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Combine Effect of Lewis Acidity and Electric Field of Proximal Redox Innocent Metal Ions on Redox Potential of Vanadyl Schiff Base Complexes: Experimental and Theoretical Study

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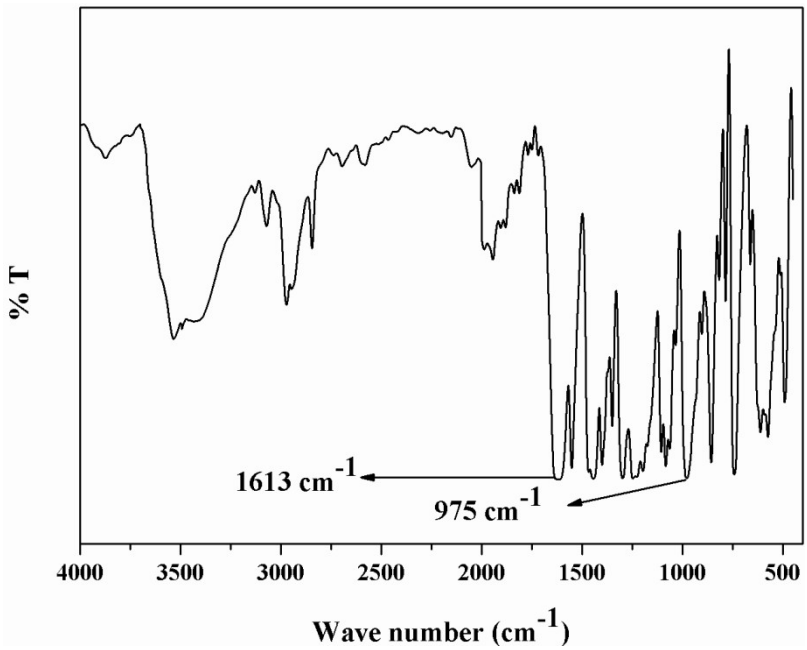

Fig. S1. IR spectrum of complex **1**

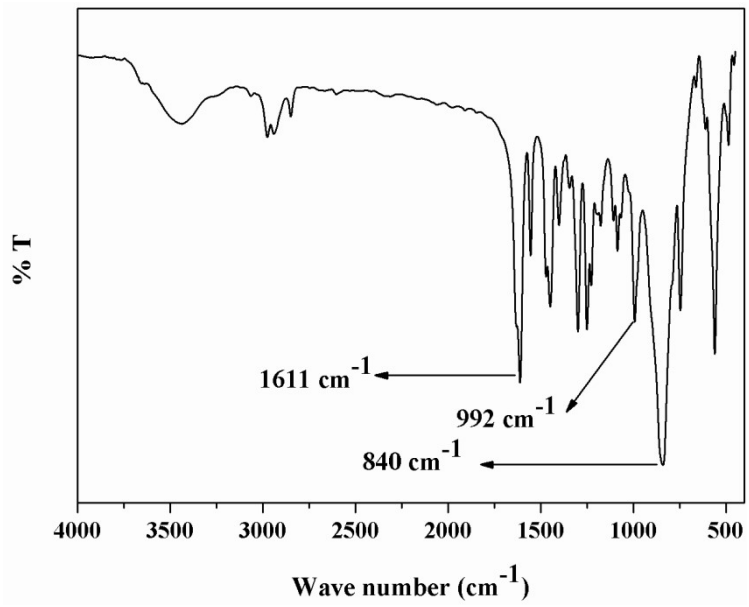

Fig. S2. IR spectrum of complex **1•K**

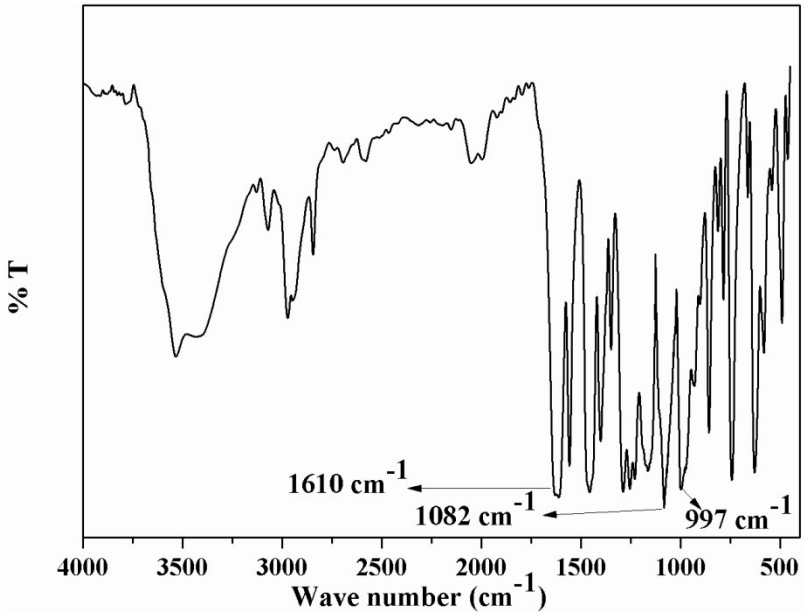

Fig. S3. IR spectrum of complex **1•Ba**

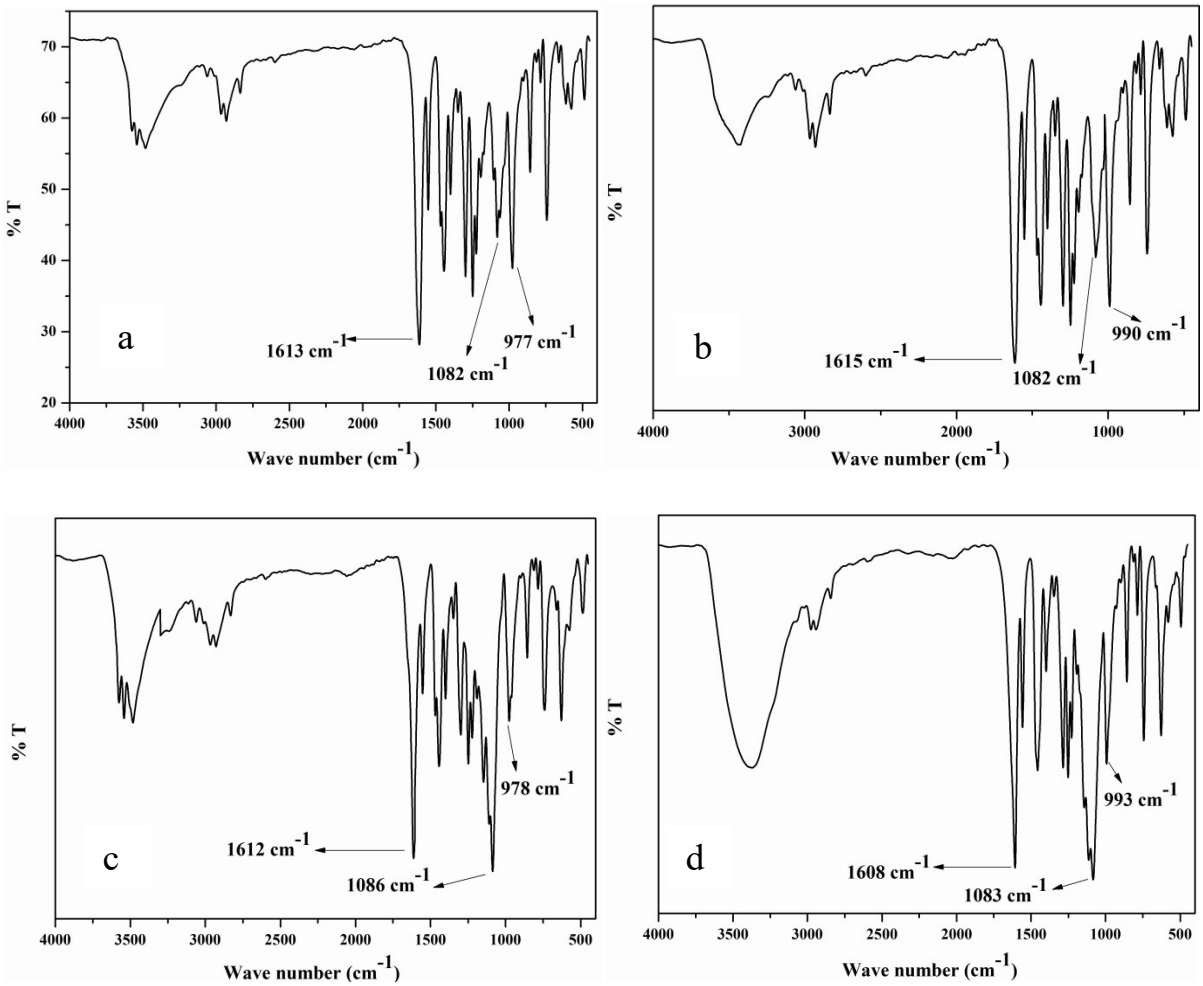

Fig. S4. IR spectra of the compounds (a) **1•Li**, (b) **1•Na**, (c) **1•Mg** and (d) **1•Ca**

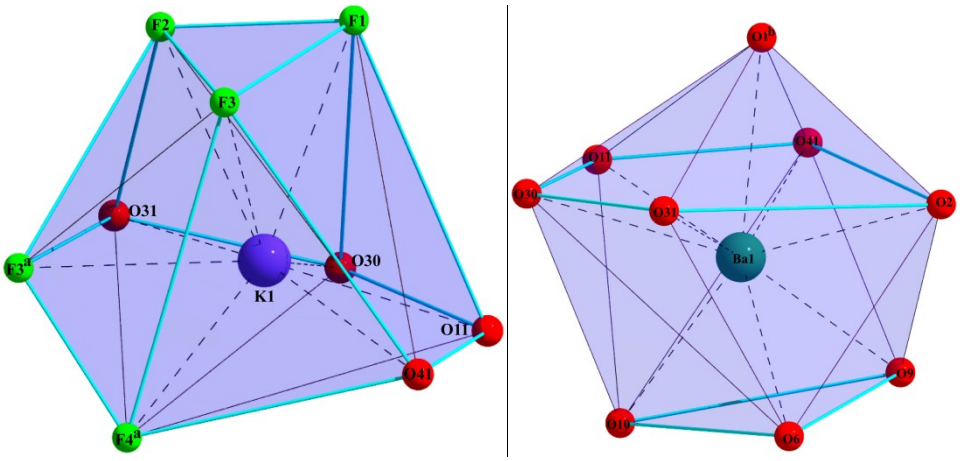

Fig. S5. Polyhedral view of the coordination sphere around the potassium and barium centres for complexes **1•K** (left) and **1•Ba** (right), respectively.

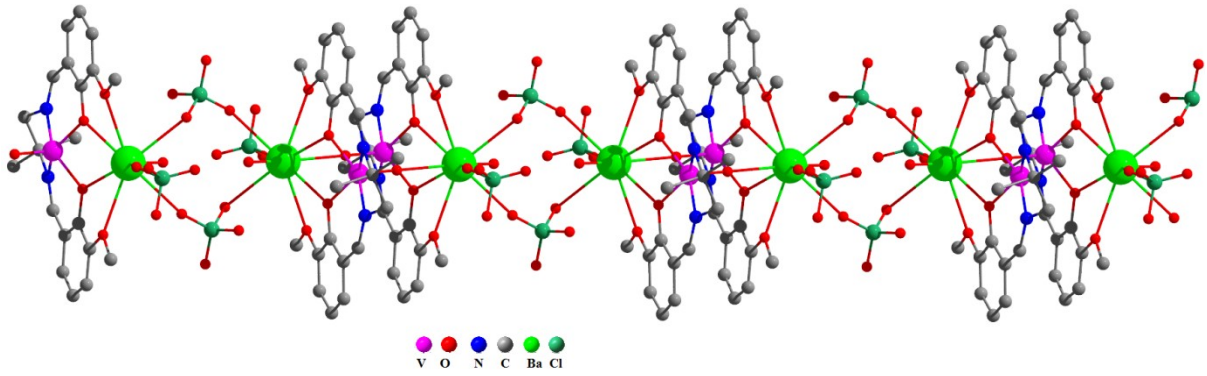

Fig. S6. Polymeric chain of complex **1•Ba.**

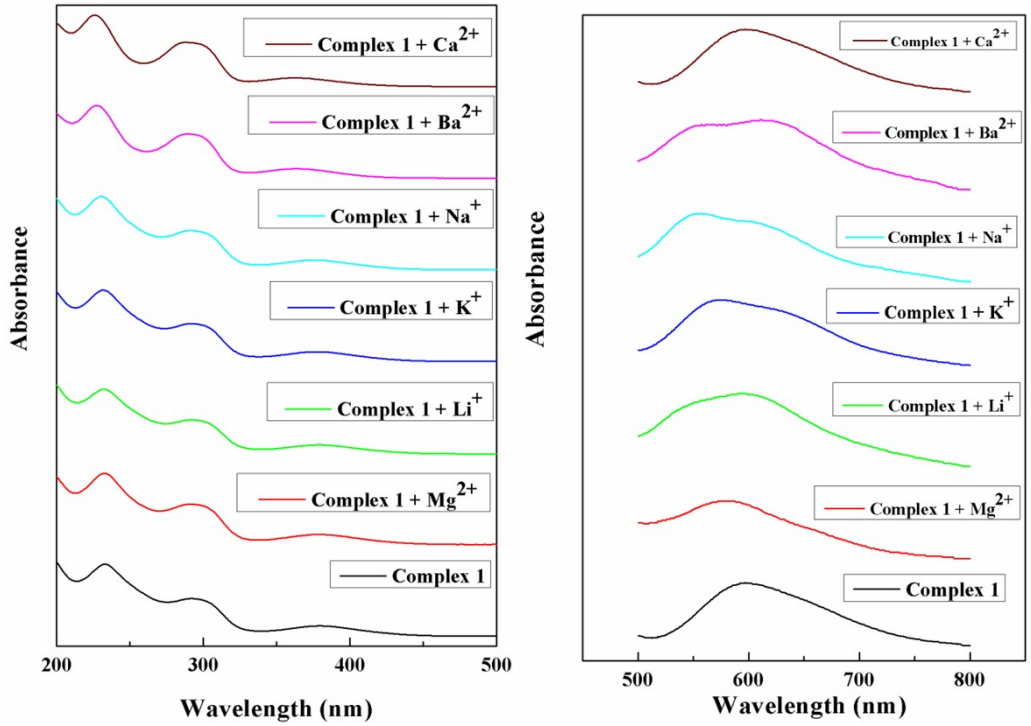

Fig. S7. CT [5 X 10^{-5} M] (left) and d–d [1 X 10^{-3} M] (right) spectra of complex **1** and complex **1•M** [M = Mg^{2+}, Li^{+}, K^{+}, Na^{+}, Ba^{2+} and Ca^{2+}] in acetonitrile solution.

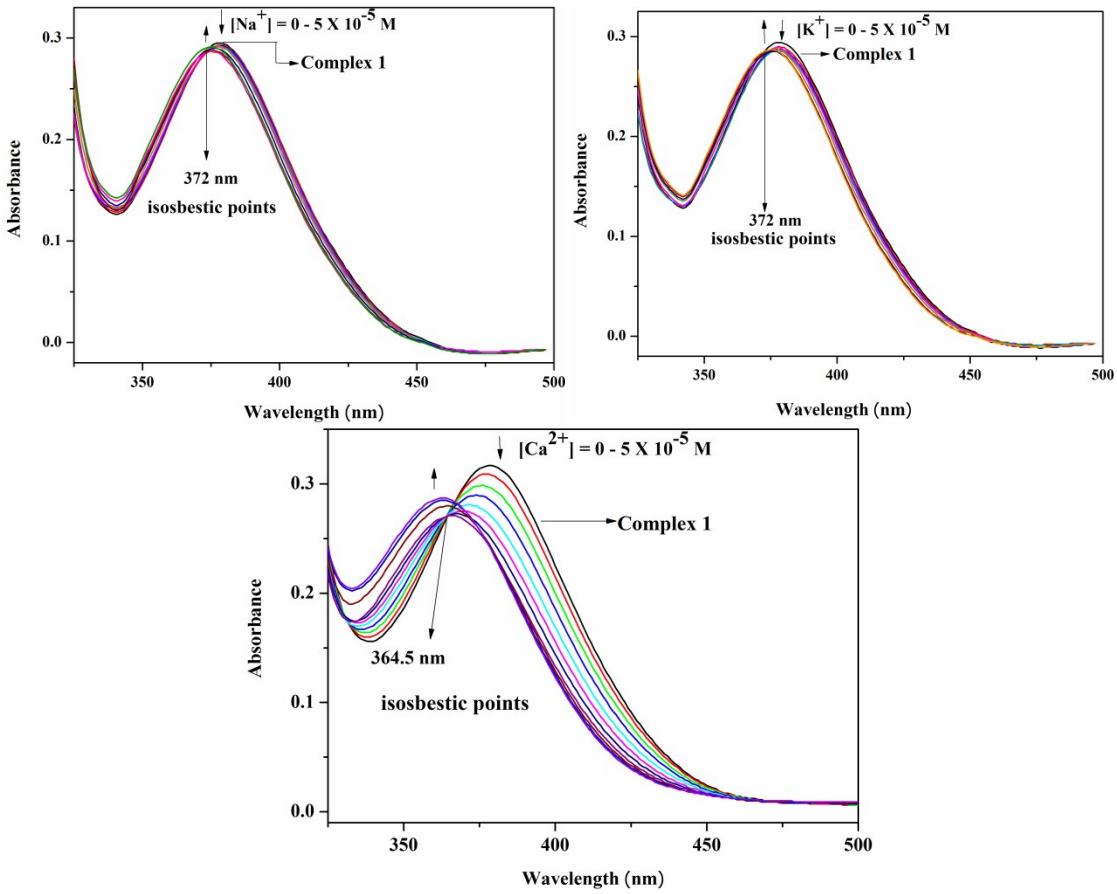

Fig. S8. Spectrophotometric titration of the fixed 5×10^{-5} M concentration of the complex **1** by 5×10^{-3} M respective metal ions in acetonitrile. The range of concentration for metal ions in the figure, indicates its final concentration in solution.

