57230700	-0.72090700	C	-2.56792900	-1.72462600	2.64940000
O	0.60213400	-1.04490500	-0.85061500	H	-1.88694800	-1.68151300	3.50830300
C	2.12586200	1.13236000	-2.27258800	H	-3.36665900	-2.44019000	2.87944800
C	1.21319100	0.96795600	-3.31464500	C	-1.26719100	-3.43000200	1.62683500
H	0.15957300	0.85768800	-3.09461800	H	-2.04258600	-4.17873700	1.82961900
C	1.64340200	0.95598500	-4.63751500	H	-0.56148900	-3.42938200	2.46655500
H	0.92224900	0.83113000	-5.43658400	C	-0.55635700	-3.79773300	0.34853300
C	2.99502100	1.10299500	-4.93667900	H	-0.20780300	-4.83517600	0.42021400
H	3.32926500	1.09305300	-5.96709300	H	-1.24701000	-3.72570900	-0.50096100
C	3.91249700	1.27144800	-3.90463600	C	1.25594400	-3.18623200	-1.05797200
H	4.96549700	1.39626100	-4.12690100	H	0.59400000	-3.02001300	-1.91731700
C	3.47705400	1.29179000	-2.58310200	H	1.59212000	-4.23018600	-1.08113300
H	4.19776200	1.43594600	-1.78486400	C	2.46571200	-2.28760900	-1.14409700
C	1.70081700	1.10918600	-0.81283100	H	3.13452600	-2.46533900	-0.29674400
H	2.46144400	1.64515100	-0.22993000	H	3.00882900	-2.51940100	-2.06798000
C	1.63535000	-0.29644800	-0.22338200	C	4.16970500	0.13877100	-0.50289900
H	1.44264300	-0.22399000	0.85449600	C	3.94268400	0.05341300	0.87085400
C	0.56401600	-2.40331400	-0.41887400	H	2.94445900	-0.14034000	1.24010000
H	1.51285500	-2.89980900	-0.65507700	C	4.99122300	0.20392500	1.77263600
H	0.41329100	-2.44909800	0.66709600	H	4.79965500	0.13113800	2.83671400
C	-0.55500400	-3.12192800	-1.13059300	C	6.28237300	0.44763300	1.31271200
H	-0.51110100	-4.18768600	-0.87542800	H	7.09834500	0.56469400	2.01562500
H	-0.43809800	-3.02287100	-2.21654400	C	6.51952800	0.53074200	-0.05551200
C	-2.92156700	-3.21572100	-1.33177800	H	7.52220600	0.71027800	-0.42462800
H	-2.86811200	-3.10547300	-2.42190300	C	5.46950700	0.37089700	-0.95465700
H	-2.91562100	-4.28642000	-1.09410900	H	5.66582000	0.42396300	-2.02040900
C	-4.19873300	-2.60794600	-0.80740800	K	-0.19835900	-0.17357800	0.33768400
H	-5.04984700	-3.17221500	-1.20747800				
C	-5.47211800	-0.60096400	-0.77831100				
H	-6.35074300	-1.12558900	-1.17309100	K⁺ / 2-Ph-18c6_c4			
H	-5.52605800	-0.61706700	0.31720500	C	0.01255100	-3.16973600	-0.87510400
C	-5.48800500	0.82174800	-1.27975100	H	-0.04339900	-4.21673500	-0.55327200
H	-6.45158100	1.27773000	-1.02187300	H	0.31140300	-3.14923800	-1.93013000
H	-5.38037600	0.84025300	-2.37132900	C	1.03689300	-2.45408100	-0.30350100
C	-4.38981100	2.91908500	-1.07048600	H	1.98330700	-3.00622800	-0.07565700
H	-4.26287900	2.99109600	-2.15771900	H	0.70809400	-2.42052100	1.01572700
H	-5.33153400	3.41261500	-0.80109600	C	2.18015100	-0.39205200	0.21541100
C	-3.25336200	3.61678200	-0.36556500	H	1.82604500	-0.24814400	1.24410900
H	-3.34433600	3.48440100	0.71965800	C	2.41174200	0.97195500	-0.42748100
H	-3.30272400	4.69006100	-0.58578500	H	3.10103000	1.50601800	0.23973900
C	-0.88641600	3.67581200	-0.18210900	C	-0.10736100	3.68221900	-0.37684300
H	-0.90074200	4.76330200	-0.32506800	H	-0.063549300	4.76149700	-0.55944600
H	-0.91843200	3.47079700	0.89535100	H	-0.35695500	3.52902200	0.68069400
C	0.38412300	3.12600000	-0.78416300	C	1.22357700	3.04795100	-0.70027800
H	1.23908600	3.60774400	-0.29565600	H	1.99546300	3.51628900	-0.07830900
H	0.42774800	3.34862400	-1.85452700	H	1.47981800	3.21260700	-1.75117500

