Supporting information

Table S1. IR spectra of pristine porphyrins and salts **1 - 4.**

Components	Cryptand	Bu_3MePI	$Cu^{II}(TPP^{2-})$	$\{Crypt(Cs^+)\}_2\{Cu^{II}(TPP^{4-})\}^{2-}$ (**1**)	$Ni^{II}(TPP^{2-})$	$\{Crypt(Cs^+)\}\{Ni(TPP)\}^-\cdot C_6H_5CH_3$ (**2**)	$\{Bu_3MeP^+\}\{Ni(TPP)\}^-\cdot C_6H_5CH_3$ (**3**)	$Fe^{II}(TPP^{2-})$	$\{Bu_3MeP^+\}\{Fe^{I}(TPP^{2-})\}^-\cdot C_6H_5CH_3$ (**4**)
$M^{II}TPP$			444w	444w	444w	444w	-	433w	420w
			524w	527w*	525w	528w*	-	523w	523w
			656m	656w	560w	557w	565w	660w	662w
			696s	700s	663w	666w	-	700s	700s
			711m	-	696s	702s	702s	719m	714m*
			728m	731m*	708m	715m	712m*	750s	750s
			742s	752s	723w	733m*	731m	803s	820m*
			793s	768m	741s	752s	752m	1000vs	989s
			833w	834w	791s	787m	781m	1068m	1068m
			898w	872w	834w	833w	843w	1171m	1175w
			995m	989m	1005vs	983s*	1005m	1201w	1198w*
			1005vs	1004m	1023w	-	1017m	1335m	1356s
			1070s	1056s 1066s*	1075m	1069s*	1060s*	1441m	1439s
			1177w	1186m	1176w	1176w	1175w	1485w	1494w*
			1310w	1296m*	1201w	1201w	1201w	1517w	-
			1347s	1355vs*	1247w	1249w	1240w*	1595m	1597m
			1369w	-	1352s	1344s	1338s	3016w	3020w
			1440m	1440m*	1437m	1439m*	1436m	3052w	3052w
			1490w	1488m*	1460w	1460w	1454s		
			1534w	1532w	1490w	1490w*	1488m*		
			1600w	1591m	1533w	1528m	1530w		
			3022w	3021w	1599m	1596m	1595w		
			3051w	3047w	3021w	3023w	3022w		
					3057w	3053w	3054w		
$Cation^+$	$Crypt(Cs^+)$			$Crypt(Cs^+)$		$Crypt(Cs^+)$	Bu_3MeP^+		Bu_3MeP^+
	476w	456w		464w		-	464w		464w
	528w	719w		527w*		528w*	712m*		714m*
	581w	767w		-		-	761m		765m
	735m	820m		731m*		733m	-		820m*
	922m	946m		914m		-	940w		944s
	948w	972m		942s		942m	-		973s*
	982m	1009w		964m		983s*	1005m*		1002w
	1038w	1079w		-		-	1060s*		1068m
	1071m	1100m		1066s*		1069s*	-		1099m
	1100s	1205w		1104vs		1106vs	1216w		1198w*
	1127s	1237w		1125s		1126m	1240w*		1230w
	1213w	1279w		-		-	1294s		1278w
	1295m	1311m		1296m*		1298w	1320m		1307m
	1329m	1384m		-		-	1381w		1384m
	1360s	1464m		1355vs*		1354s	1454s*		1460s
	1446m	2878s		1440m*		1439m	2872w		2872w
	1462m	2958s		1473m		1460w	2959w		2960w
	1490w			1488m*		1490w*			
	2790w			2806m		2807m			
	2877w			2868m		2861m			
	2943w			2939m		2941m			
Solvent $C_6H_5CH_3$				731m*		733m*	-		-
				1020w		1020w	1026w		1020w
				1488m*		1490w*	1488m*		1494w*

Abbreviation: w: weak, m: middle, s: strong, vs: very strong.

*: bands are overlapped.

IR spectra of starting metal phthalocyanines and their anion-radical salts

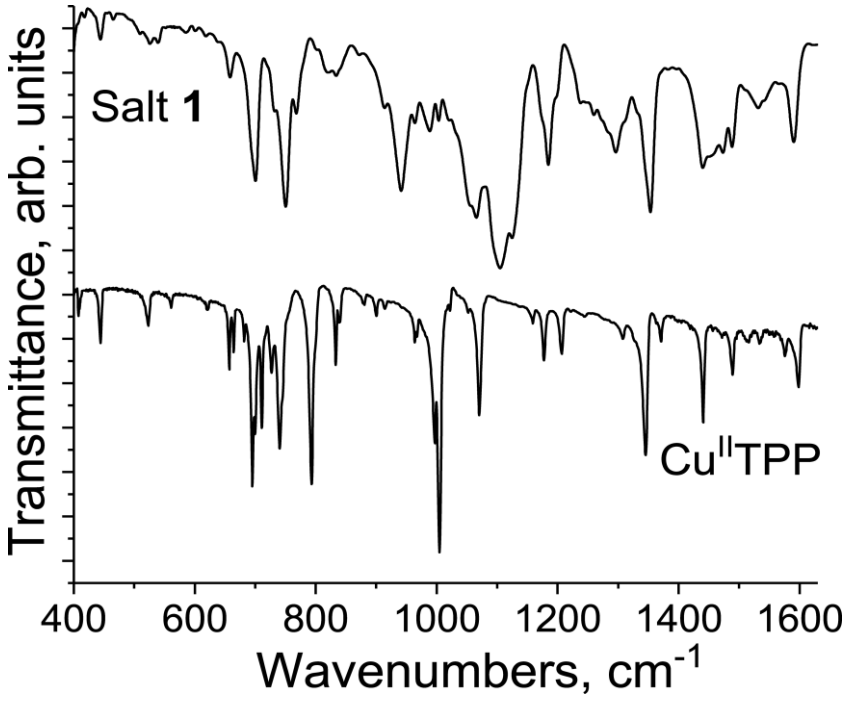

Figure S1. IR spectra of pristine $Cu^{II}(TPP^{2-})$ and salt $\{cryptand(Cs^{+})\}_2\{Cu^{II}(TPP^{4-})\}^{2-}$ (**1**) in KBr pellets. Pellet for **1** was prepared in anaerobic conditions.

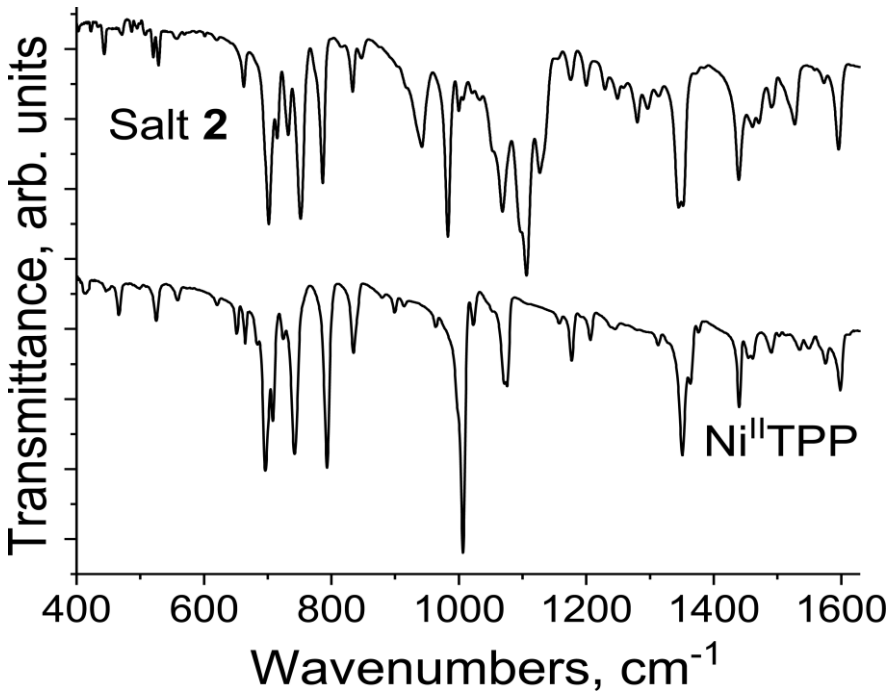

Figure S2. IR spectra of pristine $Ni^{II}(TPP^{2-})$ and salt $\{cryptand(Cs^{+})\}\{Ni(TPP)\}^{-}\cdot C_6H_5CH_3$ (**2**) in KBr pellets. Pellet for **2** was prepared in anaerobic conditions.