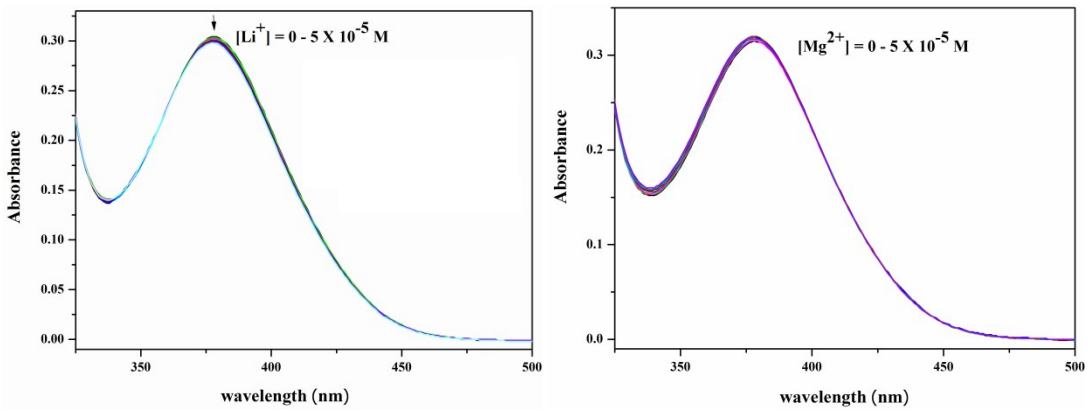

Fig. S9. Spectrophotometric titration of the fixed 5×10^{-5} M concentration of the complex **1** by 5×10^{-3} M respective metal ions in acetonitrile. The range of concentration for metal ions in the figure, indicates its final concentration in solution.

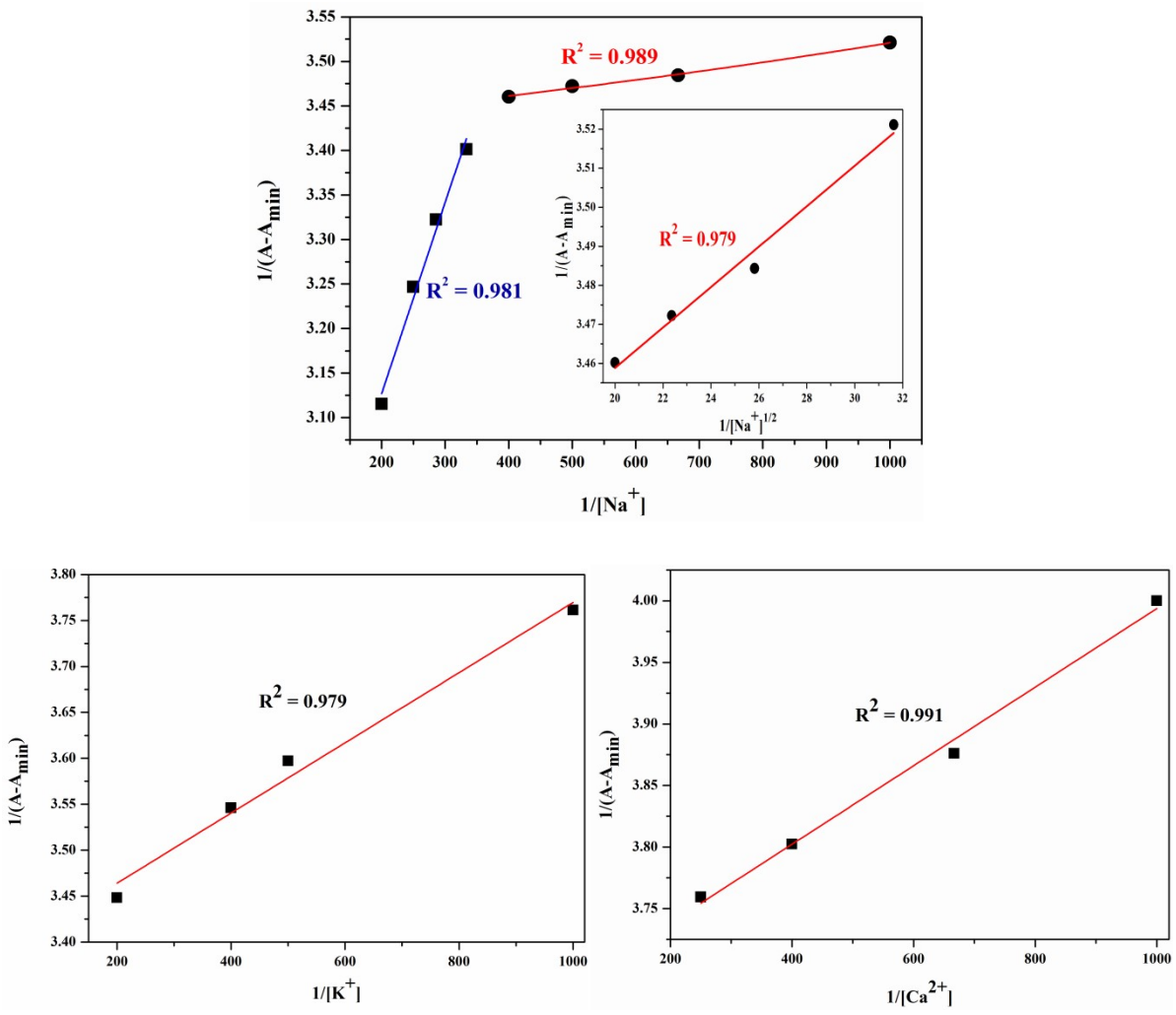

Fig. S10. Benesi−Hildebrand plot for the associative interaction of complex **1** with Na^+ (upper panel), K^+ (upper panel, left) and Ca^{2+} (lower panel, right) in acetonitrile.

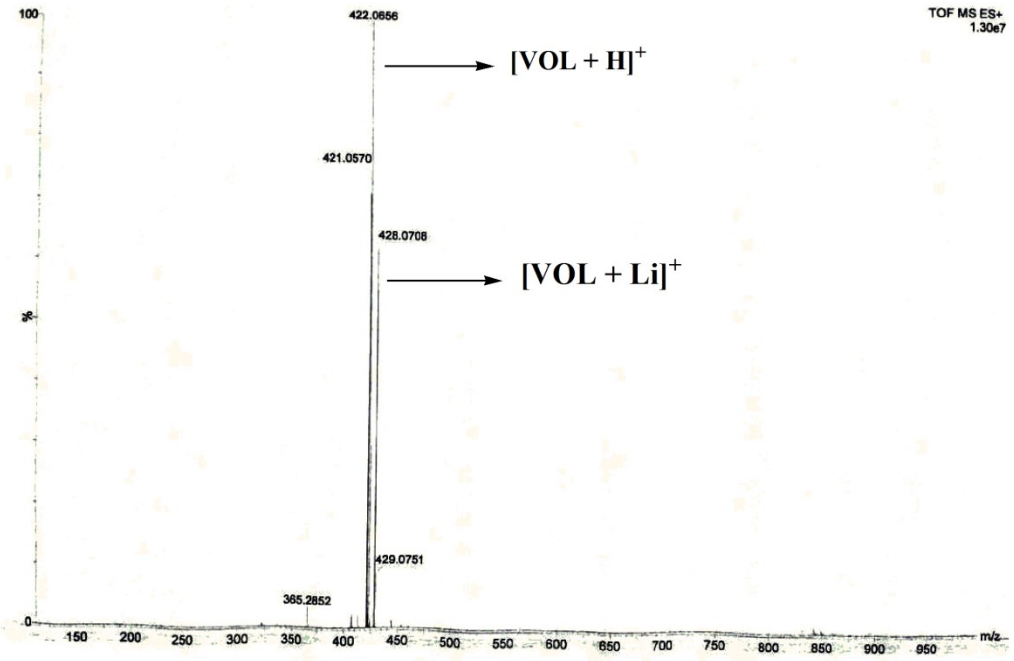

Fig. S11. Representative ESI mass spectrum of complex **1** and $LiClO_4$ mixture in acetonitrile.

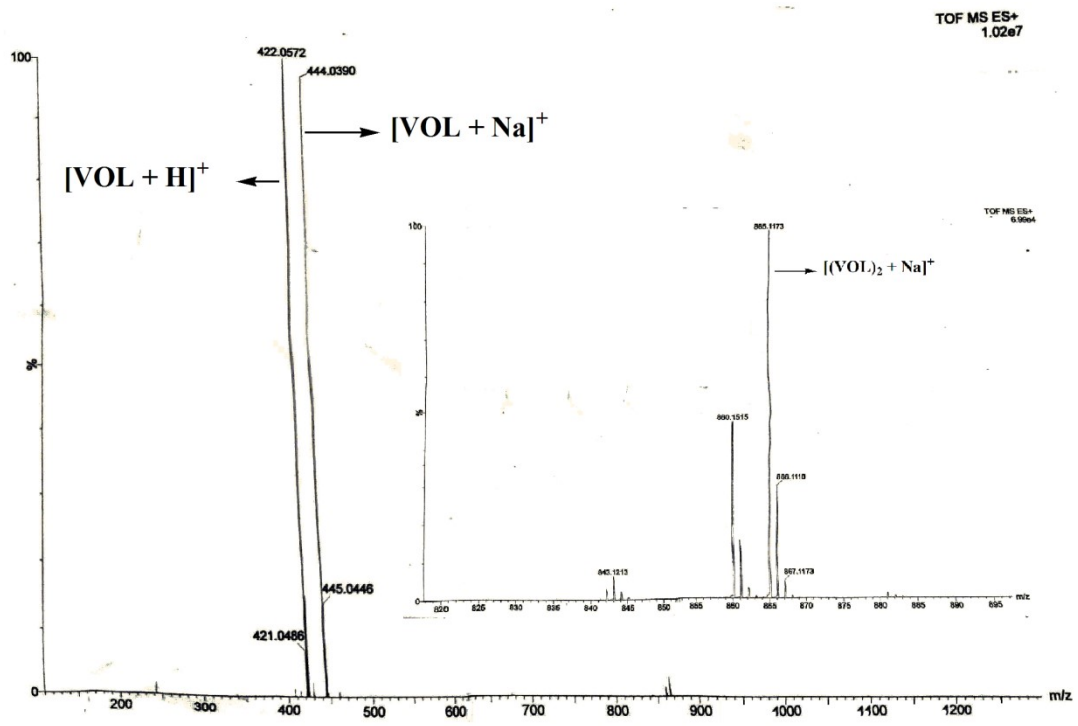

Fig. S12. Representative ESI mass spectrum of complex **1** and $NaBF_4$ mixture in acetonitrile.

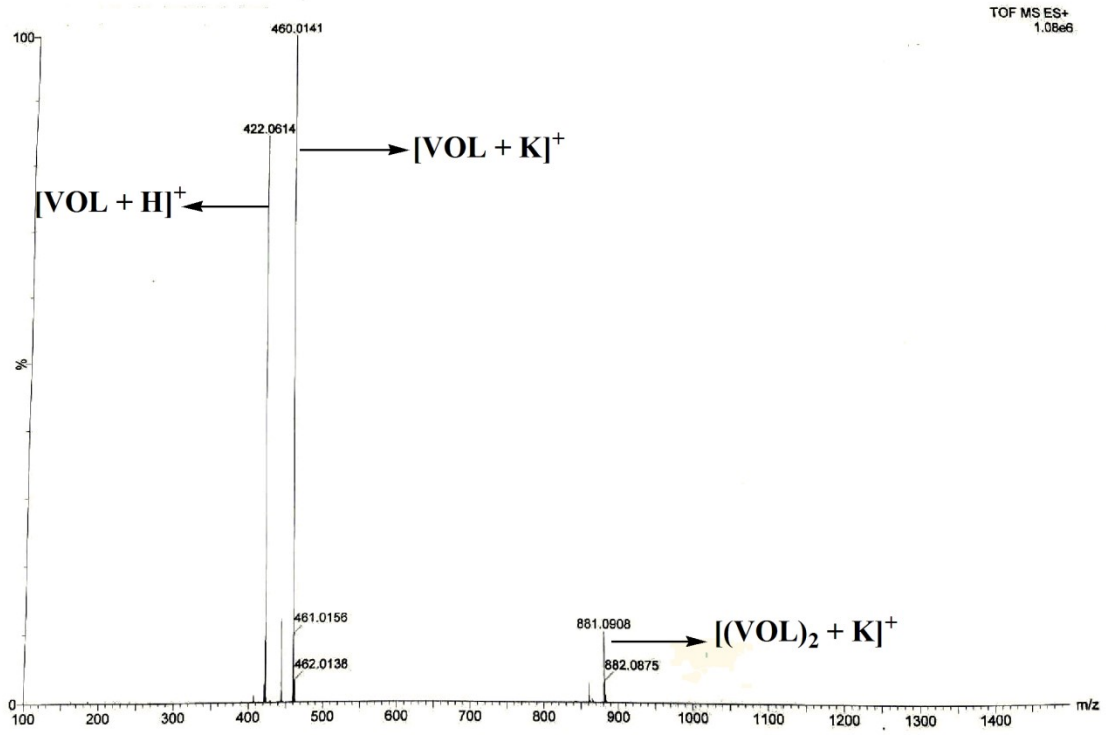

Fig. S13. Representative ESI mass spectrum of complex **1** and KPF_6 mixture in acetonitrile.

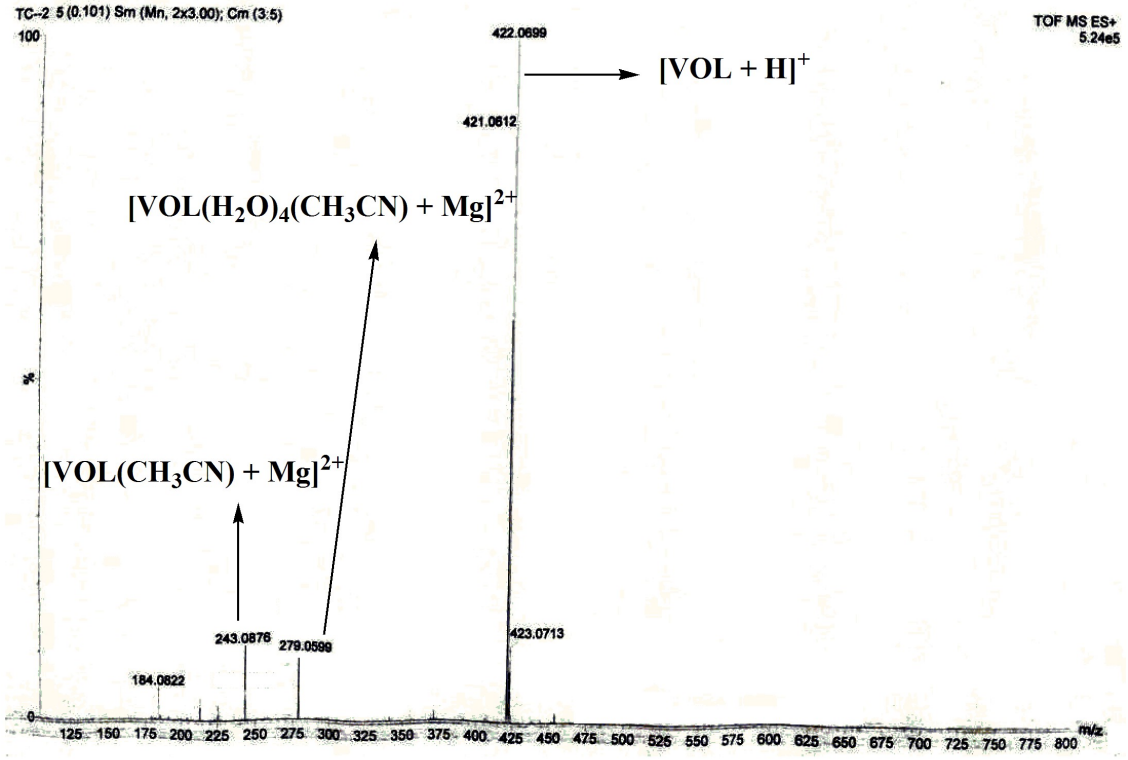

Fig. S14. Representative ESI mass spectrum of complex **1** and $Mg(ClO_4)_2$ mixture in acetonitrile.