C	-3.41850700	3.03026700	-1.87304400
H	-3.09335300	3.01539400	-2.92054000
H	-4.36475300	3.58170900	-1.81473100
C	-2.39202600	3.73003100	-1.01787800
H	-2.68559400	3.68259300	0.03815200
H	-2.34093900	4.78518500	-1.31267000
C	-4.73641000	-0.40559200	-1.54945100
H	-5.56002400	-0.91836300	-2.06094600
H	-4.98264900	-0.33978700	-0.48238400
C	-4.58285900	0.97571500	-2.13621600
H	-5.54846400	1.49323800	-2.08260300
H	-4.28737000	0.90874200	-3.19050900
C	-3.59655700	-2.46587600	-1.22849200
H	-3.82166100	-2.45416800	-0.15494300
H	-4.39570900	-3.01498300	-1.74121500
C	-2.28494300	-3.16736500	-1.47924800
H	-2.03403300	-3.13092800	-2.54655100
H	-2.38418300	-4.21950600	-1.18590900
O	1.21933600	-1.13042400	-0.52842400
O	-1.25743800	-2.54053300	-0.71500100
O	-3.52228500	-1.13169300	-1.72590800
O	1.15218500	1.64884200	-0.42014000
O	-1.12117600	3.10978200	-1.19966900
O	-3.59911700	1.69752800	-1.39867500
C	3.05777000	0.88879000	-1.80151300
C	4.44882500	0.93874900	-1.90055300
C	2.30735200	0.73400500	-2.96694900
C	5.08045200	0.82004800	-3.13474000
H	5.04590600	1.07556300	-1.00493600
C	2.93469200	0.62415900	-4.20380400
H	1.22684200	0.70990400	-2.91195500
C	4.32347700	0.66191500	-4.29124800
H	6.16154100	0.86091400	-3.19287300
H	2.33816000	0.50872300	-5.10104600
H	4.81133600	0.57610300	-5.25467600
H	3.13255400	-0.93320100	0.24980800
K	-1.21367700	0.27100700	-0.92012800

K⁺ / 2-Ph-18c6_c5

O	1.28308800	-1.47248700	-0.03340100
O	1.96238100	0.82898000	-1.43350300
O	0.16953600	3.05036400	-1.35846900
O	-2.51207900	0.75508500	2.02548600
O	-0.71310400	-1.46961000	1.95007200
O	-1.68617500	3.19173300	0.80063800
C	2.53178800	-1.41279900	-0.72844300
H	2.73552500	-2.39772200	-1.16898500
C	2.33000600	-0.46137700	-1.90380500
H	1.54241300	-0.85974000	-2.55588000
H	3.26103900	-0.40682100	-2.47955800
C	1.87456700	1.79428700	-2.47886400
H	1.13250400	1.47786600	-3.22258300
H	2.84424400	1.89327800	-2.98134700
C	1.48876700	3.13035700	-1.89442500
H	2.19693900	3.41800000	-1.10791900
H	1.52782700	3.88823400	-2.68632600
C	-0.27727300	4.28385500	-0.80031900
H	-0.27157400	5.06841300	-1.56682600
H	0.39217900	4.59220000	0.01210600
C	-1.68446200	4.11969600	-0.28201500
H	-2.34440700	3.76361100	-1.08270000
H	-2.05231600	5.09539700	0.05781300
C	-2.97897500	3.01198800	1.37480200
H	-3.36072000	3.96888800	1.75128700
H	-3.67781200	2.63784000	0.61641600
C	-2.88624400	2.03784300	2.52290600
H	-2.14899400	2.38530900	3.25729500
H	-3.86329300	1.98037300	3.01784500
C	-2.45264400	-0.24041400	3.04490000
H	-3.43550500	-0.35220600	3.51860600
H	-1.73048800	0.05387700	3.81621500
C	-2.05138500	-1.55965000	2.43335700
H	-2.73157600	-1.81790800	1.61211200
H	-2.12402600	-2.34294800	3.19768100