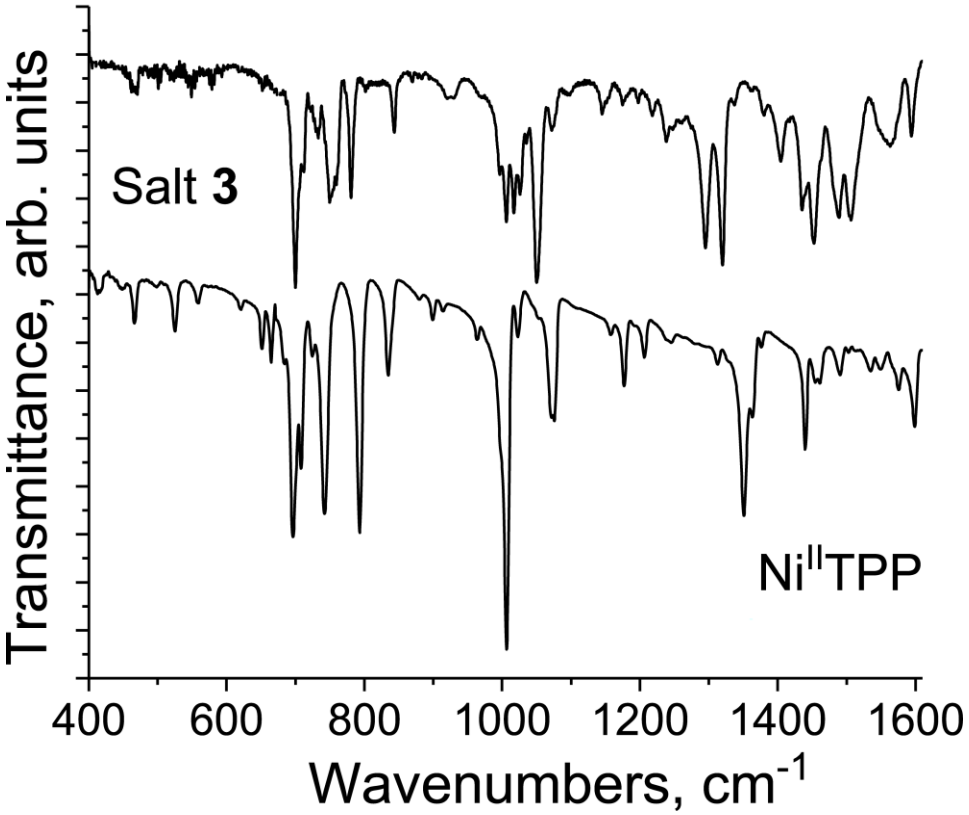

Figure S3. IR spectra of pristine $Ni^{II}(TPP^{2-})$ and salt $(Bu_3MeP^+)\{Ni(TPP)\}^-\cdot C_6H_5CH_3$ (**3**) in KBr pellets. Pellet for **3** was prepared in anaerobic conditions.

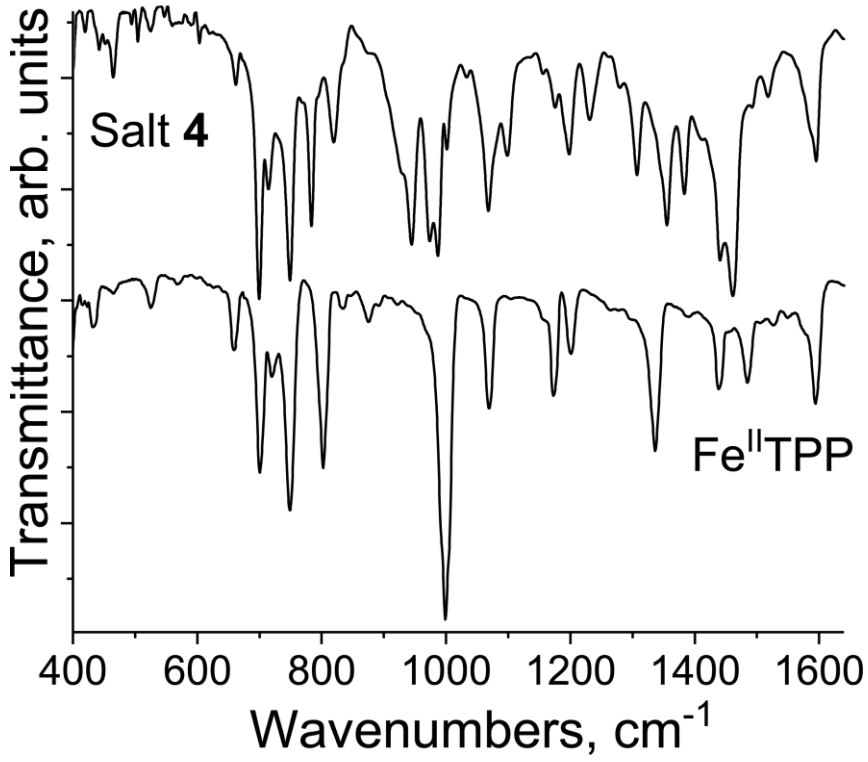

Figure S4. IR spectra of pristine $Fe^{II}(TPP^{2-})$ and salt $(Bu_3MeP^+)\{Fe^{I}(TPP^{2-})\}^-\cdot C_6H_5CH_3$ (**4**) in KBr pellets. Pellets for both compounds were prepared in anaerobic conditions.

Crystal strutures of salts 1 and 2.

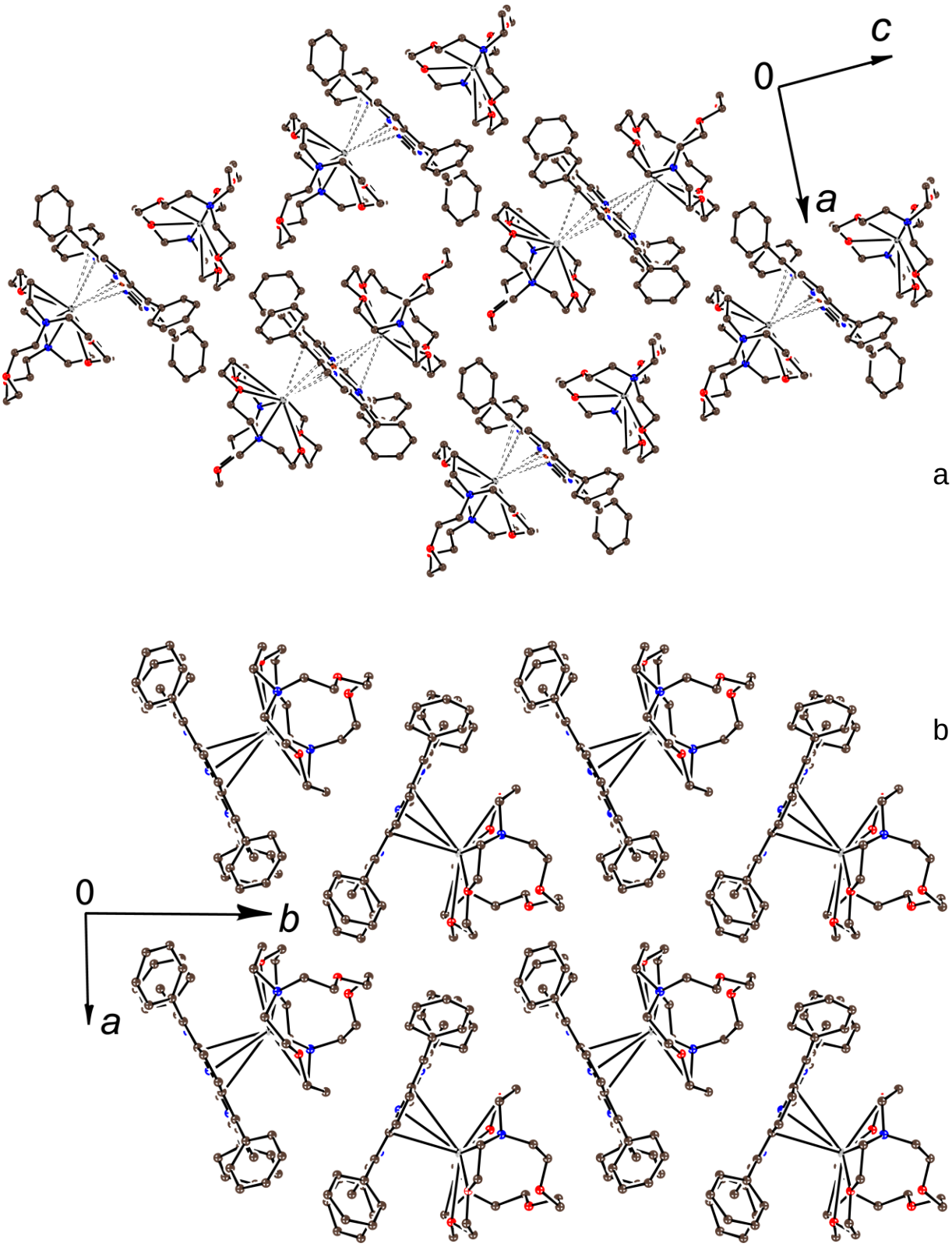

Figure S5. View on the packing of salts **1** (a) and **2** (b).