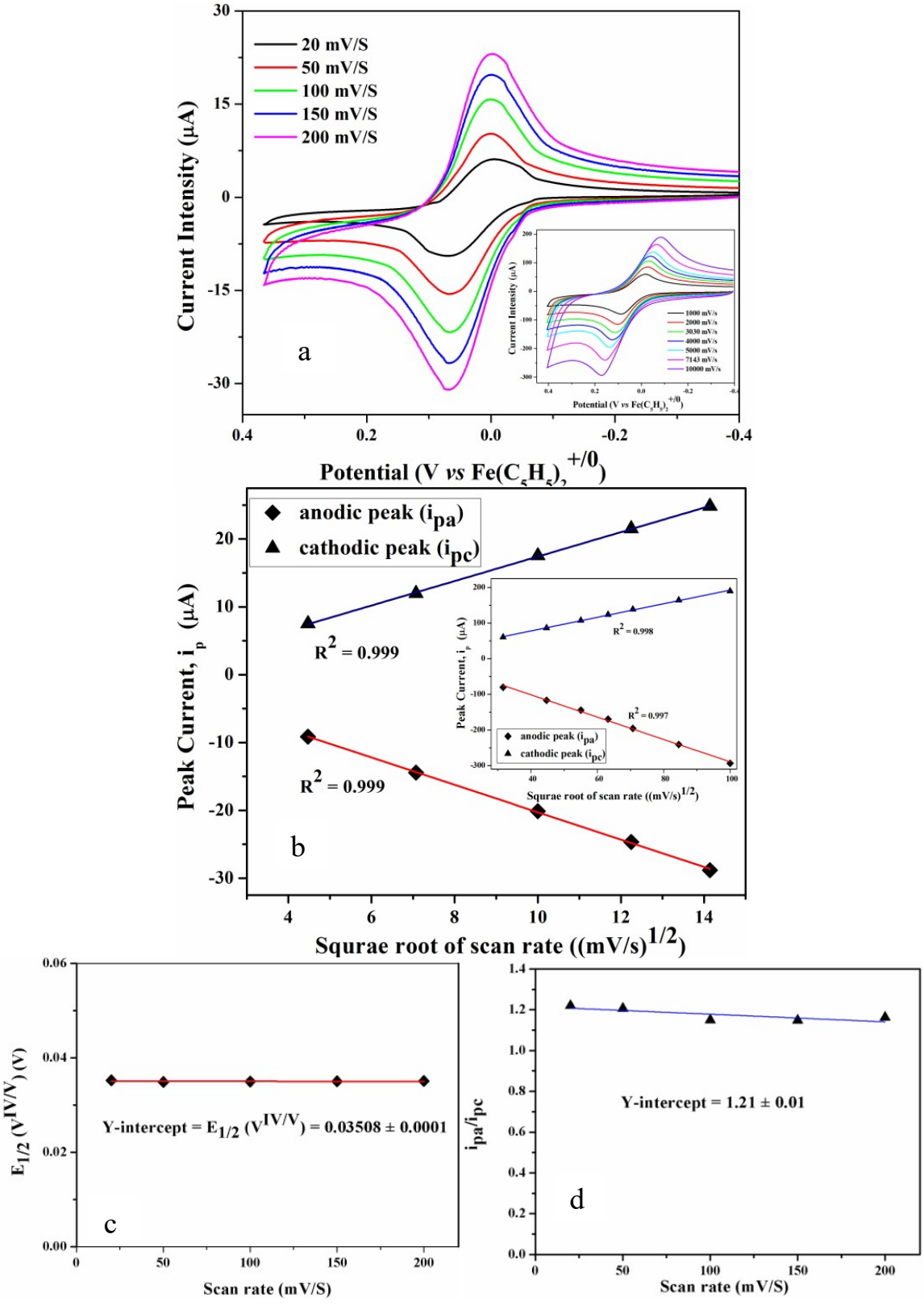

Fig. S15. Cyclic voltammograms data of complex **1** (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1**. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

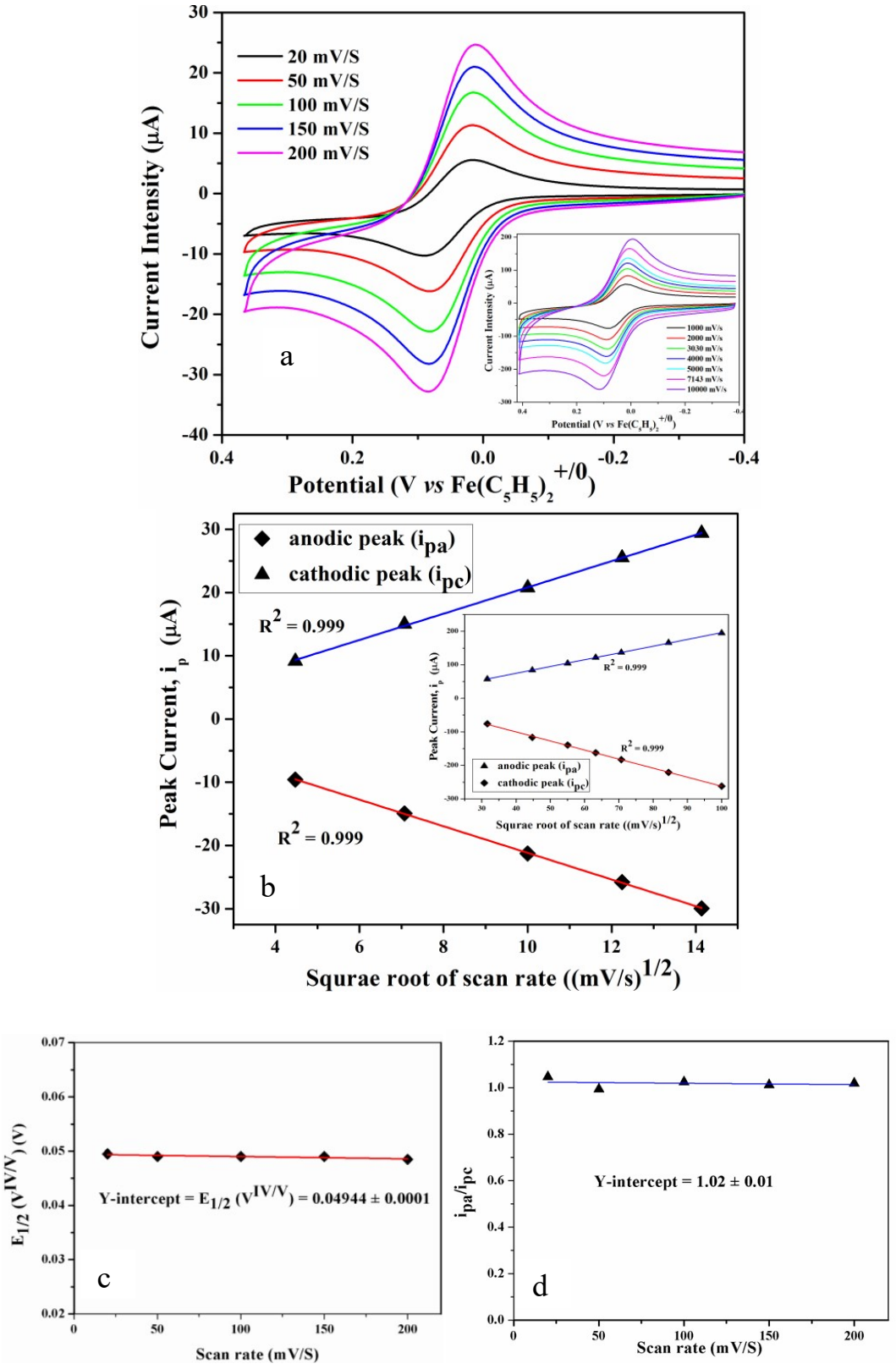

Fig. S16. Cyclic voltammograms data of complex **1** + Li^+ (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1** + Li^+. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

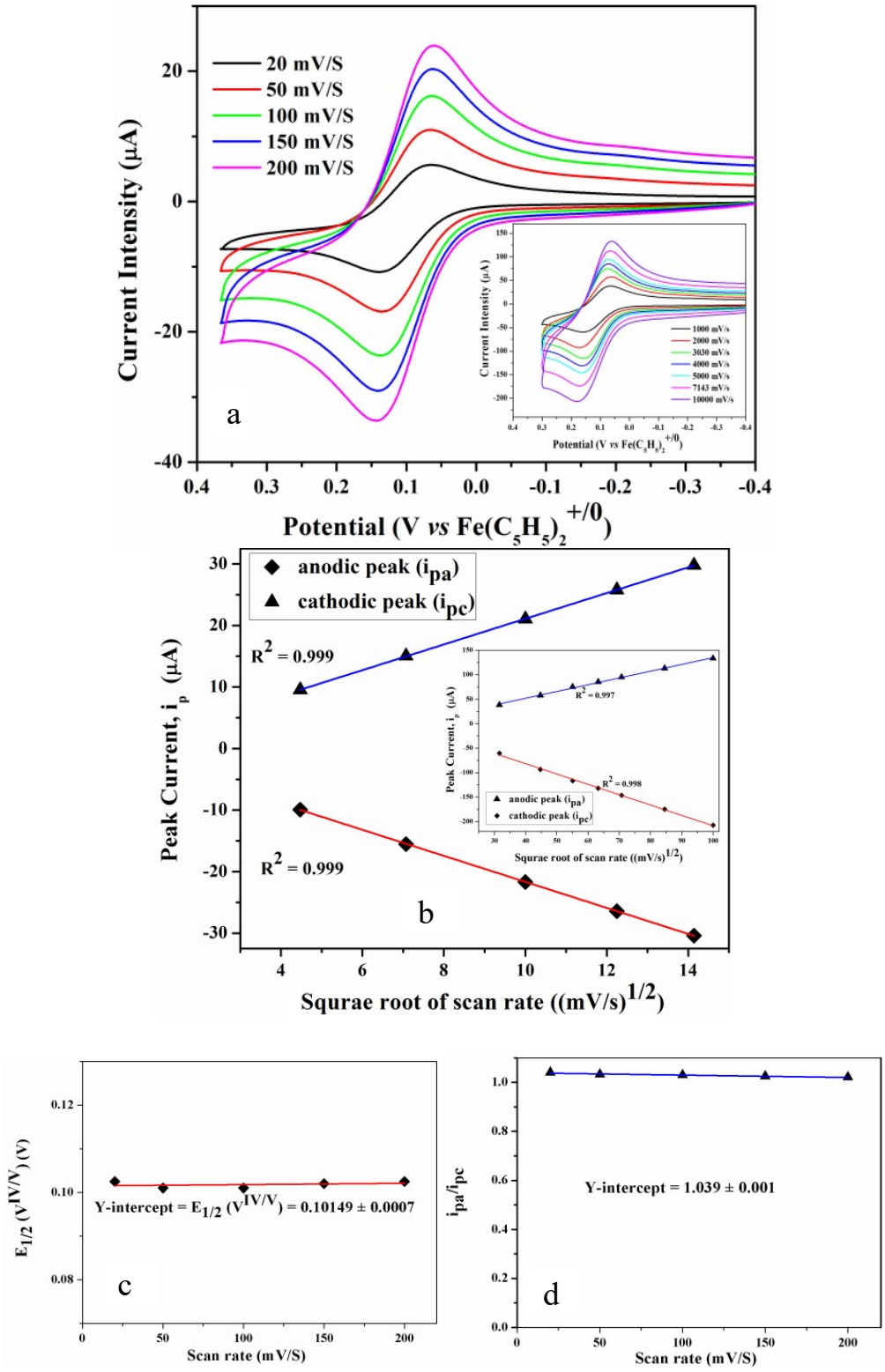

Fig. S17. Cyclic voltammograms data of complex **1**+ Na^+ (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1** + Na^+. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

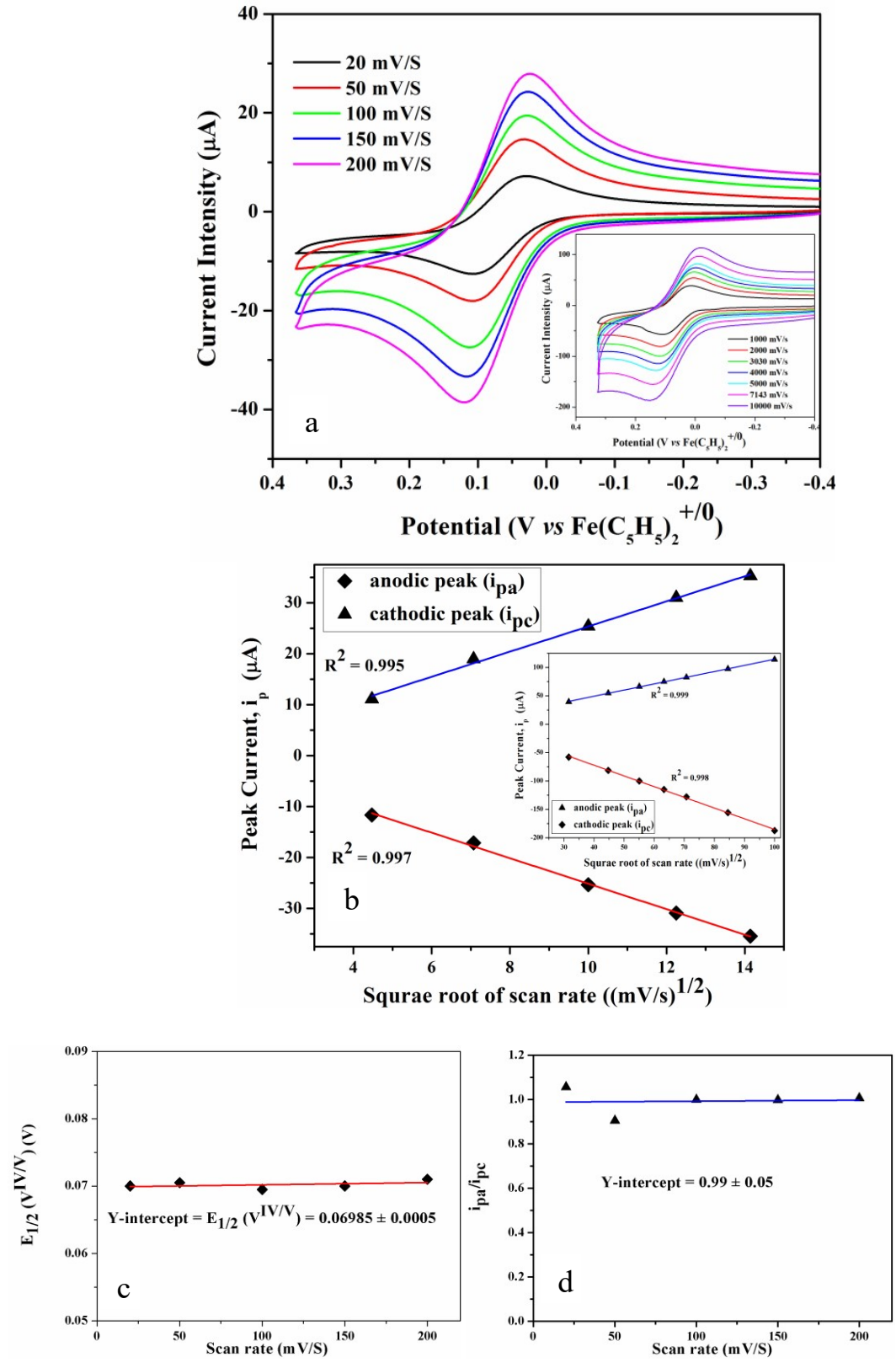

Fig. S18. Cyclic voltammograms data of complex **1**+ $\mathbf{K}^+$ (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1** + $\mathbf{K}^+$. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