C	-0.26428000	-2.67636300	1.33792200
H	-0.88844500	-2.90607000	0.46522800
H	-0.34237600	-3.51140200	2.04513600
C	1.18012600	-2.52614700	0.92550100
H	1.51757100	-3.47083200	0.48353600
H	1.80572200	-2.30984600	1.79673600
C	3.71132600	-1.04115000	0.15611100
C	3.60079300	-0.10399300	1.18365700
H	2.64365200	0.35620800	1.39011800
C	4.70836100	0.23821100	1.95246500
H	4.60615500	0.96494300	2.74975500
C	5.94528700	-0.34883900	1.70012000
H	6.80745600	-0.08192000	2.29931400
C	6.06519400	-1.28633000	0.67943900
H	7.02121400	-1.75586200	0.48098400
C	4.95262400	-1.63270000	-0.08160100
H	5.05209800	-2.37425300	-0.86739500
K	-0.31905700	0.79751700	0.26329100

K⁺ / 2-Ph-18c6_c6

O	1.68383100	-0.06127300	-1.20118000
O	1.04592800	1.29232800	1.14111600
O	-1.45179100	0.72926500	2.40993400
O	-2.17479200	-2.97868700	-0.70229800
O	0.32549500	-2.39481100	-1.96904900
O	-2.70308600	-1.76775700	1.82307600
C	2.62956200	0.84689100	-0.63128400
H	3.13824600	1.38206500	-1.44509300
C	1.82439800	1.90252800	0.12044000
H	1.16964900	2.42521800	-0.58824100
H	2.51690500	2.63329200	0.55388500
C	0.34829000	2.64064100	1.94528600
H	-0.33236400	2.83468400	1.32241000
H	1.05975100	2.92394700	2.42428100
C	-0.42554100	1.51287800	3.01579900
H	-0.86774200	2.24938200	3.69773600
H	0.24671800	0.86786700	3.59422700
C	-2.22667500	0.00424400	3.36237800
H	-2.69919600	0.69693000	4.06942500
H	-1.58087400	-0.67790900	3.92868000
C	-3.30430100	-0.77212400	2.64759600
H	-3.95547200	-1.24340400	3.39382500
H	-3.91570000	-0.09712800	2.03588500
C	-3.66030300	-2.56581700	1.13054100
H	-4.32361400	-3.06572200	1.84684700
H	-4.27441000	-1.93327800	0.47754100
C	-2.94300200	-3.61400800	0.31706400
H	-4.21149500	-4.21149500	0.96284100
H	-3.68631800	-4.28357100	-0.13277300
C	-1.47775400	-3.90754900	-1.53019500
H	-2.18972000	-4.58236500	-2.02068400
H	-0.79343800	-4.51175700	-0.92221900
C	-0.70803900	-3.15688100	-2.58789200
H	-1.38147800	-2.49497200	-3.14672500
H	-0.27467700	-3.87775200	-3.29176800
C	1.08544800	-1.63242400	-2.90361900
H	1.50476200	-2.28828600	-3.67655100
H	0.43928400	-0.89367900	-3.39454100
C	2.22185600	-0.94460800	-2.18655700
H	2.87890700	-1.68265100	-1.71704900
H	2.80689900	-0.37784800	-2.92050100
C	3.69281700	0.17681600	0.22563900
C	3.42481300	-0.95306500	0.99816500
H	2.44266300	-1.40571600	0.96819800
C	4.41503800	-1.51505300	1.79787700
H	4.19287400	-2.39558600	2.38909000
C	5.68683600	-0.95104400	1.84024200
H	6.45709100	-1.38950700	2.46317800
C	5.96500900	0.17358300	1.06986100
H	6.95446100	0.61458100	1.08737700
C	4.97475600	0.72742400	0.26449300
H	5.20420400	1.59675200	-0.34323500
K	-0.68317400	-0.73811000	0.13374800