Crystal strutures of salts 3 and 4.

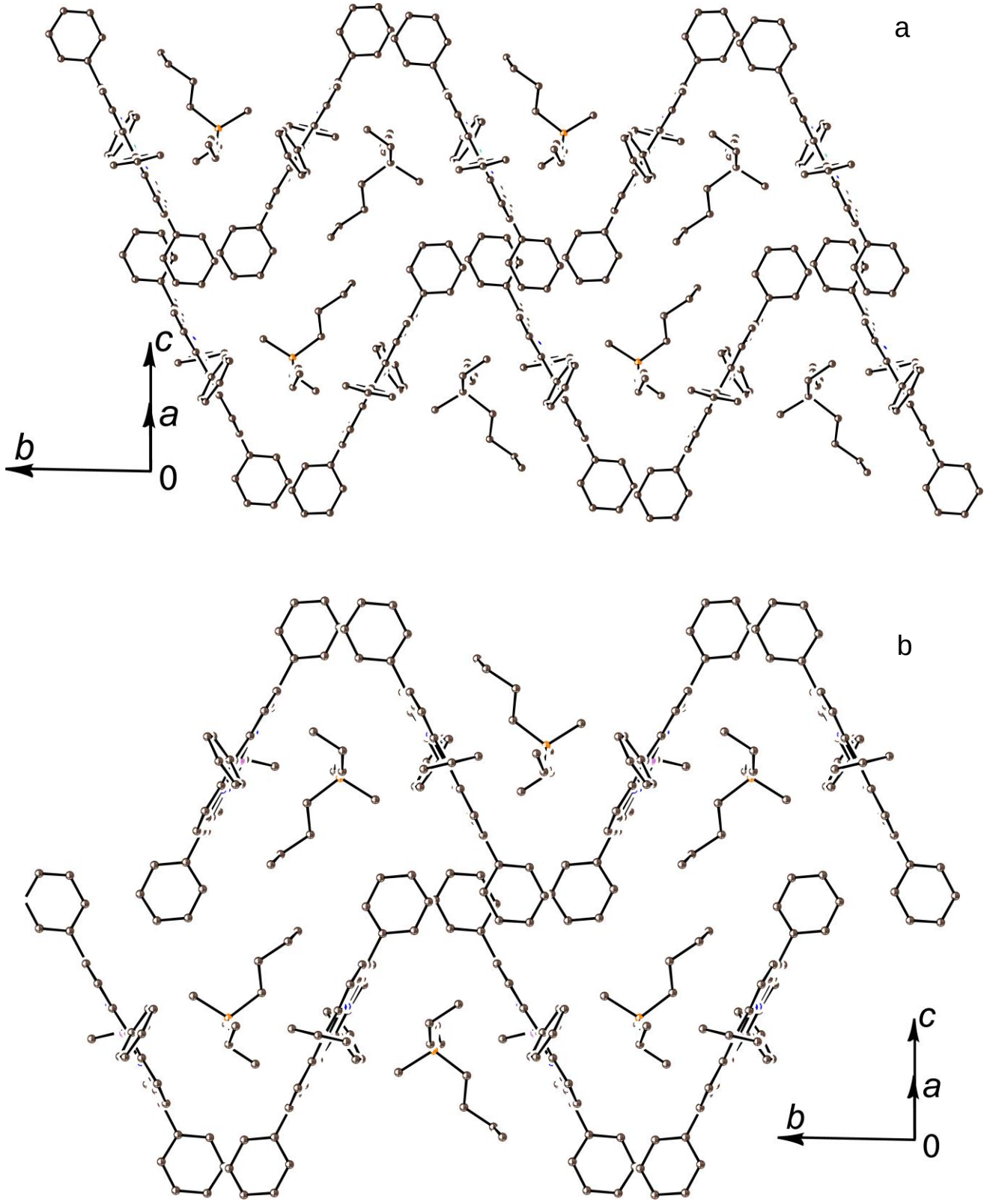

Figure S6. Crystal structures of salts **3** (a) and **4** (b): veiw on the chains of alternated $\{MTPP\}^-$ anions and Bu_3MeP^+ cations appoximately along the porphyrin planes. Solvent $C_6H_5CH_3$ molecules are not shown.

Table S2. Optical spectra of metalloporphyrins and their anionic salts **1** - **4**.

Porphyrin state in salt	Soret band	Q-band	Bands in the NIR range
$Cu^{II}(TPP^{2-})^{0}$	426	546	-
$\{Cu^{II}(TPP^{4-})\}^{2-}$ in **1**	423, ~450 (shoulder)	541, 615, 670	770, 870
$Ni^{II}(TPP^{2-})^{0}$	418	532, 624	-
$\{Ni^{I}(TPP^{2-})\}^{-}$ in **2**	285, 426	575, 650	774, 854
$\{Ni^{I}(TPP^{2-})\}^{-}$ in **3**	283, 422	578, 648	772, 850
$Fe^{II}(TPP^{2-})^{0}$	424	501, 566, 617, 678	-
$\{Fe^{I}(TPP^{2-})\}^{-}$ in **4**	440	- 574, 612, 702	-

UV-spectrum of 3

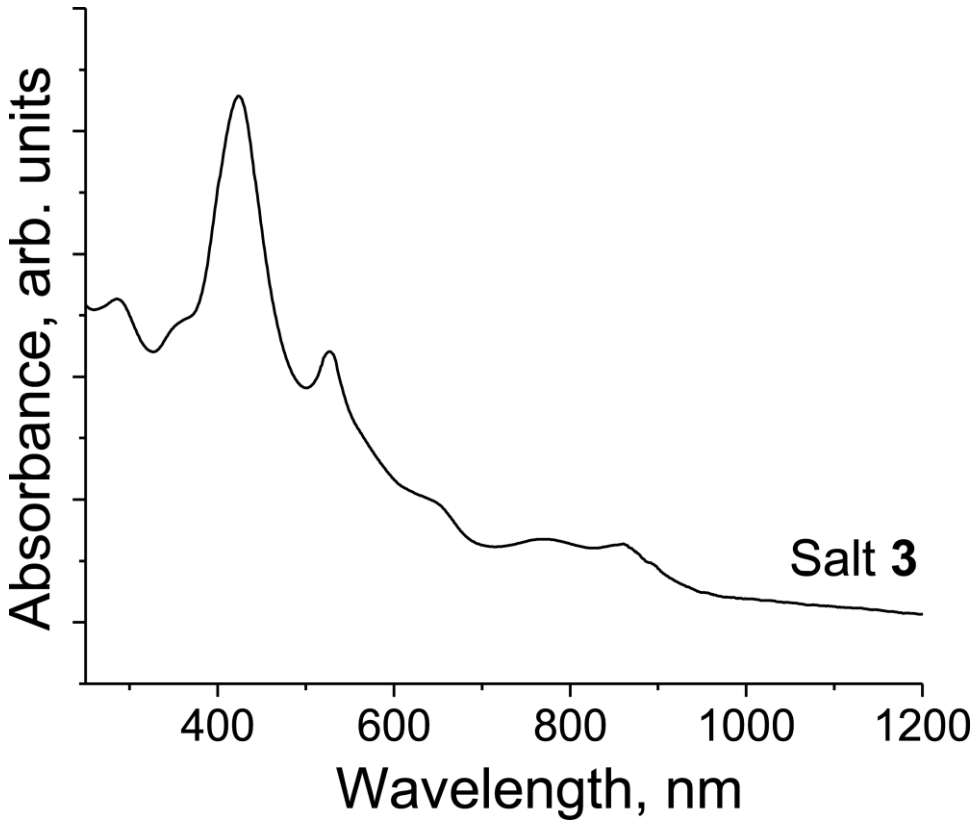

Figure S7. Spectrum of salt **3** in the UV-visible-NIR ranges in KBr pellets prepared in anaerobic conditions.