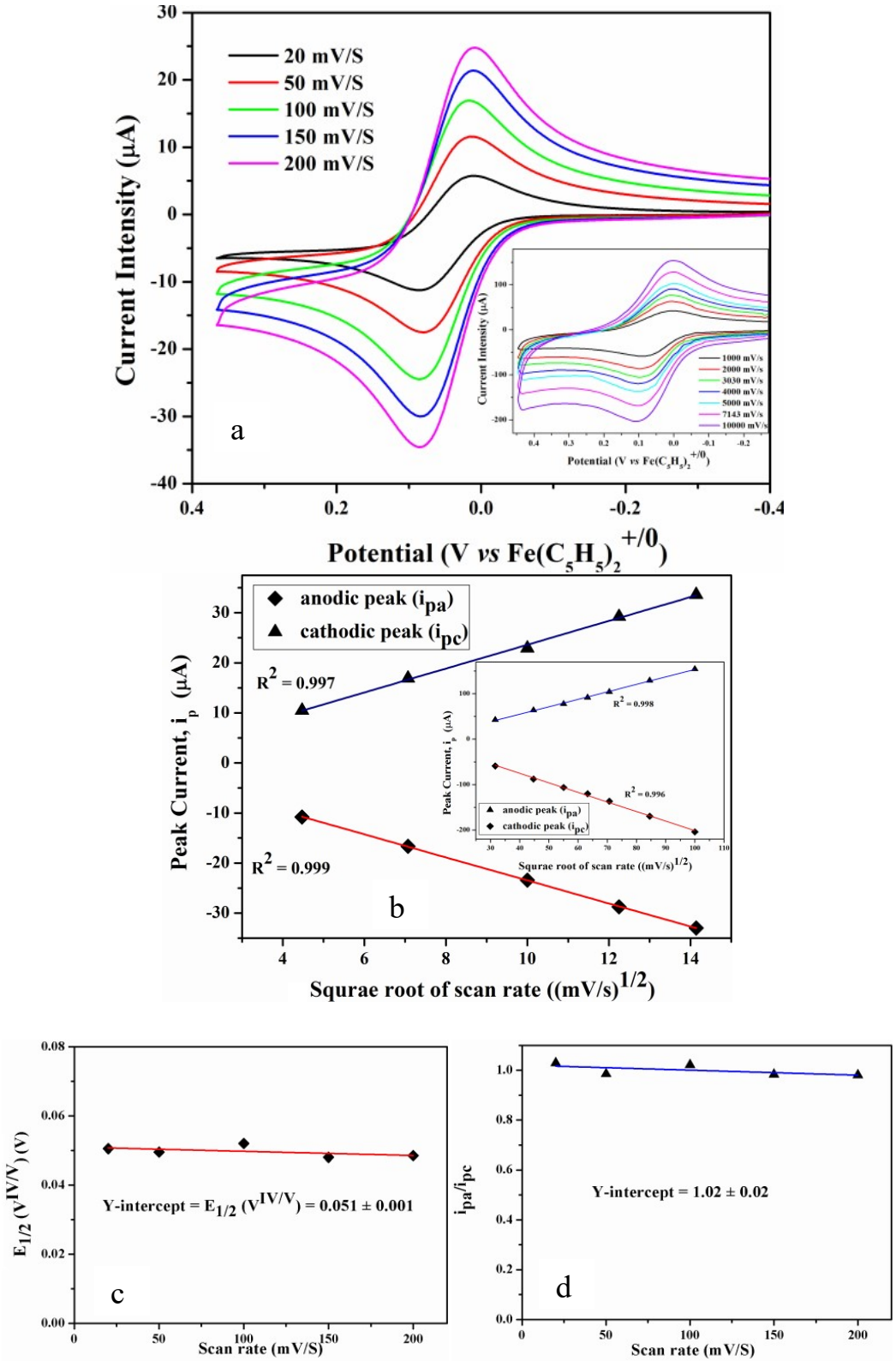

Fig. S19. Cyclic voltammograms data of complex **1**+ $\mathbf{Mg^{2+}}$ (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1** + $\mathbf{Mg^{2+}}$. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

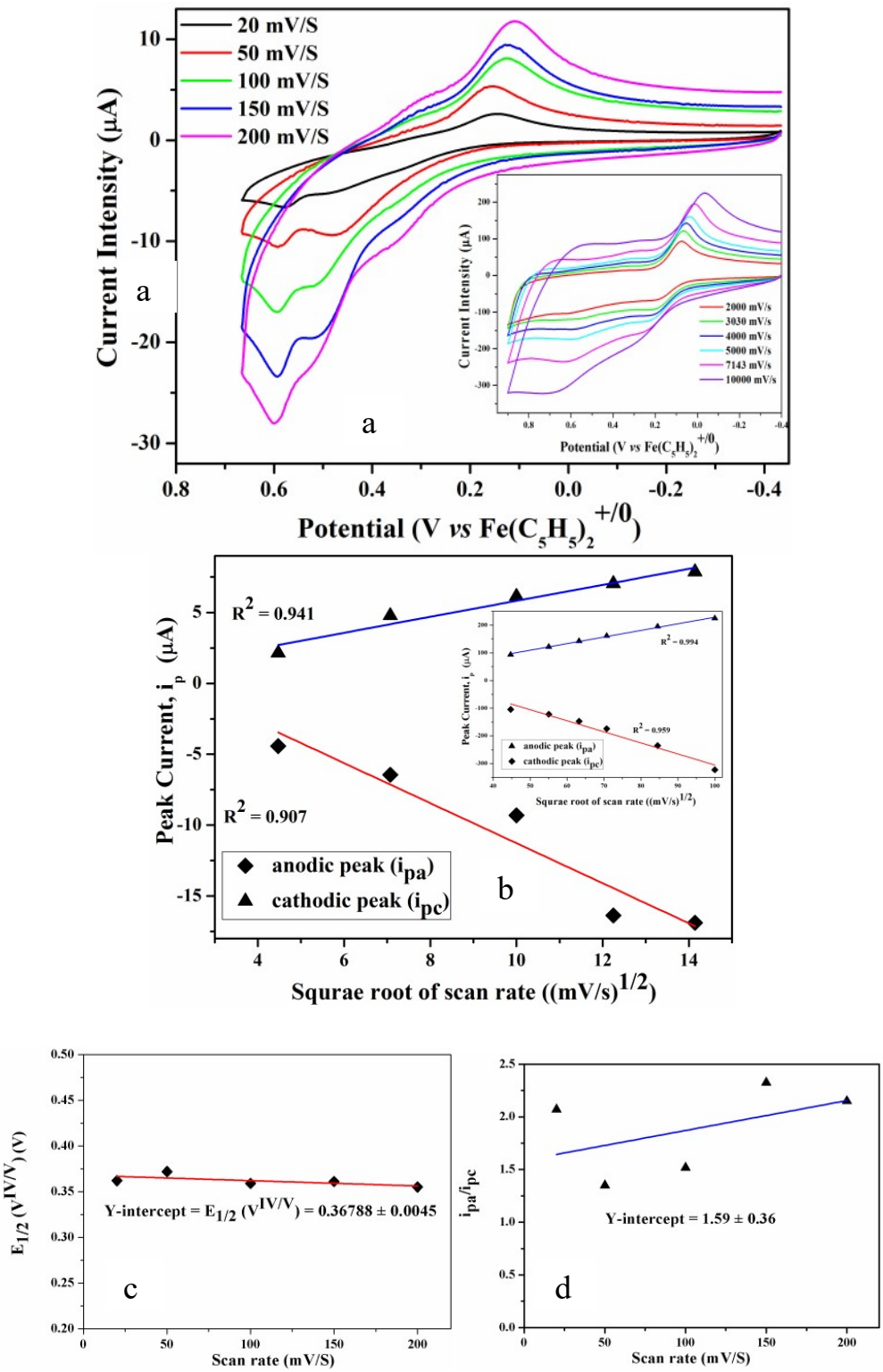

Fig. S20. Cyclic voltammograms data of complex **1**+ $\mathbf{Ca^{2+}}$ (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1** + $\mathbf{Ca^{2+}}$. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

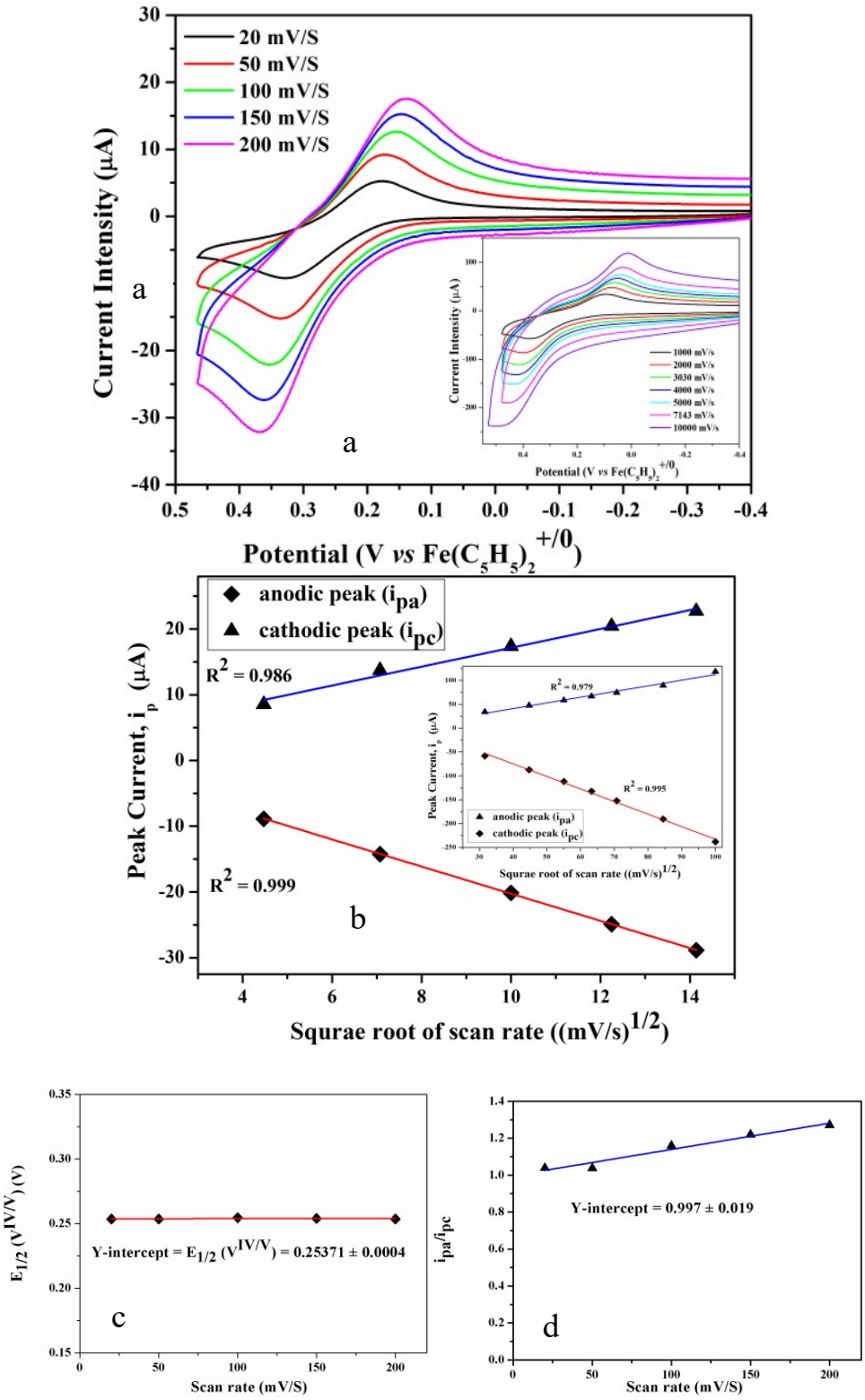

Fig. S21. Cyclic voltammograms data of complex **1**+ **Ba**$^{2+}$ (10^{-3} M) in presence of 0.1 M TBAP in acetonitrile (insert: at high scan rate). (a) scan rate dependence data for complex **1** + **Ba**$^{2+}$. (b) plot of peak current density *vs*. (scan rate)$^{1/2}$. (c) plot of $E_{1/2}$ value *vs*. scan rate. (d) plot of ratio of anodic to cathodic peak currents *vs*. scan rate.

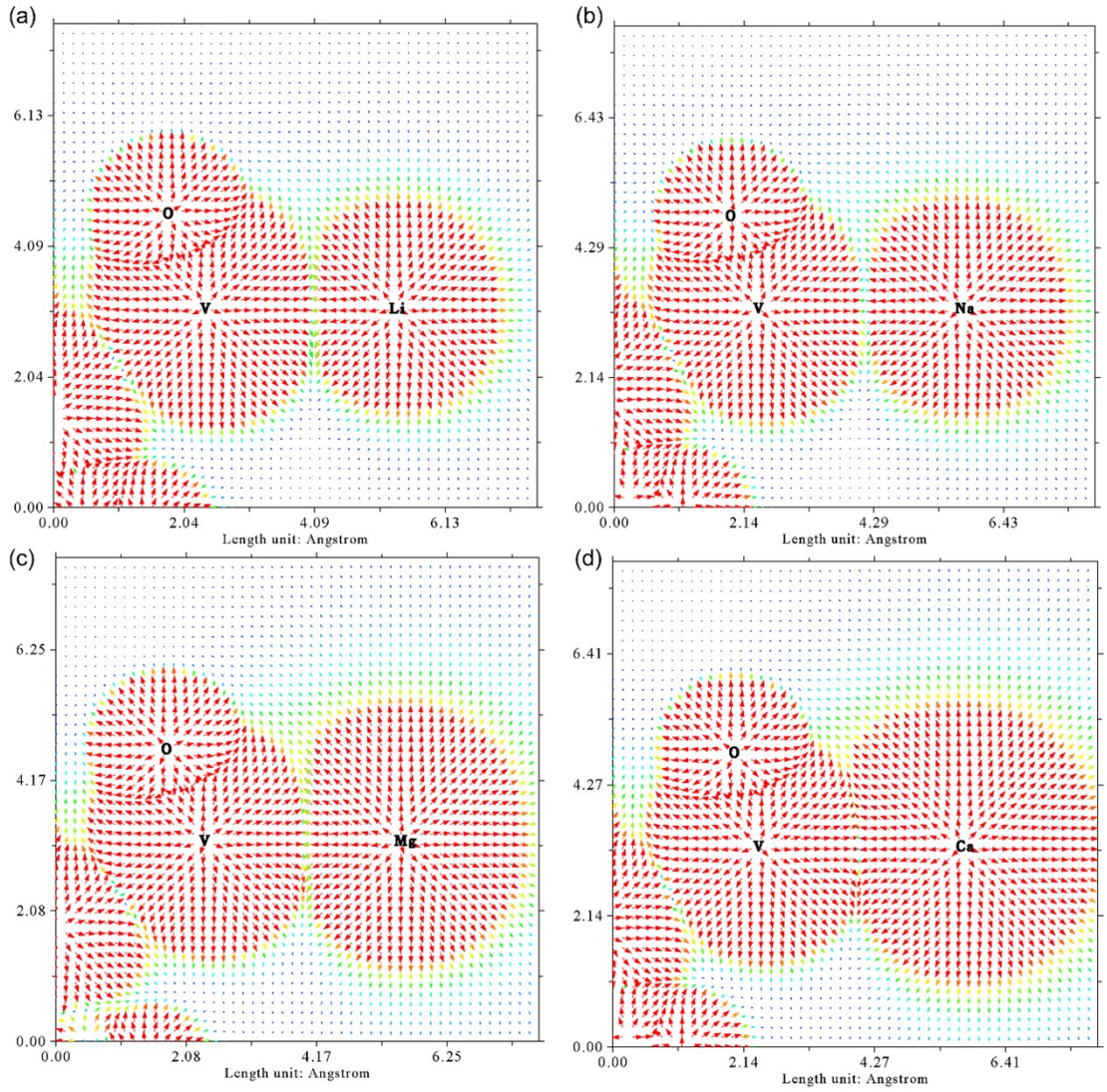

Fig. S22. Vector electric field 2D maps of Li^{+} (a), Na^{+} (b), Mg^{2+} (c) and Ca^{2+} (d) at the RI-BP86-D3/def2-TZVP (COSMO=acetonitrile) level of theory.

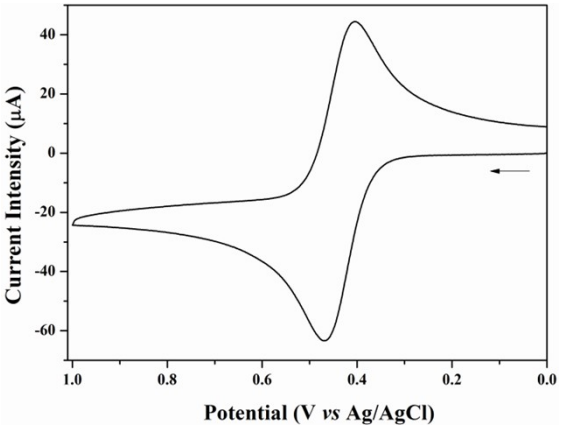

Fig. S23. Cyclic voltammograms of ferrocene (10^{-3} M) at 100 mV/s in acetonitrile.