Magnetic data for salt 1.

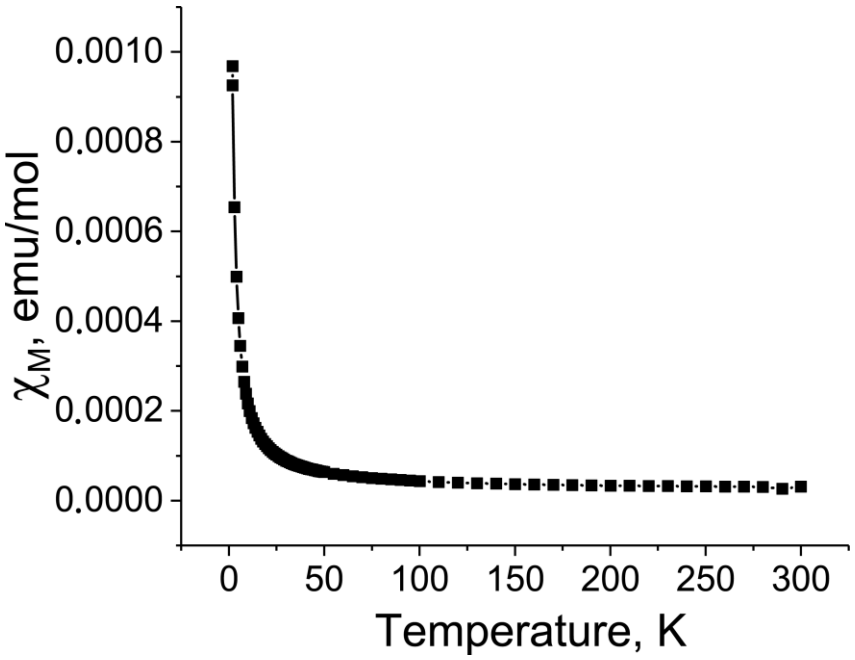

Fig. S8. Temperature dependence of molar magnetic susceptibility of polycrystalline **1** in the 1.9-300 R range.

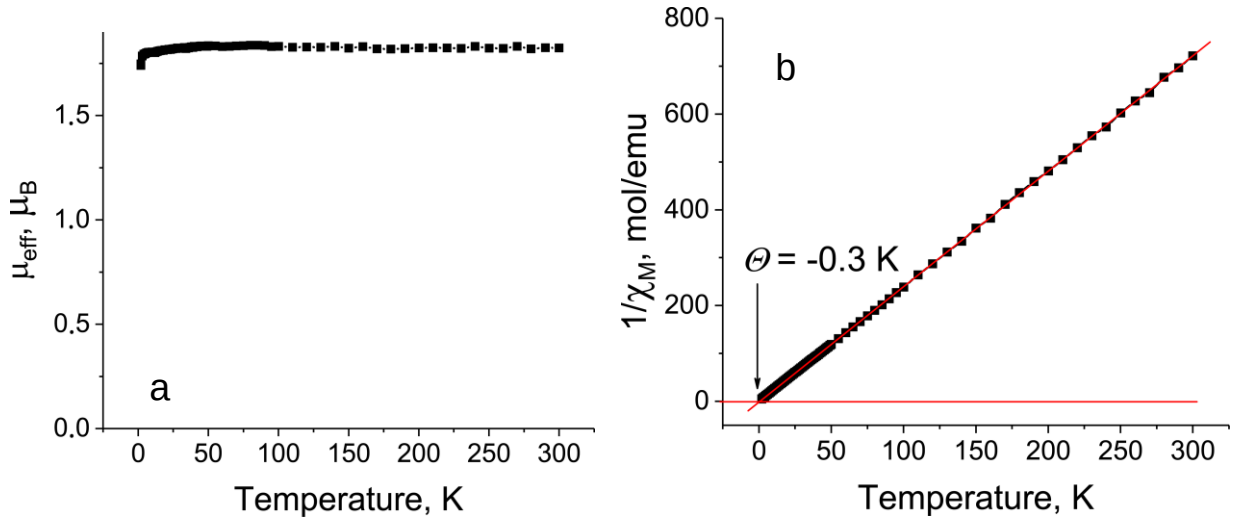

Figure S9. Magnetic data for polycrystalline salt **1**. Temperature dependence of : (a) effective magnetic moment and (b) reciprocal molar magnetic susceptibility in the 1.9-300 K range. Red line in Fig a show approximation of the dependence by the Curie-Weiss law with Weiss temperature of -0.3K.

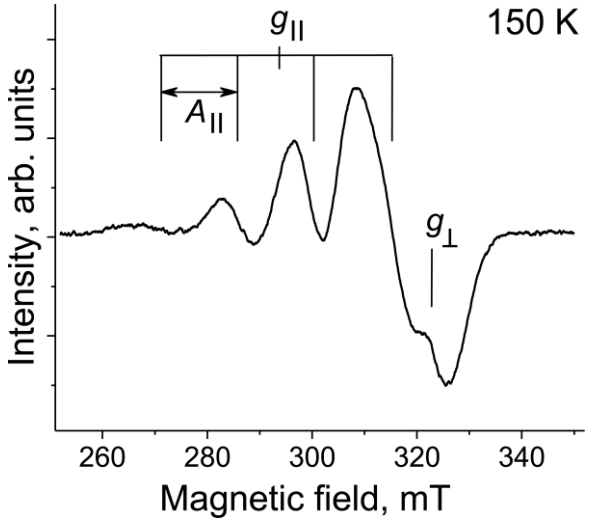

Fig. S10. EPR signal from polycrystalline **1** at 150 K. Determination of *g*-factors and $A_{||}$ is schematically shown.

Magnetic data for salt 2.

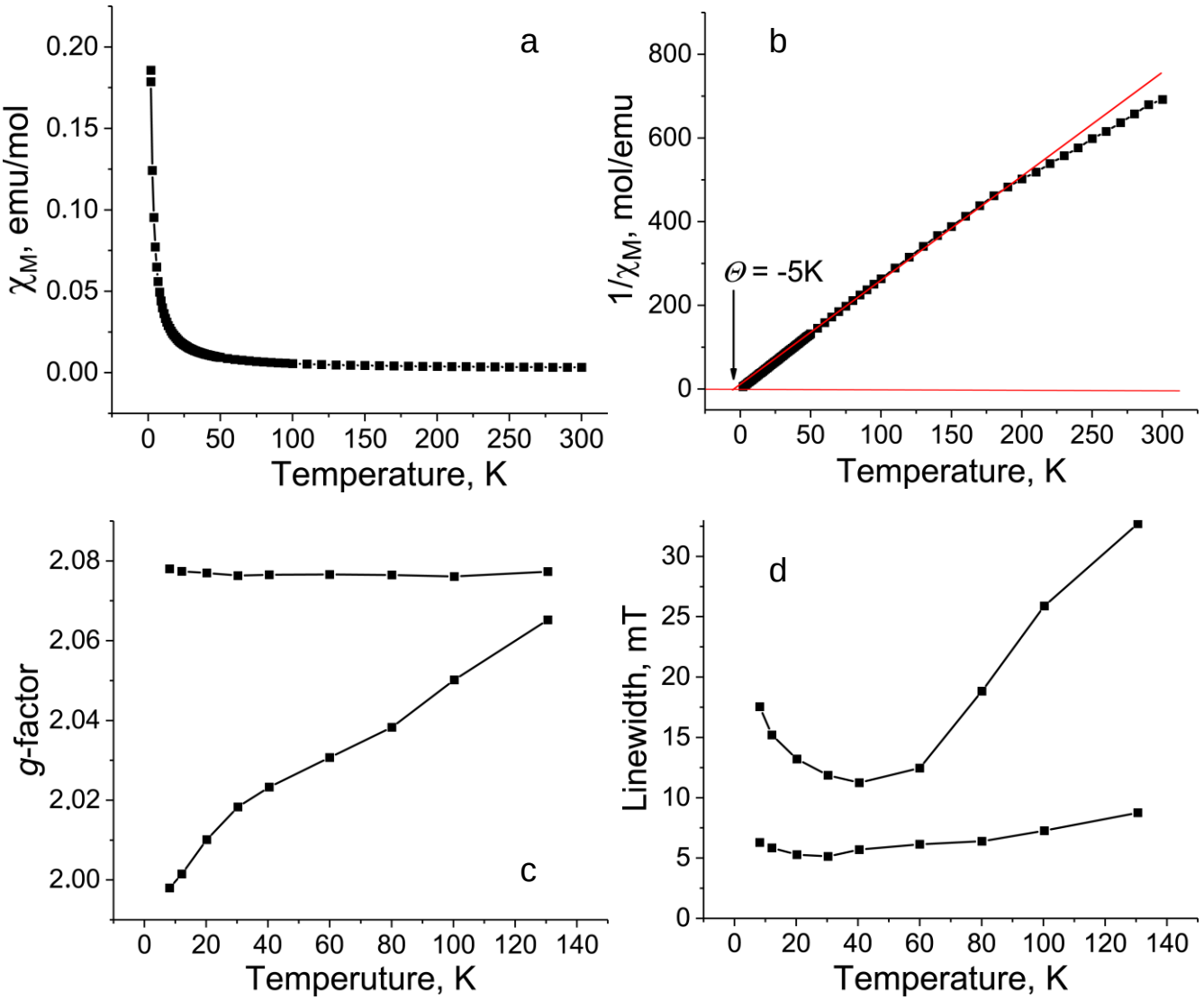

Fig. S11. Temperature dependences of molar magnetic susceptibility (a) and reciprocal molar magnetic susceptibility (b) of polycrystalline salt **2**. Red line shows the Curie-Weiss fit for 20-150 K range. Temperature dependencies of *g*-factor (c) and the linewidth (d) of two broad components of the EPR signal from polycrystalline **2**.

Theoretical calculations.

DFT calculations were performed using the PBE density functional theory[1] with the extended basis set: Fe, Ni Cu [9s9p8d/5s5p4d], C N,O, P [5s5p2d/3s3p2d], H [5s1p/3s1p], Cs {4s,1p}/{2s,1p} for the valence electrons and the SBK pseudopotential[2]. For the systems containing cryptand(Cs^+) units all-electron calculations were performed using scalar relativistic approximation which is based on full four-component one-electron Dirac equation with spin–orbit effects separated out[3]. The energy optimized extended Gaussian basis set of double-polarized quality for the large component, and the corresponding kinetically balanced basis for the small component was used: Cs [30s28p20d/8s7p4d], Ni [21s16p11d5f/6s5p3d1f], C, N, O [10s7p3d/3s2p1d], and H [6s,2p/2s1p][4]. The Hirschfeld method was applied to determine the charge on the atoms.[5] All calculations were carried out using the PRIRODA program[6] at Joint Supercomputer Center of Russian Academy of Sciences. In some cases HSEH1PBE functional implemented into GAUSSIAN 09[7] was used and the calculations have been done at Computational Center of ICPC RAS

References.

1. J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett*., 1996, **77**, 3865.
2. W. J. Stevens, H. Basch, M. Krauss, *J. Chem. Phys.*, 1984, **81**, 6026.
3. K. G. Dyall, *J. Chem. Phys.*, 1994, **100**, 2118
4. D. N. Laikov, *Chem. Phys. Lett.* 2005, **416**, 116.
5. F. L. Hirshfeld, *Theor. Chim. Acta*, 1977, **44**, 129.
6. D. N. Laikov, *Chem. Phys. Lett*. 1997, **281**, 151.
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, et. al., 09, Revision D. 01, Gaussian. Inc., Wallingford, CT., 2009

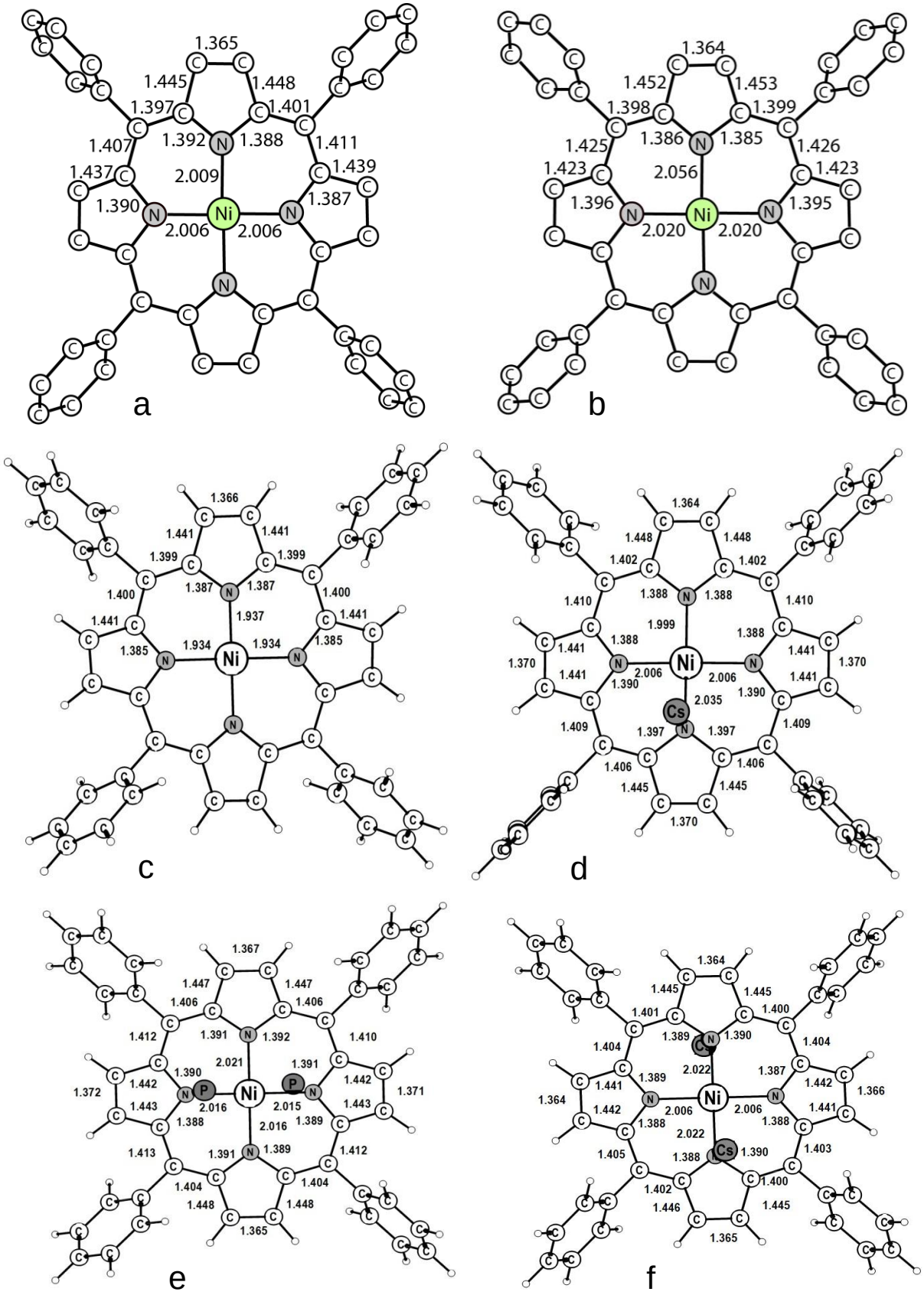

Fig. S12. Calculated structures of: (a) the $\{Ni^{I}(TPP^{2-})\}^{-}$ anion with S = 1/2 state; (b) the $\{Ni^{II}(TPP^{\bullet 3-})\}^{-}$ anion with S = 3/2 state; (c) initial $\{Ni^{II}(TPP^{2-})\}^{0}$, S = 0; (d) $[(Cs^{+})\{Ni^{I}(TPP^{2-})\}^{-}]^{0}$, S = 1/2; (c) $[(Bu_3MeP^{+})_2\{Ni^{I}(TPP^{2-})\}^{-}]^{+}$, S = 1/2; (d) $[\{Crypt(Cs^{+})\}_2\{Ni^{I}(TPP^{2-})\}^{-}]^{+}$, S = 1/2. Hydrogen atoms are omitted for (a) and (b). Only Cs and P atoms of the cations are shown in (c) and (d). All distances are shown in Å.