Table S1. Selected bond lengths (Å) and bond angles (°) of Complex **1**

Bond lengths (Å)		**Bond angles (°)**	
V(1) – O(1)	1.598(2)	O(1) – V(1) – O(11)	111.63(10)
V(1) – O(11)	1.922(2)	O(1) – V(1) – O(30)	104.54(10)
V(1) – O(30)	1.939(2)	O(1) – V(1) – N(19)	103.45(10)
V(1) – N(19)	2.073(2)	O(1) – V(1) – N(22)	109.22(10)
V(1) – N(22)	2.054(2)	O(11) – V(1) – O(30)	88.36(9)
		O(11) – V(1) – N(19)	87.86(9)
		O(11) – V(1) – N(22)	138.82(9)
		O(30) – V(1) – N(19)	151.14(9)
		O(30) – V(1) – N(22)	86.44(9)
		N(19) – V(1) – N(22)	77.82(9)

Table S2. Geometrical features of hydrogen bonding interactions (distances (Å) and angles (°)) of Complex **1**

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	∠D–H···A (°)
O(51) – H(51A) ··· O(30)	0.8700	2.4600	3.113(3)	133.00
O(51) – H(51A) ··· O(31)	0.8700	2.1500	2.953(3)	152.00
O(51) – H(51B) ··· O(11)	0.8700	2.3300	3.109(3)	149.00
O(51) – H(51B) ··· O(41)	0.8700	2.1700	2.897(3)	141.00
O(52^{k}) – H(52A^{k}) ··· O(51)	0.8700	2.0600	2.905(4)	164.00
O(52) – H(52B) ··· O(51)	0.8700	2.0700	2.939(4)	176.00

^{k} = 2-x,1-y,2-z

Table S3. SHAPE analysis for the potassium and barium centres in complexes **1•K** and **1•Ba**, respectively (the lowest values are indicated in bold).

Geometry	Symmetry	**1•K**	**1•Ba**
Enneagon	D9h	34.402	32.563
Octagonal pyramid	C8v	22.764	22.968
Heptagonal bipyramid	D7h	16.056	12.368
Johnson triangular cupola J3	C3v	**8.626**	14.450
Capped cube J8	C4v	9.779	9.022
Spherical-relaxed capped cube	C4v	9.124	7.108
Capped square antiprism J10	C4v	12.233	4.657
Spherical capped square antiprism	C4v	11.424	3.784

Tricapped trigonal prism J51	D3h	12.586	5.876
Spherical tricapped trigonal prism	D3h	12.205	4.869
Tridiminished icosahedron J63	C3v	11.164	13.735
Hula-hoop	C2v	11.366	6.433
Muffin	Cs	9.730	**2.290**

Table S4. Selected bond lengths (Å) and bond angles (°) of Complex **1•K**

Bond lengths (Å)			
V(1) – O(1)	1.598(3)	K(1) – O(31)	2.788(3)
V(1) – O(11)	1.926(2)	K(1) – O(41)	2.815(3)
V(1) – O(30)	1.946(2)	K(1) – F(3^a)	3.008(3)
V(1) – N(19)	2.054(3)	K(1) – F(4^a)	2.777(3)
V(1) – N(22)	2.053(3)	P(1) – F(1)	1.591(3)
K(1) – F(1)	2.983(3)	P(1) – F(2)	1.607(3)
K(1) – F(2)	2.884(3)	P(1) – F(3)	1.608(3)
K(1) – F(3)	2.871(3)	P(1) – F(4)	1.604(3)
K(1) – O(11)	2.705(3)	P(1) – F(5)	1.586(3)
K(1) – O(30)	2.700(2)	P(1) – F(6)	1.564(3)
Bond angles (°)			
O(1) – V(1) – O(11)	108.15(12)	F(2) – K(1) – F(3^a)	67.45(8)
O(1) – V(1) – O(30)	110.44(12)	F(2) – K(1) – F(4^a)	112.78(8)
O(1) – V(1) – N(19)	105.52(15)	F(3) – K(1) – O(11)	120.34(9)
O(1) – V(1) – N(22)	105.46(13)	F(3) – K(1) – O(30)	143.02(8)
O(11) – V(1) – O(30)	85.79(10)	F(3) – K(1) – O(31)	113.04(9)
O(11) – V(1) – N(19)	88.07(12)	F(3) – K(1) – O(41)	82.98(8)
O(11) – V(1) – N(22)	145.96(13)	F(3) – K(1) – F(3^a)	64.54(9)
O(30) – V(1) – N(19)	143.65(14)	F(3) – K(1) – F(4^a)	91.77(8)
O(30) – V(1) – N(22)	87.54 (12)	O(11) – K(1) – O(30)	58.37(7)
N(19) – V(1) – N(22)	77.90(15)	O(11) – K(1) – O(31)	115.66(7)
F(1) – K(1) – F(2)	44.54(7)	O(11) – K(1) – O(41)	56.59(7)
F(1) – K(1) – F(3)	45.02(7)	F(3^a) – K(1) – O(11)	159.43(8)
F(1) – K(1) – O(11)	90.73(7)	F(4^a) – K(1) – O(11)	113.91(8)
F(1) – K(1) – O(30)	99.62(7)	O(30) – K(1) – O(31)	57.49(7)
F(1) – K(1) – O(31)	103.97(8)	O(30) – K(1) – O(41)	113.84(7)
F(1) – K(1) – O(41)	92.07(8)	F(3^a) – K(1) – O(30)	131.57(8)
F(1) – K(1) – F(3^a)	103.39(7)	F(4^a) – K(1) – O(30)	123.65(8)
F(1) – K(1) – F(4^a)	136.55(8)	O(31) – K(1) – O(41)	162.65(8)
F(2) – K(1) – F(3)	45.68(8)	F(3^a) – K(1) – O(31)	75.75(8)
F(2) – K(1) – O(11)	131.46(8)	F(4^a) – K(1) – O(31)	96.87(9)
F(2) – K(1) – O(30)	104.25(8)	F(3^a) – K(1) – O(41)	107.29(8)

F(2) – K(1) – O(31)	70.44(7)	F(4[a]) – K(1) – O(41)	75.18(9)
F(2) – K(1) – O(41)	126.77(8)	F(3[a]) – K(1) – F(4[a])	45.86(8)

[a] = 1-x,1-y,1-z

Table S5. Selected bond lengths (Å) and bond angles (°) of Complex **1•Ba**

Bond lengths (Å)			
V(1) – O(1)	1.598(8)	Ba(1) – O(9)	2.787(14)
V(1) – O(11)	1.923(6)	Ba(1) – O(10)	2.735(15)
V(1) – O(30)	1.924(6)	Ba(1) – O(11)	2.743(5)
V(1) – N(19)	2.039(10)	Ba(1) – O(30)	2.749(6)
V(1) – N(22)	2.046(9)	Ba(1) – O(31)	2.850(7)
Ba(1) – O(2)	2.792(12)	Ba(1) – O(41)	2.852(7)
Ba(1) – O(6)	2.872(13)	Ba(1) – O(1[b])	2.686(8)
Bond angles (°)			
O(1) – V(1) – O(11)	109.0(3)	O(6) – Ba(1) – O(41)	146.0(3)
O(1) – V(1) – O(30)	110.8(3)	O(1[b]) – Ba(1) – O(6)	126.6(4)
O(1) – V(1) – N(19)	105.0(4)	O(9) – Ba(1) – O(10)	76.6(4)
O(1) – V(1) – N(22)	102.9(4)	O(9) – Ba(1) – O(11)	107.0(3)
O(11) – V(1) – O(30)	84.9(3)	O(9) – Ba(1) – O(30)	154.1(3)
O(11) – V(1) – N(19)	88.7(3)	O(9) – Ba(1) – O(31)	144.3(3)
O(11) – V(1) – N(22)	147.9(4)	O(9) – Ba(1) – O(41)	66.6(3)
O(30) – V(1) – N(19)	143.8(4)	O(1[b]) – Ba(1) – O(9)	121.2(3)
O(30) – V(1) – N(22)	87.6(3)	O(10) – Ba(1) – O(11)	72.0(3)
N(19) – V(1) – N(22)	79.2(4)	O(10) – Ba(1) – O(30)	79.0(3)
O(2) – Ba(1) – O(6)	72.9(4)	O(10) – Ba(1) – O(31)	112.2(4)
O(2) – Ba(1) – O(9)	76.6(4)	O(10) – Ba(1) – O(41)	97.6(4)
O(2) – Ba(1) – O(10)	145.1(4)	O(1[b]) – Ba(1) – O(10)	147.2(3)
O(2) – Ba(1) – O(11)	137.9(3)	O(11) – Ba(1) – O(30)	56.42(18)
O(2) – Ba(1) – O(30)	129.3(3)	O(11) – Ba(1) – O(31)	108.60(18)
O(2) – Ba(1) – O(31)	79.0(3)	O(11) – Ba(1) – O(41)	55.24(18)
O(2) – Ba(1) – O(41)	91.8(3)	O(1[b]) – Ba(1) – O(11)	76.2(2)
O(1[b]) – Ba(1) – O(2)	67.4(3)	O(30) – Ba(1) – O(31)	55.40(18)
O(6) – Ba(1) – O(9)	80.3(4)	O(30) – Ba(1) – O(41)	108.67(18)
O(6) – Ba(1) – O(10)	81.0(4)	O(1[b]) – Ba(1) – O(30)	77.0(2)
O(6) – Ba(1) – O(11)	149.0(3)	O(31) – Ba(1) – O(41)	140.1(2)
O(6) – Ba(1) – O(30)	104.4(3)	O(1[b]) – Ba(1) – O(31)	70.8(2)
O(6) – Ba(1) – O(31)	67.8(3)	O(1[b]) – Ba(1) – O(41)	69.8(2)

[b] = 1-x,1-y,1-z

Table S6. Binding constant of metal ions towards complex **1**.

Metal ions interacts with complex **1**	Binding constant (K_b) for 1:1 complexation in acetonitrile
K^+	0.88 X 10^4
Ca^{2+}	1.15 X 10^4
Ba^{2+}	1.46 X 10^4

Table S7. Experimental and theoretical (in parenthesis) distances of complexes **1•K** and **1•Ba**

	V···M	V-N	V=O
1•K	3.722 (3.983)	2.054,2.053 (2.046, 2.066)	1.598 (1.610)
1•Ba	3.829 (3.797)	2.039, 2.040 (2.038, 2.056)	1.598 (1.602)

Table S8. Crystallographic data and structure refinement parameters of complexes **1**, **1•K and 1•Ba.**

Complex	**1**	**1•K**	**1•Ba**
Chemical formula	$C_{20}H_{22}N_2O_5V$, $2(H_2O)$	$C_{40}H_{44}F_{12}K_2N_4O_{10}P_2V_2$	$C_{20}H_{22}BaCl_2N_2O_{14}V$
Formula weight	457.37	1210.81	773.57
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$I2/a$	$P\bar{1}$
a(Å)	10.1320(15)	24.8898(12)	11.5816(4)
b (Å)	19.209(2)	8.4307(4)	12.2757(4)
c(Å)	10.8529(15)	25.4214(10)	12.4432(4)
α (°)	90	90	61.585(1)
β (°)	105.233(5)	100.290(4)	62.339(1)
γ (°)	90	90	71.137(1)
V (Å^3)	2038.0(5)	5248.6(4)	1366.16(8)
Z	4	4	2
ρ_{calc}(g cm^{-3})	1.491	1.532	1.880
T (K)	132	100	100
μ (Mo Kα) (mm^{-1})	0.532	0.673	2.041
F(000)	956	2456	762
R(int)	0.058	0.063	0.025

Total reflections	15069	28657	13715
Unique reflections	4163	6009	4806
$I>2\sigma(I)$	3483	5142	4473
$R_1{}^a$, $wR_2{}^b$	0.0566, 0.1548	0.0648, 0.1856	0.0677, 0.1690
R (all)	0.0681	0.0732	0.0719
GOF^{c}on F^2	1.07	1.05	1.05
Residual electron Density, eÅ^{-3}	-0.71, 0.63	-0.96, 1.76	-1.70, 2.50

Cartesian Coordinates:

V(IV) Geometries:

1

V	6.0572662	5.1425756	-6.1792387
O	7.0091225	4.0054511	-4.9105504
O	5.0806269	5.8422284	-4.6524110
O	5.1402971	4.1768523	-7.0923822
O	7.3705459	1.9886429	-3.2543557
O	3.5759033	5.9145456	-2.4975644
N	7.8683364	5.4173546	-7.1412823
C	4.3151278	6.9030631	-4.5049630
C	8.0732040	3.2615725	-5.1089625
N	5.7937790	6.9871299	-7.0326922
C	3.4921099	6.9896536	-3.3336985
C	3.4521917	9.1216789	-5.1739219
H	3.4455645	9.9403910	-5.8958369
C	8.3196252	2.1620385	-4.2197918
C	4.2727924	7.9906076	-5.4276947
C	2.6695238	9.1753146	-4.0382286
H	2.0325862	10.0379004	-3.8424823
C	2.6883783	8.1061881	-3.1181334
H	2.0631566	8.1634471	-2.2283232
C	7.5489665	0.8943561	-2.3409805
H	8.4790614	1.0061937	-1.7612832
H	6.6880837	0.9312469	-1.6652492
H	7.5601135	-0.0706951	-2.8723852
C	5.0558991	7.9774676	-6.6282974
H	5.0126940	8.8805949	-7.2532713
C	9.4484140	1.3633592	-4.3814669
H	9.6246744	0.5249978	-3.7090956
C	2.7663475	5.9327325	-1.3107538
H	1.6942509	5.9840919	-1.5600277
H	2.9782454	4.9901355	-0.7953776
H	3.0340521	6.7788145	-0.6577404

C	8.8915865	4.6165832	-7.0382751
H	9.7641461	4.8031408	-7.6772682
C	9.0247812	3.5044267	-6.1451321
C	6.5373354	7.0735433	-8.2851834
H	6.5152741	8.0886827	-8.7094159
C	7.9874226	6.6272022	-8.0248195
C	10.3807150	1.6244179	-5.4095847
H	11.2585525	0.9861617	-5.5092515
C	10.1777322	2.6815355	-6.2730309
H	10.8945382	2.8996565	-7.0665778
C	8.7419996	7.7086149	-7.2361640
H	9.7596318	7.3659781	-7.0039355
H	8.8074911	8.6312511	-7.8290395
H	8.2277825	7.9317083	-6.2907351
C	8.6712404	6.3338894	-9.3638499
H	8.5550144	7.2041162	-10.0238148
H	9.7482730	6.1552600	-9.2495423
H	8.2148153	5.4620421	-9.8525738
H	6.0670087	6.3826074	-9.0032726

1•Li$^+$

V	6.9907476	4.3392785	6.7264897
O	5.4463117	3.8870271	6.7557148
O	7.4218813	5.4368324	8.2860732
O	8.1926094	3.1642678	7.7093991
O	7.5086463	6.2376615	10.7426779
O	9.4467713	1.9876378	9.6086202
N	7.1365163	6.0259009	5.5868135
N	7.7748765	3.5449117	5.0291526
C	7.1306281	6.7124452	8.4826181
C	7.1615241	7.1913083	9.8228082
C	6.8534620	8.5197191	10.0972320
H	6.8539472	8.8866188	11.1226691
C	6.5440562	9.4084207	9.0453698
H	6.3078685	10.4460933	9.2799219
C	6.5577795	8.9751654	7.7327603
H	6.3474479	9.6682336	6.9167078
C	6.8492623	7.6193282	7.4252025
C	6.9692410	7.2351129	6.0431260
H	6.9560652	8.0671300	5.3274159
C	7.4791001	5.8077331	4.1370427
C	6.5819187	6.6098600	3.1909703
H	6.7898194	7.6863080	3.2439094
H	6.7703962	6.2912550	2.1566969
H	5.5213587	6.4386184	3.4218323
C	8.9616997	6.1670859	3.9553965
H	9.5929094	5.5681968	4.6266721
H	9.2684320	5.9770724	2.9179553
H	9.1271622	7.2294427	4.1811605
C	7.2652685	4.2962893	3.8821655
H	6.1866035	4.0900703	3.8004385

H	7.7514017	3.9936343	2.9429808
C	8.5798476	2.5330812	4.8918433
H	8.8644718	2.2301713	3.8749122
C	9.1608568	1.7816674	5.9740161
C	10.0075884	0.6813583	5.6787140
H	10.1528947	0.3912343	4.6371039
C	10.6404680	-0.0088083	6.6971964
H	11.2824612	-0.8590633	6.4686839
C	10.4799196	0.3877718	8.0422913
H	11.0061198	-0.1547369	8.8262814
C	9.6629168	1.4685237	8.3549643
C	8.9633252	2.1583498	7.3279557
C	7.5725091	6.6401377	12.1246248
H	8.3215275	7.4337699	12.2673489
H	6.5889304	6.9847170	12.4775706
H	7.8711384	5.7452563	12.6794102
C	10.1196797	1.3517493	10.7152473
H	9.8148905	1.9076290	11.6072512
H	9.8064006	0.3013673	10.8074301
H	11.2114206	1.4116366	10.5934537
Li	8.2979196	4.0701277	9.4648059