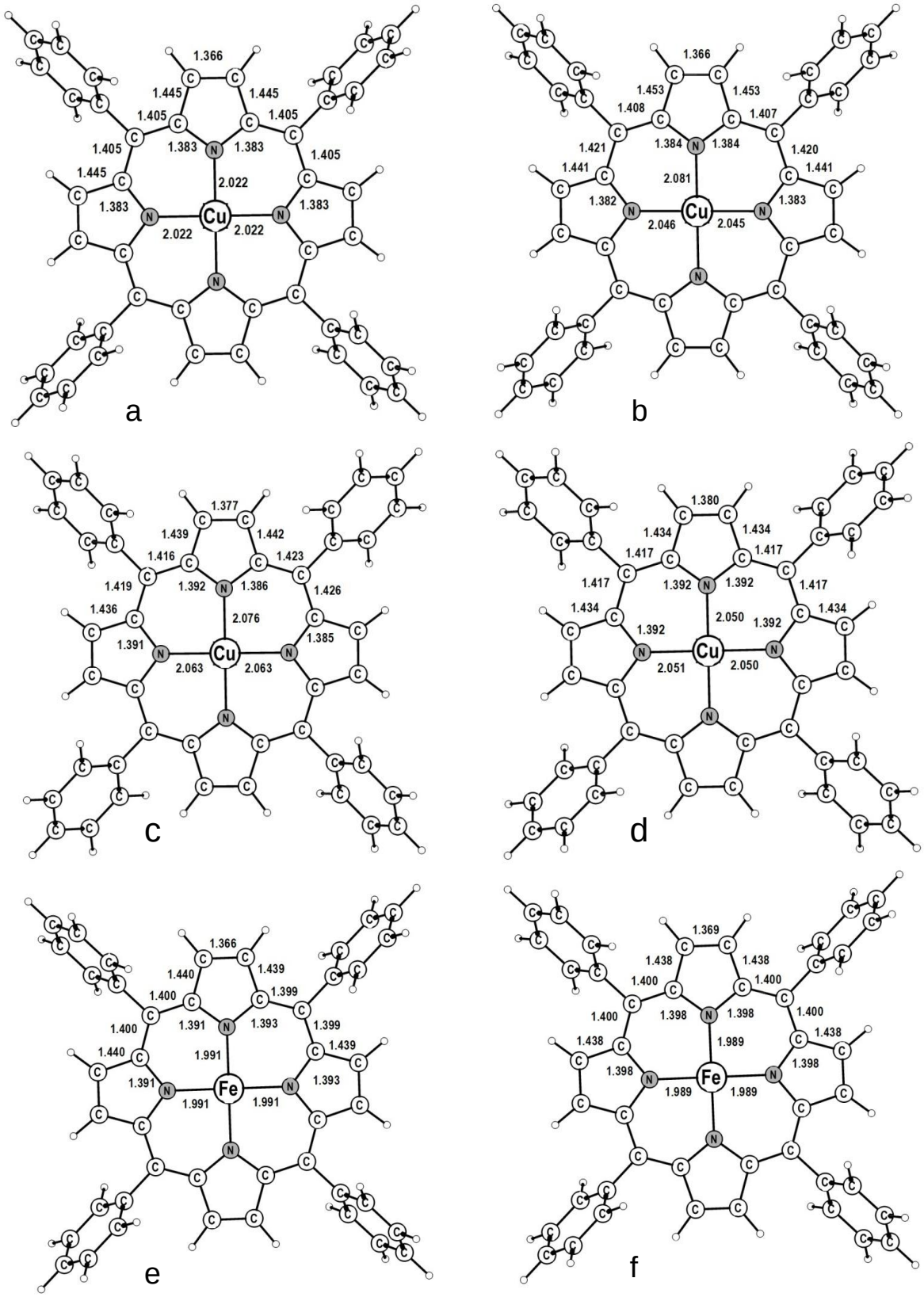

Fig. S13. Calculated structure of the complexes (a) $\{Cu^{II}(TPP^{2-})\}^{0}$, S = 1/2; (b) $\{Cu^{II}(TPP^{\bullet 3-})\}^{-}$, S = 1; (c) $\{Cu^{II}(TPP^{4-})\}^{2-}$, S = 1/2; (d) $\{Cu^{II}(TPP^{4-})\}^{2-}$, S = 3/2; (e) $\{Fe^{II}(TPP^{2-})\}^{0}$, S = 1; (f) $\{Fe^{I}(TPP^{2-})\}^{-}$, S = 1/2. Hydrogen atoms are omitted. All distances are shown in Å.

Table S3. Calculated length of the bonds in metal tetraphenylporphyrins. Types of bonds are given according to Scheme 1.

Complex	Spin state	The average length of the bonds, Å						
		M-N	1	2	Difference 2-1	3	4	Difference 4-3
$Ni^{II}(TPP^{2-})^0$	S = 0	1.934	1.400		0	1.441		0
$\{Ni^{I}(TPP^{2-})\}^-$	S = 1/2	2.007	1.407	1.397	0.010	1.446	1.438	0.008
$\{Ni^{II}(TPP^{\bullet 3-})\}^-$	S = 3/2	2.038	1.425	1.398	0.027	1.453	1.423	0.030
$\{[Crypt(Cs^+)][Ni^{I}(TPP^{2-})]^-\}$	S = 1/2	2.011	1.410	1.404	0.006	1.446	1.441	0.005
$\{[Cryp(Cs^+)]_2[Ni^{I}(TPP^{2-})]^-\}^+$	S = 1/2	2.014	1.404	1.401	0.003	1.445	1.442	0.003
$\{[Bu_3MeP^+]_2[Ni^{I}(TPP^{2-})]^-\}^+$	S = 1/2	2.017	1.412	1.406	0.006	1.447	1.442	0.005
$\{Cu^{II}(TPP^{2-})\}^0$	S = 1/2	2.022	1.405	1.405	0	1.445	1.445	0
$\{Cu^{II}(TPP^{3-})\}^-$	S = 1	2.063	1.421	1.408	0.013	1.453	1.441	0.012
$\{Cu^{II}(TPP^{4-})\}^{2-}$	S = 1/2	2.070	1.419	1.416	0.003	1.439	1.436	0.003
$\{Cu^{II}(TPP^{4-})\}^{2-}$	S = 3/2	2.070	1.417	1.417	0	1.434	1.434	0
$\{Fe^{II}(TPP^{2-})\}$	S = 1	1.991	1.400	1.399	0.001	1.440	1.440	0
$\{Fe^{I}(TPP^{2-})\}^-$	S = 1/2	1.989	1.400	1.400	0	1.438	1.438	0

Charge on the Fe^{II} atom is appreciably higher in $Fe^{II}(TPP^{2-})\}^0$ compared to the neutral $\{Ni^{II}(TPP^{2-})\}^0$ complex. That leads to its greater electron affinity, 1.96 eV, compared to that of the nickel analog, 1.64 eV. The excited quintet S = 2 state of $\{Fe^{II}(TPP^{2-})\}^0$ is positioned by 0.38 eV higher, than the ground S = 1 state. The spin density on the metal atom increases from 2.097 (S =1) to 3.537 (S = 2). Due to the population of a strongly delocalized x^2-y^2 orbital, charge on the metal atom increases in the excited state to 0.255. In both complexes $\{Fe^{II}(TPP^{2-})\}^0$ (S = 1) and $\{Fe^{I}(TPP^{2-})\}^-$ (S = 1/2), the value of a spin density on the metal atom is higher than the formal theoretical values, that is due to the noticeable nonequivalence of similar orbitals populated with the electrons with opposite spin orientations.

Cartesian coordinates of the considered systems

$\{Ni^{II}(TPP^{2-})\}^{0}$

charge=0 mult=1

28	2.62588179	10.54135049	18.39888505
7	2.84595201	8.64655336	18.69031759
7	3.51350086	10.37511136	16.68904647
6	3.03160457	14.95192695	12.09318729
6	7.25436714	5.15905959	15.41236571
6	3.52100341	11.29544912	15.65422098
6	4.33781735	10.82340891	14.56440099
1	4.51186774	11.36574824	13.64070353
6	4.87541077	9.63166237	14.95978334
1	5.56785086	8.99641306	14.41763484
6	4.32594636	9.33570629	16.25886588
6	4.50292234	8.11922957	16.92642645
6	3.72101791	7.79154228	18.03998124
6	3.59352915	6.45180387	18.55584289
1	4.17133293	5.59885916	18.21484937
6	2.59850199	6.48075476	19.49142956
1	2.21310618	5.66074824	20.08866339
6	2.15986693	7.84995705	19.59268052
6	2.97662384	12.58404139	15.70151239
6	3.00076312	13.41818043	14.46083687
6	3.88419266	14.50456201	14.32155887
1	4.57014250	14.74416684	15.13603266
6	3.89933867	15.26481531	13.14665135
1	4.59528953	16.10044189	13.05297880
6	2.15200117	13.87022911	12.21973355
1	1.47225241	13.61819312	11.40381240
6	2.13897982	13.10719815	13.39293314
1	1.45306701	12.26363937	13.49014427
6	5.45127532	7.09748716	16.38701226
6	5.19742442	6.42619539	15.17664955
1	4.28666274	6.65363691	14.61979413
6	6.09190180	5.46421277	14.69393388
1	5.87647619	4.94856672	13.75632949
6	7.51462500	5.81867357	16.61945819
1	8.41816167	5.58766393	17.18650774
6	6.61864155	6.77808980	17.10475632
1	6.82264097	7.29146091	18.04619241
7	2.40358926	12.44349140	18.10585834
7	1.74003944	10.69501932	20.11096407
6	-0.82168857	5.39029494	22.96402634
6	1.01477272	16.41793869	23.11643976
6	1.16517034	9.67592551	20.85683798
6	0.52039953	10.21263877	22.02870356
1	-0.03075972	9.62861756	22.75816069
6	0.76573112	11.55632119	22.03543514
1	0.44469596	12.29457641	22.76317011
6	1.49177024	11.85455666	20.82641158
6	1.73066691	13.15882500	20.37849065
6	2.08715051	13.40973790	19.04922233

6	2.03746558	14.71375425	18.43722444
1	1.83194555	15.64035297	18.96256827
6	2.24922060	14.53229094	17.10032977
1	2.25383686	15.28147206	16.31579393
6	2.52356209	13.13058827	16.90694970
6	1.28488091	8.30922052	20.58382186
6	0.55962084	7.30747177	21.42349574
6	-0.48034751	6.54648090	20.85773058
1	-0.75021603	6.70724427	19.81238602
6	-1.16733143	5.59752235	21.62321558
1	-1.97500907	5.02006143	21.16988416
6	0.21614443	6.13742876	23.53435124
1	0.49825454	5.97627798	24.57639171
6	0.90137471	7.08930281	22.77073123
1	1.71767270	7.66163095	23.21502884
6	1.47481840	14.29663391	21.31445476
6	2.35355608	14.52930527	22.38835401
1	3.22077250	13.87915675	22.51772929
6	2.12711643	15.58388522	23.28025245
1	2.82256595	15.75326519	24.10424948
6	0.12947915	16.18999267	22.05581002
1	-0.74541561	16.82955393	21.92572109
6	0.35752453	15.13814496	21.16125219
1	-0.34088522	14.95662253	20.34223946
1	0.83676643	17.23895790	23.81294990
1	3.04346646	15.54579115	11.17772474
1	-1.35580780	4.64883380	23.56055049
1	7.95180780	4.40942191	15.03487045

$\{Ni^{I}(TPP^{2-})\}^{-}$ *S* = 1/2

charge=-1 mult=2

28	2.62373609	10.52008283	18.39795084
7	2.81404076	8.54360182	18.68632455
7	3.42894269	10.33666905	16.56690054
6	4.61572407	15.46625588	12.71535432
6	5.87566865	4.70179706	14.38644874
6	3.76720763	11.36037464	15.69292493
6	4.56260254	10.85207243	14.59500762
1	4.98520527	11.45329618	13.79611523
6	4.71252512	9.51179305	14.80142492
1	5.26716947	8.80226836	14.19497088
6	4.00936016	9.19453367	16.02348202
6	3.98816966	7.91494636	16.58459223
6	3.43174240	7.62554611	17.84448247
6	3.41463577	6.31108873	18.42425874
1	3.80652394	5.41191866	17.95925081
6	2.78779657	6.42306116	19.64009735
1	2.62576454	5.64312023	20.37722461
6	2.41719546	7.80545847	19.79115701
6	3.45955031	12.71753490	15.85234091
6	3.85649913	13.66794815	14.77294228
6	4.77529473	14.70912295	15.01849497
1	5.19981659	14.81110514	16.01869251

6	5.15105746	15.59626855	14.00402677
1	5.87097418	16.38913743	14.21984214
6	3.70124522	14.43780242	12.45518998
1	3.27162762	14.32699938	11.45684887
6	3.32657370	13.55133197	13.47142851
1	2.60999446	12.75432750	13.26511647
6	4.63940500	6.80141914	15.82811619
6	4.09381398	6.33568452	14.61627511
1	3.18093637	6.79895823	14.23752170
6	4.70464850	5.29746440	13.90218432
1	4.26118274	4.95149845	12.96574691
6	6.42947875	5.15474754	15.59122953
1	7.34585328	4.70201884	15.97660528
6	5.81674044	6.19206092	16.30367134
1	6.25068452	6.54493169	17.24086805
7	2.43308472	12.49643485	18.10901039
7	1.81911407	10.70260051	20.22941639
6	0.57805976	5.56257390	24.05098392
6	-0.59010734	16.34446733	22.43093202
6	1.47334119	9.67831220	21.09996991
6	0.68109454	10.18877043	22.19929944
1	0.25402428	9.58818846	22.99628961
6	0.54263689	11.53106893	21.99830156
1	-0.00664170	12.24280273	22.60706321
6	1.24737991	11.84705318	20.77684876
6	1.27265127	13.12742030	20.21751352
6	1.82151584	13.41557827	18.95416823
6	1.83336796	14.72911726	18.37218483
1	1.44480277	15.62881312	18.83895403
6	2.44887259	14.61516087	17.15076609
1	2.60367422	15.39373689	16.41068489
6	2.81969234	13.23286424	16.99931053
6	1.77256645	8.31983246	20.93592979
6	1.36314894	7.36668623	22.00826137
6	0.43850737	6.33347205	21.75118280
1	0.02056890	6.23934707	20.74745534
6	0.05002136	5.44342551	22.75826016
1	-0.67405937	4.65686723	22.53347910
6	1.49823714	6.58290389	24.32259820
1	1.92238227	6.68508029	25.32419572
6	1.88583306	7.47213955	23.31361779
1	2.60623251	8.26322346	23.52920476
6	0.62984170	14.24269443	20.97883138
6	1.18687201	14.70754790	22.18574729
1	2.10213354	14.24252393	22.55654347
6	0.58409628	15.74690471	22.90504474
1	1.03623316	16.09215823	23.83758908
6	-1.15532405	15.89224477	21.23118694
1	-2.07438562	16.34636030	20.85390829
6	-0.55063796	14.85374390	20.51355761
1	-0.99355309	14.50128787	19.58040871
1	-1.06132657	17.15490302	22.99106308
1	4.90832069	16.15879087	11.92335453

1	0.27554813	4.86779834	24.83727813
1	6.35311042	3.89220196	13.83038998

{$Ni^{I}(TPP^{2-})$}$^{-}$ *S* = 3/2

charge=-1 mult=4

28	2.62373155	10.51952316	18.39778601
7	2.86588853	8.50177024	18.71080443
7	3.52481641	10.34614735	16.59796300
6	4.59112743	15.48379672	12.70560586
6	5.81100415	4.65427520	14.34736541
6	3.84334092	11.38076222	15.71694574
6	4.62599397	10.88234775	14.63872337
1	5.03697042	11.47436244	13.82702495
6	4.78407421	9.51678558	14.84776433
1	5.34433449	8.81899244	14.23346432
6	4.09585943	9.19690636	16.05159379
6	4.05260147	7.89054529	16.62200333
6	3.48098030	7.59496937	17.86409025
6	3.42500634	6.26290012	18.44206194
1	3.81526826	5.36024736	17.98207339
6	2.79567781	6.37600685	19.64649198
1	2.59152118	5.58633599	20.36314822
6	2.43416091	7.77334255	19.80783635
6	3.48863825	12.75175885	15.87706125
6	3.87637189	13.69180857	14.78336022
6	4.80776627	14.72674803	15.00358275
1	5.25897474	14.82674282	15.99236825
6	5.15849700	15.61451580	13.97883195
1	5.88333836	16.40776218	14.17641673
6	3.66984731	14.45409115	12.46815428
1	3.21522480	14.34365642	11.48093567
6	3.32015136	13.56918917	13.49383071
1	2.59899032	12.77158182	13.30649139
6	4.66621556	6.77890609	15.83768241
6	4.14275987	6.40467425	14.58279847
1	3.27751066	6.94390383	14.19299499
6	4.70473547	5.35574777	13.84751143
1	4.27166804	5.07945162	12.88334422
6	6.34778754	5.01806333	15.58821156
1	7.21511711	4.48616703	15.98624787
6	5.78488788	6.06993220	16.32147040
1	6.21411215	6.35648341	17.28321062
7	2.38058092	12.53689947	18.08429394
7	1.72279321	10.69325251	20.19764221
6	0.67094625	5.56159669	24.09978694
6	-0.59537726	16.37984355	22.43003790
6	1.41212157	9.65988446	21.08269533
6	0.63220639	10.15812554	22.16316871
1	0.22820294	9.56667291	22.97878094
6	0.46662804	11.52212216	21.95047673
1	-0.09465986	12.21914216	22.56468572
6	1.14836306	11.84139805	20.74278537
6	1.18545724	13.14631419	20.16898959