1•Na$^+$

V	7.1092651	4.3759189	6.8053271
O	5.5743980	3.8944528	6.8936752
O	7.5014501	5.5442356	8.3249738
O	8.3414384	3.1849812	7.7413622
O	7.5003258	6.4312865	10.7855850
O	9.5118436	1.7792766	9.6114838
N	7.1793945	6.0483848	5.6153718
N	7.8160759	3.5711800	5.0724919
C	7.1520067	6.8072913	8.4885313
C	7.1414818	7.3331098	9.8156793
C	6.7844373	8.6574747	10.0450591
H	6.7619947	9.0541820	11.0589891
C	6.4530097	9.5057679	8.9674952
H	6.1788630	10.5409572	9.1696957
C	6.4908144	9.0313810	7.6708047
H	6.2587536	9.6887639	6.8312783
C	6.8360435	7.6789644	7.4085300
C	6.9631398	7.2609916	6.0394998
H	6.9049588	8.0701365	5.3005826
C	7.5076271	5.8175706	4.1657464
C	6.6180569	6.6182072	3.2107988
H	6.8436496	7.6920398	3.2397958
H	6.7973618	6.2766362	2.1821860
H	5.5556344	6.4686218	3.4481388
C	8.9931132	6.1604413	3.9723285
H	9.6222654	5.5636035	4.6471912
H	9.2928306	5.9557353	2.9355280
H	9.1679721	7.2239004	4.1856862

C	7.2758927	4.3096886	3.9327047
H	6.1936235	4.1103682	3.8865199
H	7.7324863	3.9921870	2.9834910
C	8.6007252	2.5486708	4.9072538
H	8.8440167	2.2436077	3.8801459
C	9.1915730	1.7741521	5.9634358
C	9.9750836	0.6435074	5.6136338
H	10.0836922	0.3830461	4.5595263
C	10.5856059	-0.1157419	6.5934569
H	11.1821412	-0.9878565	6.3270389
C	10.4483851	0.2370905	7.9516794
H	10.9450227	-0.3668606	8.7093447
C	9.6933068	1.3456138	8.3213265
C	9.0339714	2.1355073	7.3316935
C	7.5101403	6.8926881	12.1510782
H	8.2344383	7.7104126	12.2837443
H	6.5076358	7.2245867	12.4595430
H	7.8129547	6.0299931	12.7532695
C	10.1254590	1.0068561	10.6633886
H	9.8417521	1.5002451	11.5985825
H	9.7465098	-0.0258823	10.6614341
H	11.2210898	1.0068676	10.5622716
Na	8.5072881	4.1303603	9.9807214

1•K$^+$

V	7.2616202	4.4116362	6.8962559
K	9.1679878	4.3598400	10.3024979
O	5.7469500	3.8901938	7.0654127
O	7.6192326	5.6513868	8.3782570
O	8.5497091	3.2162223	7.7567512
O	7.4452583	6.6042019	10.8433599
O	9.6588749	1.6438467	9.5823405
N	7.2447756	6.0646606	5.6569306
N	7.8613164	3.5883135	5.1209166
C	7.1839847	6.8922300	8.5122789
C	7.0874044	7.4514661	9.8256564
C	6.6536241	8.7611238	10.0069832
H	6.5742412	9.1773027	11.0100145
C	6.3176839	9.5696267	8.9022258
H	5.9871268	10.5943429	9.0703613
C	6.4182498	9.0634273	7.6219888
H	6.1738775	9.6827747	6.7572628
C	6.8400040	7.7245831	7.4081412
C	6.9835748	7.2772156	6.0526219
H	6.8800047	8.0625259	5.2937264
C	7.5359490	5.8197505	4.2026530
C	6.6351954	6.6193597	3.2567024
H	6.8837279	7.6884786	3.2530478
H	6.7764899	6.2506017	2.2316584
H	5.5770228	6.4983418	3.5272201
C	9.0200136	6.1442330	3.9689198

H	9.6603853	5.5471288	4.6327510
H	9.2918942	5.9280422	2.9266343
H	9.2094749	7.2076914	4.1692306
C	7.2780398	4.3162025	3.9972176
H	6.1923887	4.1294205	4.0022724
H	7.6883175	3.9803448	3.0333852
C	8.6104484	2.5471942	4.9192510
H	8.7904568	2.2316860	3.8820977
C	9.2225612	1.7517955	5.9447167
C	9.9206957	0.5825089	5.5462290
H	9.9678513	0.3344696	4.4846217
C	10.5174105	-0.2316480	6.4886468
H	11.0483314	-1.1345618	6.1880968
C	10.4405745	0.1038877	7.8544121
H	10.9143159	-0.5487188	8.5857404
C	9.7726666	1.2520298	8.2722836
C	9.1435499	2.1158498	7.3211657
C	7.3046985	7.0905038	12.1923244
H	7.9706022	7.9475410	12.3747750
H	6.2621091	7.3742863	12.4004951
H	7.5915952	6.2566776	12.8416997
C	10.2182919	0.7728256	10.5855989
H	9.9830079	1.2371370	11.5490439
H	9.7575095	-0.2251718	10.5392708
H	11.3099195	0.6897900	10.4729509

1•Mg^{2+}

V	5.8459138	5.0499563	-6.8640062
O	6.5302174	3.8284976	-5.4994543
O	4.7436035	5.4233179	-5.2749993
O	5.0948280	4.2885662	-8.0560804
O	6.7356407	2.5345459	-3.3373595
O	3.9922897	5.2488493	-2.8509933
N	7.7776300	5.3784139	-7.4158330
C	4.3027029	6.5710468	-4.7600991
C	7.7327398	3.3008193	-5.3055973
N	5.7331470	7.0189163	-7.2824976
C	3.8252784	6.5072369	-3.4344972
C	3.8233852	8.9530258	-4.7850874
H	3.8565400	9.9161568	-5.2958693
C	7.8792874	2.5274668	-4.1366919
C	4.3719734	7.8159530	-5.4278658
C	3.2746327	8.8513649	-3.5156940
H	2.8515231	9.7300602	-3.0308244
C	3.2939038	7.6281685	-2.8149824
H	2.9075632	7.5815404	-1.7982076
C	6.7862106	1.8037485	-2.0784906
H	7.5833495	2.2116921	-1.4442999
H	5.8109534	1.9590669	-1.6078859
H	6.9421676	0.7365944	-2.2769553
C	5.1023868	7.9727722	-6.6656243

H	5.1634729	8.9892750	-7.0760977
C	9.0788982	1.8898609	-3.8628351
H	9.2018637	1.2712275	-2.9752697
C	3.5071911	5.0615696	-1.4907955
H	2.4249929	5.2369229	-1.4594164
H	3.7249409	4.0192845	-1.2403344
H	4.0406430	5.7346984	-0.8082283
C	8.8052335	4.6332601	-7.1145516
H	9.7759864	4.8755890	-7.5659403
C	8.8400519	3.5680258	-6.1393559
C	6.5660849	7.2371881	-8.4667922
H	6.6391523	8.3022739	-8.7284095
C	7.9829029	6.6530937	-8.2045628
C	10.1631887	2.0679315	-4.7496518
H	11.1031317	1.5605083	-4.5368028
C	10.0618143	2.9090777	-5.8468591
H	10.9288363	3.0922645	-6.4826041
C	8.7798388	7.6252312	-7.3225249
H	9.7734118	7.2181652	-7.0926235
H	8.9092446	8.5805641	-7.8480543
H	8.2545302	7.8118180	-6.3750926
C	8.6757911	6.3861208	-9.5416284
H	8.6864751	7.3090832	-10.1366629
H	9.7180073	6.0713548	-9.4004617
H	8.1414150	5.6102165	-10.1061361
Mg	5.2465601	3.9479366	-3.9401711
H	6.0947535	6.7034306	-9.3061503

1•Ca^{2+}

V	6.0180606	5.1373026	-6.4294056
O	6.8977179	4.0706052	-5.0361478
O	5.0629754	5.7106042	-4.8120065
O	5.1477190	4.2007308	-7.3936677
O	7.2056413	2.3075696	-3.1877839
O	3.8346380	5.7252009	-2.5505585
N	7.8633300	5.4065932	-7.2644475
C	4.3324042	6.8046840	-4.5731013
C	7.9869472	3.3086502	-5.1576078
N	5.7910361	7.0210839	-7.1325358
C	3.6326237	6.8451516	-3.3474387
C	3.4789394	9.0307737	-5.0861188
H	3.4352338	9.8887833	-5.7579419
C	8.1897265	2.3237980	-4.1672567
C	4.2778397	7.9179746	-5.4474229
C	2.7654433	9.0318638	-3.8988054
H	2.1469147	9.8872769	-3.6304301
C	2.8442534	7.9391263	-3.0143179
H	2.2942164	7.9663562	-2.0754161
C	7.3085041	1.2874493	-2.1568810
H	8.2318138	1.4254017	-1.5799483
H	6.4380589	1.4318824	-1.5093516

H	7.2732134	0.2898715	-2.6130486
C	5.0560497	7.9821197	-6.6614090
H	5.0246609	8.9314230	-7.2121558
C	9.2967783	1.4870629	-4.2208868
H	9.4525897	0.7143767	-3.4699919
C	3.1136558	5.6582513	-1.2895789
H	2.0323639	5.6797011	-1.4756214
H	3.3930806	4.7008173	-0.8369570
H	3.4198537	6.4845024	-0.6354188
C	8.8717718	4.5993778	-7.1067891
H	9.7846599	4.7808584	-7.6879597
C	8.9473275	3.4947403	-6.1801885
C	6.5835104	7.1660041	-8.3554809
H	6.6031657	8.2064186	-8.7100015
C	8.0206385	6.6616484	-8.0856217
C	10.2380838	1.6494547	-5.2569058
H	11.1056272	0.9917206	-5.2905697
C	10.0801975	2.6435991	-6.2083592
H	10.8288286	2.7861734	-6.9884547
C	8.7800261	7.6775797	-7.2184796
H	9.7845382	7.3012168	-6.9830605
H	8.8781137	8.6285682	-7.7587282
H	8.2492380	7.8621592	-6.2737536
C	8.7288046	6.4126749	-9.4185792
H	8.6722603	7.3230357	-10.0298932
H	9.7924663	6.1795245	-9.2803102
H	8.2499378	5.5912659	-9.9683295
Ca	5.5264008	4.1103933	-3.2218845
H	6.1144009	6.5403467	-9.1308997

1•Ba^{2+}

V	6.1461275	5.2140307	-6.1262929
O	7.1528368	4.1475008	-4.8025571
O	5.2319974	5.9372057	-4.5367990
O	5.2220801	4.2111235	-6.9686932
O	7.5320555	2.1607687	-3.1115462
O	3.6864476	6.0072833	-2.3965939
N	7.9192320	5.4365399	-7.1429449
C	4.3609020	6.9506526	-4.4543831
C	8.1311853	3.2861437	-5.0954750
N	5.8444466	7.0253227	-7.0100799
C	3.5204945	7.0271016	-3.3120742
C	3.3375846	9.0381405	-5.2493885
H	3.2772103	9.8179891	-6.0097292
C	8.3680334	2.2017624	-4.2098235
C	4.2553447	7.9746043	-5.4335943
C	2.5229330	9.0804446	-4.1330247
H	1.8102367	9.8928521	-3.9964309
C	2.6131838	8.0707409	-3.1596924
H	1.9701025	8.1167613	-2.2828286
C	7.6895386	1.0527148	-2.1920507

H	8.6891421	1.0688292	-1.7367851
H	6.9285882	1.1947048	-1.4169952
H	7.5129640	0.0995269	-2.7088140
C	5.0591417	7.9835736	-6.6269262
H	4.9796618	8.8763694	-7.2613149
C	9.3730324	1.2758372	-4.4695704
H	9.5384525	0.4378736	-3.7950049
C	2.7743101	5.9625028	-1.2707673
H	1.7363236	5.8934072	-1.6235265
H	3.0313926	5.0561737	-0.7122627
H	2.9096497	6.8428049	-0.6281231
C	8.8793027	4.5617429	-7.1145842
H	9.7255106	4.6874052	-7.8007805
C	8.9734211	3.4288939	-6.2306499
C	6.6035237	7.1229051	-8.2563171
H	6.5832094	8.1419069	-8.6688044
C	8.0517575	6.6738276	-7.9851044
C	10.1919712	1.4185807	-5.6051059
H	10.9779348	0.6877519	-5.7913629
C	10.0067275	2.4865956	-6.4639847
H	10.6518220	2.6179118	-7.3335307
C	8.7851179	7.7219109	-7.1328033
H	9.7988784	7.3720731	-6.8963729
H	8.8560213	8.6685605	-7.6851391
H	8.2529311	7.9051356	-6.1886183
C	8.7680449	6.4351294	-9.3154311
H	8.6739971	7.3363996	-9.9352340
H	9.8409331	6.2468431	-9.1795394
H	8.3207536	5.5908818	-9.8580413
Ba	5.8805265	4.3189715	-2.4779402
H	6.1392653	6.4390361	-8.9844726

V(V) Geometries:

1

V	6.0655227	5.1068862	-6.1697388
O	7.1087670	4.2666868	-4.9150462
O	4.7276241	5.6398986	-5.0525393
O	5.4861923	4.0034845	-7.1586290
O	7.4639708	2.3939480	-3.0712658
O	3.2353323	5.5753213	-2.8612848
N	7.8406225	5.4284482	-7.2024338
C	4.2365444	6.7905478	-4.6012070
C	8.0923413	3.3845265	-5.1045966
N	5.7955092	6.9494798	-7.0394699
C	3.4136818	6.7842205	-3.4427237
C	3.9018538	9.2078018	-4.8270333
H	4.0761911	10.1315878	-5.3790286
C	8.3207406	2.3829146	-4.1228651
C	4.4734575	8.0036036	-5.2951411
C	3.1239325	9.1963678	-3.6800088

H	2.6866079	10.1211266	-3.3048212
C	2.8792062	7.9961070	-2.9915562
H	2.2591662	8.0146179	-2.0969717
C	7.6592247	1.4032526	-2.0430919
H	8.6518551	1.5081388	-1.5788884
H	6.8802949	1.5979941	-1.2995989
H	7.5401943	0.3869274	-2.4487033
C	5.2051277	7.9908634	-6.5267624
H	5.2429982	8.9298643	-7.0927637
C	9.3694636	1.4794388	-4.3129221
H	9.5470807	0.6922754	-3.5822940
C	2.4028396	5.5121783	-1.6850183
H	1.3796222	5.8498377	-1.9091554
H	2.3903766	4.4570894	-1.3955056
H	2.8293601	6.1167440	-0.8704142
C	8.8263131	4.5804819	-7.1439349
H	9.6698578	4.7235865	-7.8286636
C	8.9509220	3.4820944	-6.2296444
C	6.4829494	7.0431607	-8.3236254
H	6.4177877	8.0563016	-8.7434552
C	7.9447211	6.6280275	-8.0947542
C	10.2108286	1.5725033	-5.4376259
H	11.0225355	0.8546856	-5.5525126
C	10.0221909	2.5679873	-6.3796876
H	10.6852837	2.6610047	-7.2399366
C	8.7053649	7.7173277	-7.3242859
H	9.7306696	7.3830677	-7.1171779
H	8.7479207	8.6360730	-7.9242257
H	8.2165094	7.9421737	-6.3664917
C	8.6071602	6.3228572	-9.4399147
H	8.4751319	7.1888280	-10.1018147
H	9.6868728	6.1538676	-9.3384011
H	8.1470529	5.4460549	-9.9150434
H	6.0005068	6.3384860	-9.0172342

1•Li$^+$

V	7.2386868	4.4256786	6.9196290
O	5.6660047	4.2607048	7.0725048
O	7.7717364	5.6372733	8.2129412
O	8.0478412	2.9622790	7.6751297
O	7.8584891	6.5758704	10.7040017
O	9.1185063	1.4419027	9.5987878
N	7.2045738	6.0230420	5.6127680
N	7.8284222	3.5950147	5.1395496
C	7.2700803	6.8563672	8.4421220
C	7.3151963	7.3890208	9.7573993
C	6.8076565	8.6677551	9.9917150
H	6.8129078	9.0783939	10.9997588
C	6.2918392	9.4443174	8.9388040
H	5.9070740	10.4407009	9.1537325
C	6.2870716	8.9580548	7.6441367

H	5.9171037	9.5657157	6.8181004
C	6.7684572	7.6534742	7.3797076
C	6.8792127	7.2167177	6.0181154
H	6.7080001	7.9884093	5.2597008
C	7.4619724	5.7689644	4.1574998
C	6.5277439	6.5511539	3.2329198
H	6.7704769	7.6213148	3.2139275
H	6.6492415	6.1732173	2.2091216
H	5.4783461	6.4218529	3.5304979
C	8.9362495	6.1007543	3.8825469
H	9.6036519	5.5285506	4.5407701
H	9.1799497	5.8642599	2.8383456
H	9.1175433	7.1700947	4.0538742
C	7.2014529	4.2619816	4.0015600
H	6.1202039	4.0646929	4.0449728
H	7.5951261	3.8863590	3.0476940
C	8.7489851	2.6937037	4.9526167
H	9.0193732	2.4476556	3.9184572
C	9.4154764	1.9609816	5.9872642
C	10.4040955	1.0150812	5.6401577
H	10.6938996	0.9055997	4.5949369
C	10.9837196	0.2334654	6.6275000
H	11.7559080	-0.4911879	6.3719008
C	10.5760630	0.3556349	7.9649390
H	11.0400319	-0.2764057	8.7196954
C	9.5833817	1.2685054	8.3358474
C	9.0088020	2.1014790	7.3393148
C	7.9773273	7.0958181	12.0471274
H	8.5898316	8.0088154	12.0564804
H	6.9849211	7.2977279	12.4764060
H	8.4771955	6.3093653	12.6207578
C	9.6503412	0.5873071	10.6372249
H	9.1164301	0.8691073	11.5497468
H	9.4575327	-0.4700551	10.4059454
H	10.7282088	0.7607545	10.7680673
Li	7.5986572	3.6973573	10.6023787

1•Na $^{+}$

V	7.1838995	4.4287500	6.8782877
O	5.6076165	4.3070480	7.0220866
O	7.7682701	5.5877310	8.2109198
O	7.9866000	2.9760615	7.6500329
O	7.7413306	6.4204290	10.7208424
O	9.2145036	1.6961442	9.6119300
N	7.2376552	6.0325101	5.5974273
N	7.7540419	3.5742098	5.1054030
C	7.2819533	6.8132460	8.4478250
C	7.2785025	7.2961717	9.7798323
C	6.8066739	8.5827896	10.0365681
H	6.7777724	8.9625920	11.0560808
C	6.3666255	9.4073171	8.9850372

H	6.0066233	10.4096268	9.2144761
C	6.3982604	8.9609994	7.6755475
H	6.0783766	9.6057254	6.8567444
C	6.8456592	7.6495559	7.3881627
C	6.9678547	7.2349644	6.0188846
H	6.8482455	8.0274897	5.2721372
C	7.4978037	5.7758214	4.1421824
C	6.6108145	6.6108646	3.2176760
H	6.9040984	7.6683438	3.2136937
H	6.7257430	6.2390603	2.1909629
H	5.5533075	6.5279674	3.5027853
C	8.9891874	6.0368670	3.8853515
H	9.6205777	5.4259288	4.5445038
H	9.2316362	5.7978586	2.8414823
H	9.2205846	7.0943368	4.0687986
C	7.1645287	4.2826057	3.9709388
H	6.0746088	4.1378726	4.0068450
H	7.5448949	3.8980274	3.0153982
C	8.6110274	2.6114053	4.9179907
H	8.8471554	2.3320765	3.8839992
C	9.2690460	1.8747436	5.9568498
C	10.2124419	0.8770400	5.6289823
H	10.4501916	0.6900421	4.5816889
C	10.8233211	0.1487671	6.6393292
H	11.5578958	-0.6173164	6.3940213
C	10.5131618	0.3892940	7.9884171
H	11.0167123	-0.1882897	8.7613022
C	9.5731069	1.3604595	8.3397340
C	8.9344562	2.1005600	7.3146599
C	7.7581098	6.8724448	12.0973041
H	8.4083615	7.7515936	12.2059377
H	6.7388157	7.1020978	12.4378393
H	8.1624303	6.0378775	12.6780949
C	9.7478872	0.8891671	10.6920816
H	9.2776674	1.2720818	11.6027133
H	9.4774338	-0.1660073	10.5494233
H	10.8392224	1.0026819	10.7567330
Na	8.6443058	4.1549651	10.1531548

1•K$^+$

V	7.3371994	4.4815790	6.9634671
K	9.3901072	4.3428779	10.3743544
O	5.7713434	4.2826680	7.1305185
O	7.8425336	5.7223960	8.2433155
O	8.2240665	3.0557428	7.6976957
O	7.7321520	6.6285273	10.7606433
O	9.3271105	1.5401514	9.5957882
N	7.2727608	6.0603662	5.6354995
N	7.8379914	3.6068865	5.1647609
C	7.2668280	6.9129911	8.4656146
C	7.2167700	7.4308123	9.7850754

C	6.6469028	8.6865123	10.0011686
H	6.5840041	9.0892627	11.0101828
C	6.1537303	9.4505544	8.9293837
H	5.7202443	10.4293725	9.1311786
C	6.2266935	8.9722715	7.6335888
H	5.8649053	9.5672561	6.7949042
C	6.7715082	7.6903419	7.3864437
C	6.9220859	7.2502230	6.0292131
H	6.7446006	8.0128466	5.2635054
C	7.5283750	5.7905916	4.1831745
C	6.6316892	6.6012831	3.2465986
H	6.9132533	7.6617733	3.2239832
H	6.7504141	6.2132359	2.2263626
H	5.5749141	6.5114044	3.5324349
C	9.0158787	6.0640114	3.9153868
H	9.6570366	5.4749762	4.5847690
H	9.2578435	5.8050488	2.8760412
H	9.2344677	7.1279149	4.0753273
C	7.2086316	4.2957728	4.0398887
H	6.1217587	4.1397823	4.1098176
H	7.5656910	3.9031561	3.0785748
C	8.6693084	2.6297514	4.9437427
H	8.8602931	2.3504978	3.9004177
C	9.3344037	1.8578523	5.9495549
C	10.1901809	0.8020573	5.5665380
H	10.3776395	0.6255215	4.5071717
C	10.7677029	-0.0015165	6.5372702
H	11.4345391	-0.8144507	6.2525094
C	10.4968804	0.2168366	7.8974842
H	10.9613525	-0.4279755	8.6411221
C	9.6436339	1.2467543	8.3034403
C	9.0609763	2.0863153	7.3201790
C	7.6633255	7.1132567	12.1225496
H	8.2426096	8.0406210	12.2352783
H	6.6181045	7.2739225	12.4226491
H	8.1030017	6.3254279	12.7423036
C	9.7796778	0.6206628	10.6199093
H	9.3396769	0.9840129	11.5535832
H	9.4176572	-0.3958859	10.4114583
H	10.8765445	0.6283481	10.6932768

1•Mg^{2+}

V	5.9904422	5.0825641	-6.5772619
O	6.8073139	4.2893083	-5.0608325
O	4.6812637	5.4502107	-5.2820360
O	5.5409162	3.9324331	-7.5634075
O	6.8965706	2.5765215	-3.2069919
O	4.0153393	5.3764002	-2.7893777
N	7.8393070	5.4962656	-7.2761992
C	4.3264270	6.6219855	-4.7478012
C	7.8890548	3.4972103	-5.1023013

N	5.6867326	6.9148258	-7.3058923
C	3.8544038	6.5999121	-3.4211754
C	3.8593402	9.0023697	-4.8739878
H	3.8866742	9.9445693	-5.4209460
C	7.9779995	2.5458874	-4.0735582
C	4.4027454	7.8433365	-5.4669079
C	3.3192719	8.9439379	-3.5947984
H	2.9082252	9.8430285	-3.1383839
C	3.3312861	7.7500432	-2.8482426
H	2.9478465	7.7466248	-1.8296467
C	6.8627886	1.5936297	-2.1247545
H	7.7378208	1.7304503	-1.4790743
H	5.9458206	1.8043533	-1.5679988
H	6.8284318	0.5855107	-2.5534105
C	5.0613371	7.9118598	-6.7400333
H	5.0629625	8.8787028	-7.2565523
C	9.0776571	1.7023210	-4.0116870
H	9.1678994	0.9451553	-3.2347796
C	3.3321815	5.1707051	-1.5085897
H	2.2596056	5.3451307	-1.6459135
H	3.5195028	4.1268925	-1.2426033
H	3.7631724	5.8387667	-0.7544327
C	8.8654990	4.7297329	-7.0311517
H	9.8002915	4.9272622	-7.5683185
C	8.9069335	3.6570810	-6.0667961
C	6.4862401	7.0669917	-8.5248738
H	6.4133658	8.0862207	-8.9261694
C	7.9527992	6.7152565	-8.1605937
C	10.0955902	1.8403579	-4.9771285
H	10.9574442	1.1767910	-4.9241301
C	10.0293135	2.8030448	-5.9763046
H	10.8397778	2.9075706	-6.6973789
C	8.5835111	7.8351806	-7.3252682
H	9.5996829	7.5531236	-7.0209441
H	8.6371935	8.7529136	-7.9249574
H	7.9958726	8.0381897	-6.4195582
C	8.7445369	6.4284941	-9.4344932
H	8.6543973	7.2921183	-10.1064114
H	9.8129818	6.2887333	-9.2259039
H	8.3549458	5.5403786	-9.9493016
Mg	5.4698765	4.1128666	-3.5417048
H	6.1056873	6.3605286	-9.2769430

1•Ca^{2+}

V	6.0988014	5.1019800	-6.3513830
O	6.9960637	4.2739354	-4.9054865
O	4.8122143	5.5586421	-5.0494379
O	5.5889548	3.9327443	-7.2836152
O	7.1685377	2.3637754	-3.1707397
O	3.7799714	5.6269610	-2.6381821
N	7.8882022	5.4960512	-7.1999026

C	4.3009077	6.7326854	-4.6452545
C	8.0169234	3.4135966	-5.0840292
N	5.7295582	6.8891379	-7.1955207
C	3.6744572	6.7841764	-3.3827358
C	3.7041622	9.0647397	-5.0217518
H	3.7267667	9.9523382	-5.6536194
C	8.1578911	2.3848891	-4.1338151
C	4.3538725	7.8915086	-5.4600600
C	3.0566858	9.0858825	-3.7941833
H	2.5633161	9.9944568	-3.4526702
C	3.0473841	7.9524992	-2.9637118
H	2.5583798	8.0019910	-1.9927868
C	7.2669594	1.3457209	-2.1259535
H	8.2047070	1.4749175	-1.5728995
H	6.4133824	1.5190108	-1.4636307
H	7.1963715	0.3489493	-2.5770426
C	5.0527509	7.8926298	-6.7112212
H	5.0197948	8.8170763	-7.2990777
C	9.2219992	1.4963684	-4.2300379
H	9.3414295	0.6862724	-3.5132131
C	3.0437760	5.5549199	-1.3761185
H	1.9770065	5.7200549	-1.5657032
H	3.2019688	4.5387328	-1.0002054
H	3.4502638	6.2879100	-0.6694451
C	8.8917749	4.6785405	-7.0543483
H	9.7873798	4.8458416	-7.6631582
C	8.9570105	3.5736840	-6.1321993
C	6.4999852	7.0105314	-8.4366679
H	6.3914538	8.0105068	-8.8765744
C	7.9751600	6.7086398	-8.0872134
C	10.1589589	1.6488117	-5.2684367
H	10.9902790	0.9484572	-5.3328460
C	10.0433544	2.6732850	-6.1973169
H	10.7856791	2.7921294	-6.9860247
C	8.5860626	7.8447373	-7.2571350
H	9.6130048	7.5869465	-6.9678783
H	8.6073219	8.7644704	-7.8559019
H	8.0066168	8.0315080	-6.3428385
C	8.7672281	6.4448758	-9.3656677
H	8.6450240	7.3058873	-10.0354835
H	9.8414748	6.3401549	-9.1657830
H	8.4026707	5.5458764	-9.8803101
Ca	5.3982092	4.0012367	-3.2382389
H	6.1241727	6.2630743	-9.1504525

1•Ba^{2+}

V	6.2087218	5.1705322	-6.0501319
O	7.2485594	4.2829142	-4.7597079
O	5.0102525	5.7851259	-4.7727237
O	5.5570946	4.0315672	-6.9336186
O	7.6004848	2.2928482	-3.0336611

O	3.5265245	5.8400516	-2.5593621
N	7.9164424	5.4726348	-7.1230542
C	4.3156578	6.9034010	-4.5102181
C	8.1549386	3.3348688	-5.0730863
N	5.8183947	6.9368010	-7.0124466
C	3.4963923	6.9540523	-3.3595759
C	3.5929899	9.1610743	-5.1036631
H	3.6246742	10.0054876	-5.7922274
C	8.3815804	2.2780063	-4.1628343
C	4.3635266	8.0131928	-5.3861977
C	2.7978513	9.1990453	-3.9683425
H	2.2040667	10.0836550	-3.7429926
C	2.7470182	8.1005783	-3.0971105
H	2.1196982	8.1516805	-2.2092757
C	7.8012954	1.2235755	-2.0677854
H	8.8285315	1.2503809	-1.6822475
H	7.0955648	1.4170880	-1.2535077
H	7.5743675	0.2535804	-2.5280792
C	5.1188899	7.9548802	-6.6007554
H	5.0779606	8.8387176	-7.2480471
C	9.3369878	1.3076399	-4.4563501
H	9.5055421	0.4776488	-3.7734554
C	2.5539534	5.7597166	-1.4780759
H	1.5396832	5.8830988	-1.8781202
H	2.6637686	4.7546981	-1.0585450
H	2.7728157	6.5149559	-0.7123843
C	8.8445624	4.5609686	-7.1343381
H	9.6599311	4.6660189	-7.8579796
C	8.9352774	3.4272351	-6.2565159
C	6.5349110	7.0138428	-8.2873824
H	6.4287302	8.0062556	-8.7448832
C	8.0084262	6.6849444	-8.0005505
C	10.0988705	1.3931598	-5.6340436
H	10.8434539	0.6255317	-5.8399465
C	9.9193141	2.4459641	-6.5154267
H	10.5283850	2.5303608	-7.4151309
C	8.6749480	7.7986608	-7.1802773
H	9.7070913	7.5163425	-6.9357374
H	8.6902792	8.7266451	-7.7667309
H	8.1358106	7.9844949	-6.2414553
C	8.7511300	6.4305527	-9.3106128
H	8.6225834	7.3073843	-9.9579979
H	9.8296527	6.3013694	-9.1521036
H	8.3510367	5.5508628	-9.8328320
Ba	5.8579499	4.3410975	-2.3616137
H	6.1097076	6.2585598	-8.9647673

Control files:

V(IV):

1

```
$cosmo
  epsilon=   36.600
rsolv= 1.30
  refind=   1.3440
$cosmo_atoms
# radii in Angstrom units
v  1
\
   radius=  2.2230
o  2-6
\
   radius=  1.7200
n  7,10
\
   radius=  1.8300
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
   radius=  2.0000
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-50
\
   radius=  1.3000
$cosmo_out file=out.ccf
$title
$operating system unix
$symmetry c1
$coord    file=coord
$user-defined bonds    file=coord
$atoms
v  1
\
   basis =v def2-TZVP
\
jbas  =v def2-TZVP
o  2-6
\
   basis =o def2-TZVP
\
   jbas  =o def2-TZVP
n  7,10
\
   basis =n def2-TZVP
\
jbas  =n def2-TZVP
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
basis =c def2-TZVP
\
   jbas  =c def2-TZVP
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-50
\
```

```
   basis =h def2-TZVP
\
   jbas  =h def2-TZVP
$basis    file=basis
$rundimensions
   dim(fock,dens)=671197
   natoms=50
   nshell=400
   nbf(CAO)=1156
   nbf(AO)=1014
dim(trafo[SAO<-->AO/CAO])=1440
   rhfshells=2
$uhfmo_alpha   file=alpha
$uhfmo_beta   file=beta
$uhf
$alpha shells
 a       1-110                                  ( 1 )
$beta shells
 a       1-109                                  ( 1 )
$scfiterlimit      900
$thize     0.10000000E-04
$thime        5
$scfdump
$scfintunit
 unit=30       size=0        file=twoint
$scfdiis
$maxcor      500
$drvopt
   cartesian  on
   basis      off
   global     off
   hessian    on
   dipole     on
   nuclear polarizability
$interconversion  off
   qconv=1.d-7
   maxiter=25
$optimize
   internal   off
   cartesian  on
   global     off
   basis      off   logarithm
$coordinateupdate
   dqmax=0.3
   interpolate  on
   statistics    5
$forceupdate
   ahlrichs numgeo=0  mingeo=3 maxgeo=4 modus=<g|dq> dynamic
fail=0.3
   threig=0.005  reseig=0.005  thrbig=3.0  scale=1.00
damping=0.0
```

```
$forceinit on
   diag=default
$energy    file=energy
$grad    file=gradient
$forceapprox    file=forceapprox
$lock off
$dft
   functional b-p
   gridsize   m3
$scfconv   6
$scfdamp   start=0.700  step=0.050  min=0.050
$scforbitalshift  closedshell=.05
$ricore        0
$rij
$jbas    file=auxbasis
$disp3
$marij
$last step     ridft
$last SCF energy change = -.32885964E-07
$ssquare from ridft
          0.758 (not to be modified here)
$charge from ridft
          0.000 (not to be modified here)
$dipole from ridft
  x     1.87171617170861    y     2.33151846621786    z    -
0.66530913608722    a.u.
   | dipole | =    7.7854145991  debye
$optinfo       file=optinfo
$hessapprox   file=hessapprox
$orbital_max_rnorm 0.83291368338185E-04
$subenergy  Etot         E1                  Ej
Ex                  Ec                  En                  Disp
-2205.983904926    -9262.144045727     4138.742493120    -
210.8326326196    -8.408883327443     3136.722907742    -
.6374411323413E-01
$end
$TMPDIR /home/tony/TMP
```

1•Li$^+$ (as example of monocationic)

```
$cosmo
  epsilon=   36.600
  rsolv= 1.30
  refind=   1.3440
$cosmo_atoms
# radii in Angstrom units
v  1
\
   radius=  2.2230
o  2-6
\
```

```
   radius=  1.7200
n  7-8
\
   radius=  1.8300
c  9-11,13,15,17-18,20-21,25,29,32,34-35,37,39,41-43,47
\
   radius=  2.0000
h  12,14,16,19,22-24,26-28,30-31,33,36,38,40,44-46,48-50
\
   radius=  1.3000
li 51
\
   radius=  1.5700
$cosmo_out file=out.ccf
$title
$operating system unix
$symmetry c1
$coord    file=coord
$user-defined bonds    file=coord
$atoms
v  1
\
   basis =v def2-TZVP
\
jbas  =v def2-TZVP
o  2-6
\
   basis =o def2-TZVP
\
   jbas  =o def2-TZVP
n  7-8
\
   basis =n def2-TZVP
\
jbas  =n def2-TZVP
c  9-11,13,15,17-18,20-21,25,29,32,34-35,37,39,41-43,47
\
basis =c def2-TZVP
\
   jbas  =c def2-TZVP
h  12,14,16,19,22-24,26-28,30-31,33,36,38,40,44-46,48-50
\
   basis =h def2-TZVP
\
   jbas  =h def2-TZVP
li 51
\
   basis =li def2-TZVP
\
   jbas  =li def2-TZVP
$basis    file=basis
```

```
$rundimensions
   dim(fock,dens)=687495
   natoms=51
   nshell=408
   nbf(CAO)=1170
   nbf(AO)=1028
dim(trafo[SAO<-->AO/CAO])=1454
   rhfshells=2
$uhfmo_alpha   file=alpha
$uhfmo_beta   file=beta
$uhf
$alpha shells
 a       1-111                                  ( 1 )
$beta shells
 a       1-110                                  ( 1 )
$scfiterlimit      900
$thize     0.10000000E-04
$thime        5
$scfdump
$scfintunit
 unit=30       size=0        file=twoint
$scfdiis
$maxcor      500
$drvopt
   cartesian  on
   basis      off
   global     off
   hessian    on
   dipole     on
   nuclear polarizability
$interconversion  off
   qconv=1.d-7
   maxiter=25
$optimize
   internal   off
   cartesian  on
   global     off
   basis      off   logarithm
$coordinateupdate
   dqmax=0.3
   interpolate  on
   statistics    5
$forceupdate
   ahlrichs numgeo=0  mingeo=3 maxgeo=4 modus=<g|dq> dynamic
fail=0.3
   threig=0.005  reseig=0.005  thrbig=3.0  scale=1.00
damping=0.0
$forceinit on
   diag=default
$energy    file=energy
$grad    file=gradient
```

```
$forceapprox    file=forceapprox
$lock off
$dft
   functional b-p
   gridsize   m3
$scfconv   6
$scfdamp   start=0.700  step=0.050  min=0.050
$scforbitalshift  closedshell=.05
$ricore        0
$rij
$jbas    file=auxbasis
$disp3
$marij
$last step     ridft
$last SCF energy change = -.88273737E-07
$ssquare from ridft
          0.758 (not to be modified here)
$charge from ridft
          1.000 (not to be modified here)
$dipole from ridft
  x    17.72687438411231    y     9.11032611295741    z
14.86591083223811    a.u.
   | dipole | =   63.1993270160  debye
$optinfo       file=optinfo
$hessapprox   file=hessapprox
$orbital_max_rnorm 0.77239137056946E-04
$subenergy  Etot         E1                  Ej
Ex                  Ec                  En                  Disp
-2213.456573680    -9478.442657178     4231.801600192    -
212.5072647536    -8.458856438270     3254.221678359    -
.7107386187977E-01
$end
$TMPDIR /home/tony/TMP
```

1•Mg^{2+}(as example of dicationic)

```
$cosmo
  epsilon=   36.600
  rsolv= 1.30
  refind=   1.3440
$cosmo_atoms
# radii in Angstrom units
v  1
\
   radius=  2.2230
o  2-6
\
   radius=  1.7200
n  7,10
\
   radius=  1.8300
```

```
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
radius=  2.0000
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-49,51
\
   radius=  1.3000
mg 50
\
   radius=  1.6380
$cosmo_out file=out.ccf
$title
$operating system unix
$symmetry c1
$coord    file=coord
$user-defined bonds    file=coord
$atoms
v  1
\
   basis =v def2-TZVP
\
jbas  =v def2-TZVP
o  2-6
\
   basis =o def2-TZVP
\
   jbas  =o def2-TZVP
n  7,10
\
   basis =n def2-TZVP
\
jbas  =n def2-TZVP
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
basis =c def2-TZVP
\
   jbas  =c def2-TZVP
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-49,51
\
   basis =h def2-TZVP
\
   jbas  =h def2-TZVP
mg 50
\
   basis =mg def2-TZVP
\
   jbas  =mg def2-TZVP
$basis    file=basis
$rundimensions
   dim(fock,dens)=712344
   natoms=51
   nshell=412
```

```
   nbf(CAO)=1191
   nbf(AO)=1046
dim(trafo[SAO<-->AO/CAO])=1481
   rhfshells=2
$uhfmo_alpha   file=alpha
$uhfmo_beta   file=beta
$uhf
$alpha shells
 a       1-115                                  ( 1 )
$beta shells
 a       1-114                                  ( 1 )
$scfiterlimit      900
$thize     0.10000000E-04
$thime        5
$scfdump
$scfintunit
 unit=30       size=0        file=twoint
$scfdiis
$maxcor      500
$drvopt
   cartesian  on
   basis      off
   global     off
   hessian    on
   dipole     on
   nuclear polarizability
$interconversion  off
   qconv=1.d-7
   maxiter=25
$optimize
   internal   off
   cartesian  on
   global     off
   basis      off   logarithm
$coordinateupdate
   dqmax=0.3
   interpolate  on
   statistics    5
$forceupdate
   ahlrichs numgeo=0  mingeo=3 maxgeo=4 modus=<g|dq> dynamic
fail=0.3
   threig=0.005  reseig=0.005  thrbig=3.0  scale=1.00
damping=0.0
$forceinit on
   diag=default
$energy    file=energy
$grad    file=gradient
$forceapprox    file=forceapprox
$lock off
$dft
   functional b-p
```

```
   gridsize   m3
$scfconv   6
$scfdamp   start=0.700  step=0.050  min=0.050
$scforbitalshift  closedshell=.05
$ricore        0
$rij
$jbas    file=auxbasis
$disp3
$marij
$last step     ridft
$last SCF energy change = -.10832446E-05
$ssquare from ridft
          0.759 (not to be modified here)
$charge from ridft
          2.000 (not to be modified here)
$dipole from ridft
  x    23.65136279607759    y    19.01574015961478    z   -
15.24425270857046    a.u.
   | dipole | =   86.3217670359  debye
$optinfo       file=optinfo
$hessapprox   file=hessapprox
$orbital_max_rnorm 0.12464097804783E-03
$subenergy  Etot         E1                  Ej
Ex                  Ec                 En                  Disp
-2405.897859058    -10361.55495729     4613.654407609    -
226.5682132149    -8.847413946725     3577.492354904    -
.7403711689598E-01
$end
$TMPDIR /home/tony/TMP
```

V(V):

1

```
$cosmo
  epsilon=   36.600
  rsolv= 1.30
  refind=   1.3440
$cosmo_atoms
# radii in Angstrom units
v  1
\
   radius=  2.2230
o  2-6
\
   radius=  1.7200
n  7,10
\
   radius=  1.8300
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
```

```
radius=  2.0000
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-50
\
   radius=  1.3000
$cosmo_out file=out.ccf
$title
$operating system unix
$symmetry c1
$coord    file=coord
$user-defined bonds    file=coord
$atoms
v  1
\
   basis =v def2-TZVP
\
jbas  =v def2-TZVP
o  2-6
\
   basis =o def2-TZVP
\
   jbas  =o def2-TZVP
n  7,10
\
   basis =n def2-TZVP
\
jbas  =n def2-TZVP
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
basis =c def2-TZVP
\
   jbas  =c def2-TZVP
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-50
\
   basis =h def2-TZVP
\
   jbas  =h def2-TZVP
$basis    file=basis
$rundimensions
   dim(fock,dens)=671197
   natoms=50
   nshell=400
   nbf(CAO)=1156
   nbf(AO)=1014
dim(trafo[SAO<-->AO/CAO])=1440
rhfshells=1
$scfmo   file=mos
$closed shells
 a       1-109                                  ( 2 )
$scfiterlimit      900
$thize     0.10000000E-04
$thime        5
```

```
$scfdump
$scfintunit
 unit=30       size=0        file=twoint
$scfdiis
$maxcor      500
$scforbitalshift  automatic=.1
$drvopt
   cartesian  on
   basis      off
   global     off
   hessian    on
   dipole     on
   nuclear polarizability
$interconversion  off
   qconv=1.d-7
   maxiter=25
$optimize
   internal   off
   cartesian  on
   global     off
   basis      off   logarithm
$coordinateupdate
   dqmax=0.3
   interpolate  on
   statistics    5
$forceupdate
   ahlrichs numgeo=0  mingeo=3 maxgeo=4 modus=<g|dq> dynamic
fail=0.3
   threig=0.005  reseig=0.005  thrbig=3.0  scale=1.00
damping=0.0
$forceinit on
   diag=default
$energy    file=energy
$grad    file=gradient
$forceapprox    file=forceapprox
$lock off
$dft
   functional b-p
   gridsize   m3
$scfconv   6
$scfdamp   start=0.700  step=0.050  min=0.050
$ricore        0
$rij
$jbas    file=auxbasis
$disp3
$marij
$last step     ridft
$last SCF energy change = -.96050371E-07
$charge from ridft
          1.000 (not to be modified here)
$dipole from ridft
```

```
  x    13.28170757308317    y    12.36129045918187    z   -
10.78659039443983    a.u.
   | dipole | =   53.6520792389  debye
$optinfo       file=optinfo
$hessapprox   file=hessapprox
$orbital_max_rnorm 0.23259775810665E-04
$subenergy  Etot         E1                  Ej
Ex                  Ec                  En                  Disp
-2205.818689920    -9301.862057852     4143.105571060    -
210.5453558895    -8.378585786658     3171.926537956    -
.6479940720604E-01
$end
$TMPDIR /home/tony/TMP
```

1•Li^{+} (as example of monocationic)

```
$cosmo
  epsilon=   36.600
  rsolv= 1.30
  refind=   1.3440
$cosmo_atoms
# radii in Angstrom units
v  1
\
   radius=  2.2230
o  2-6
\
   radius=  1.7200
n  7-8
\
   radius=  1.8300
c  9-11,13,15,17-18,20-21,25,29,32,34-35,37,39,41-43,47
\
   radius=  2.0000
h  12,14,16,19,22-24,26-28,30-31,33,36,38,40,44-46,48-50
\
   radius=  1.3000
li 51
\
   radius=  1.5700
$cosmo_out file=out.ccf
$title
$operating system unix
$symmetry c1
$coord    file=coord
$user-defined bonds    file=coord
$atoms
v  1
\
   basis =v def2-TZVP
\
```

```
jbas  =v def2-TZVP
o  2-6
\
   basis =o def2-TZVP
\
   jbas  =o def2-TZVP
n  7-8
\
   basis =n def2-TZVP
\
jbas  =n def2-TZVP
c  9-11,13,15,17-18,20-21,25,29,32,34-35,37,39,41-43,47
\
basis =c def2-TZVP
\
   jbas  =c def2-TZVP
h  12,14,16,19,22-24,26-28,30-31,33,36,38,40,44-46,48-50
\
   basis =h def2-TZVP
\
   jbas  =h def2-TZVP
li 51
\
   basis =li def2-TZVP
\
   jbas  =li def2-TZVP
$basis    file=basis
$rundimensions
   dim(fock,dens)=687495
   natoms=51
   nshell=408
   nbf(CAO)=1170
   nbf(AO)=1028
dim(trafo[SAO<-->AO/CAO])=1454
rhfshells=1
$scfmo   file=mos
$closed shells
 a       1-110                                  ( 2 )
$scfiterlimit      900
$thize     0.10000000E-04
$thime        5
$scfdump
$scfintunit
 unit=30       size=0        file=twoint
$scfdiis
$maxcor      500
$scforbitalshift  automatic=.1
$drvopt
   cartesian  on
   basis      off
   global     off
```

```
   hessian    on
   dipole     on
   nuclear polarizability
$interconversion  off
   qconv=1.d-7
   maxiter=25
$optimize
   internal   off
   cartesian  on
   global     off
   basis      off   logarithm
$coordinateupdate
   dqmax=0.3
   interpolate  on
   statistics    5
$forceupdate
   ahlrichs numgeo=0  mingeo=3 maxgeo=4 modus=<g|dq> dynamic
fail=0.3
   threig=0.005  reseig=0.005  thrbig=3.0  scale=1.00
damping=0.0
$forceinit on
   diag=default
$energy    file=energy
$grad    file=gradient
$forceapprox    file=forceapprox
$lock off
$dft
   functional b-p
   gridsize   m3
$scfconv   6
$scfdamp   start=0.700  step=0.050  min=0.050
$ricore        0
$rij
$jbas    file=auxbasis
$disp3
$marij
$last step     ridft
$last SCF energy change = -.12509190E-07
$charge from ridft
          2.000 (not to be modified here)
$dipole from ridft
  x    31.01894848339543    y    16.30484486798923    z
31.02627920662462    a.u.
   | dipole | =  118.9658521651  debye
$optinfo       file=optinfo
$hessapprox   file=hessapprox
$orbital_max_rnorm 0.39225834080954E-04
$subenergy  Etot         E1                  Ej
Ex                Ec                En                  Disp
```

```
-2213.268334993    -9431.612376765     4194.342995294    -
212.1803442829    -8.423563515285     3244.692904477    -
.8795020041439E-01
$end
$TMPDIR /home/tony/TMP
```

1•Mg^{2+} (as example of dicationic)

```
$cosmo
  epsilon=   36.600
  rsolv= 1.30
  refind=   1.3440
$cosmo_atoms
# radii in Angstrom units
v  1
\
   radius=  2.2230
o  2-6
\
   radius=  1.7200
n  7,10
\
   radius=  1.8300
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
radius=  2.0000
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-49,51
\
   radius=  1.3000
mg 50
\
   radius=  1.6380
$cosmo_out file=out.ccf
$title
$operating system unix
$symmetry c1
$coord    file=coord
$user-defined bonds    file=coord
$atoms
v  1
\
   basis =v def2-TZVP
\
jbas  =v def2-TZVP
o  2-6
\
   basis =o def2-TZVP
\
   jbas  =o def2-TZVP
n  7,10
\
```

```
   basis =n def2-TZVP
\
jbas  =n def2-TZVP
c  8-9,11-12,14-16,18,20,24,26,28,32,34-35,37-38,40,42,46
\
basis =c def2-TZVP
\
   jbas  =c def2-TZVP
h  13,17,19,21-23,25,27,29-31,33,36,39,41,43-45,47-49,51
\
   basis =h def2-TZVP
\
   jbas  =h def2-TZVP
mg 50
\
   basis =mg def2-TZVP
\
   jbas  =mg def2-TZVP
$basis    file=basis
$rundimensions
   dim(fock,dens)=712344
   natoms=51
   nshell=412
   nbf(CAO)=1191
   nbf(AO)=1046
dim(trafo[SAO<-->AO/CAO])=1481
rhfshells=1
$scfmo   file=mos
$closed shells
 a       1-114                                  ( 2 )
$scfiterlimit      900
$thize     0.10000000E-04
$thime        5
$scfdump
$scfintunit
 unit=30       size=0        file=twoint
$scfdiis
$maxcor      500
$scforbitalshift  automatic=.1
$drvopt
   cartesian  on
   basis      off
   global     off
   hessian    on
   dipole     on
   nuclear polarizability
$interconversion  off
   qconv=1.d-7
   maxiter=25
$optimize
   internal   off
```

```
   cartesian  on
   global     off
   basis      off   logarithm
$coordinateupdate
   dqmax=0.3
   interpolate  on
   statistics    5
$forceupdate
   ahlrichs numgeo=0  mingeo=3 maxgeo=4 modus=<g|dq> dynamic
fail=0.3
   threig=0.005  reseig=0.005  thrbig=3.0  scale=1.00
damping=0.0
$forceinit on
   diag=default
$energy    file=energy
$grad    file=gradient
$forceapprox    file=forceapprox
$lock off
$dft
   functional b-p
   gridsize   m3
$scfconv   6
$scfdamp   start=0.700  step=0.050  min=0.050
$ricore        0
$rij
$jbas    file=auxbasis
$disp3
$marij
$last step     ridft
$last SCF energy change = -.33855940E-07
$charge from ridft
          3.000 (not to be modified here)
$dipole from ridft
  x    35.05183388506157    y    29.37000920167475    z   -
25.53353405932103    a.u.
   | dipole | =  133.1261721939  debye
$optinfo       file=optinfo
$hessapprox   file=hessapprox
$orbital_max_rnorm 0.41495683479115E-04
$subenergy  Etot         E1                  Ej
Ex                 Ec                 En                 Disp
-2405.678975099    -10365.79119650     4599.867180985    -
226.2519958355    -8.813062630628     3595.385012229    -
.7491334974965E-01
$end
$TMPDIR /home/tony/TMP
```