6	1.75877680	13.44218752	18.92777494
6	1.81112873	14.77371379	18.34834410
1	1.41494883	15.67520309	18.80559126
6	2.44642205	14.66192541	17.14693581
1	2.64993953	15.45124489	16.42978336
6	2.81430063	13.26591355	16.98845483
6	1.76658078	8.28902168	20.92236270
6	1.38212186	7.34996713	22.01825828
6	0.43986946	6.32367733	21.80494150
1	-0.02042958	6.22815796	20.81989993
6	0.09112611	5.43728218	22.83156269
1	-0.64245808	4.65069839	22.64002339
6	1.60293054	6.58311758	24.33049088
1	2.06709419	6.68863666	25.31378986
6	1.95086540	7.46646021	23.30279589
1	2.67969248	8.25840382	23.48459548
6	0.56442884	14.25700138	20.94908142
6	1.08579556	14.64084758	22.20183244
1	1.95533331	14.11006334	22.59366921
6	0.51633827	15.68900657	22.93253514
1	0.94774540	15.97304108	23.89519393
6	-1.13004242	16.00644781	21.19112770
1	-2.00142933	16.53006288	20.79100095
6	-0.55955877	14.95548086	20.46245312
1	-0.98656260	14.66132922	19.50201461
1	-1.04044720	17.19841523	22.99958074
1	4.86443437	16.17515722	11.90568745
1	0.39890854	4.87144141	24.90118096
1	6.25024973	3.83498943	13.77433750

$(Cs^{+})\{Ni^{I}(TPP^{2-})\}^{-}$ $S = 1/2$
charge=0 mult=2

28	2.61951340	7.38450385	19.77515550
7	4.38256371	7.41498939	20.73238368
7	3.18529464	5.76463675	18.75025450
6	-0.58246686	3.01134334	14.20910867
6	9.13453581	3.17633508	19.31886493
6	2.50432216	5.17316342	17.69545927
6	3.36726884	4.25166858	16.98590604
1	3.08990270	3.68581842	16.10203648
6	4.57451551	4.27131480	17.62101803
1	5.47460229	3.72558277	17.35580108
6	4.45506279	5.20482458	18.72177815
6	5.49949041	5.49703764	19.60963864
6	5.43264757	6.52141637	20.57567387
6	6.46669745	6.77784788	21.54622672
1	7.37382015	6.19432138	21.66688560
6	6.05081027	7.84557739	22.29804108
1	6.58315814	8.33556450	23.10739343
6	4.76678297	8.24390815	21.78001248
6	1.17468936	5.42805669	17.33243358
6	0.56414084	4.59559768	16.25179133
6	0.14869836	5.17307920	15.03625911

1	0.28063293	6.24633286	14.88711985
6	-0.41608494	4.38961465	14.02395233
1	-0.72339691	4.85653952	13.08603255
6	-0.17684303	2.42447295	15.41386951
1	-0.30778495	1.35216822	15.57170647
6	0.39291668	3.20831523	16.42362303
1	0.70385063	2.74847445	17.36324880
6	6.75818449	4.69712260	19.51092741
6	6.75225089	3.31239351	19.76710552
1	5.81513569	2.82958973	20.04947948
6	7.92867922	2.55995652	19.67440971
1	7.90281388	1.48908508	19.88523969
6	9.15447752	4.55257648	19.05975819
1	10.08812270	5.04240540	18.77600253
6	7.97869146	5.30456297	19.15773301
1	7.99665796	6.37622954	18.95131828
7	0.83545665	7.36368537	18.85739152
7	2.10118909	9.11694066	20.70817750
6	5.68944646	11.61020061	25.55853265
6	-3.97379581	11.49011018	20.42297922
6	2.81343191	9.77163464	21.71572951
6	2.03939875	10.87169063	22.24346969
1	2.35107674	11.52768040	23.05108648
6	0.82889712	10.85590664	21.60113979
1	-0.02796696	11.49626061	21.78929592
6	0.85436283	9.74579086	20.67647999
6	-0.26559440	9.31396104	19.94479926
6	-0.26405832	8.17364949	19.11707228
6	-1.40666811	7.73824196	18.35513533
1	-2.38564031	8.20722986	18.36337546
6	-0.99750029	6.66582225	17.60633910
1	-1.59612736	6.05786169	16.93558028
6	0.39236849	6.44474290	17.91668718
6	4.05618233	9.37161318	22.23672957
6	4.62692969	10.15086658	23.38063478
6	4.64095180	9.60433273	24.67789786
1	4.23127298	8.60507154	24.83499506
6	5.16606251	10.32612488	25.75558618
1	5.16310950	9.88419433	26.75375463
6	5.68426765	12.16594031	24.27388568
1	6.09500754	13.16379593	24.10751071
6	5.15811973	11.44074707	23.19809326
1	5.16337602	11.87635468	22.19597633
6	-1.54767192	10.07073815	20.10251039
6	-1.71594203	11.35276180	19.54817004
1	-0.89531937	11.79808013	18.98050345
6	-2.91498554	12.05812250	19.70504013
1	-3.02369637	13.05009815	19.26199391
6	-3.82213172	10.21366814	20.97919863
1	-4.64073915	9.76241734	21.54304547
6	-2.62206151	9.51173511	20.82024568
1	-2.50592584	8.51859757	21.25751328
1	-4.90994785	12.03704307	20.54717501

1	-1.02496223	2.39985880	13.42071947
1	6.09894264	12.17272589	26.39926137
1	10.05165233	2.58924211	19.24471534
55	3.24961559	11.01315264	18.49223733

$[(Bu_3MeP^+)_2\{Ni^I(TPP^{2-})\}^-]^+$, S =1/2
charge=1 mult=2

28	0.16839528	-0.42099121	0.92708390
7	-0.07278467	-0.97015113	2.85062746
7	2.16938921	-0.62114390	1.12307680
6	6.29682011	0.75544945	-3.73347282
6	5.01337016	-2.16290501	6.77818629
6	3.13272245	-0.24236254	0.19351076
6	4.43872172	-0.18557490	0.81330422
1	5.35713003	0.11593042	0.31937006
6	4.27637542	-0.55790912	2.11853666
1	5.03879815	-0.62140167	2.88884290
6	2.86982696	-0.83970234	2.30545019
6	2.30800727	-1.24487609	3.52955116
6	0.91921887	-1.32186626	3.76070289
6	0.33018719	-1.74836523	5.00590142
1	0.87612479	-2.11568393	5.86909267
6	-1.02812435	-1.62343623	4.86779944
1	-1.79020943	-1.82690390	5.61342865
6	-1.27141423	-1.13361436	3.53287055
6	2.89449331	0.04370038	-1.16213862
6	4.07000000	0.28889923	-2.05291499
6	4.23852423	1.52686285	-2.70366030
1	3.49866918	2.31442961	-2.54910429
6	5.34111636	1.75906122	-3.53289621
1	5.45571752	2.72846478	-4.02109561
6	6.14233489	-0.48063799	-3.09454783
1	6.88180029	-1.26939069	-3.24461148
6	5.04141390	-0.70978293	-2.26171316
1	4.92996548	-1.67416574	-1.76187676
6	3.23777845	-1.56138023	4.65844791
6	4.15318801	-2.62657349	4.55653055
1	4.16980002	-3.22614884	3.64495347
6	5.02970935	-2.92648667	5.60502172
1	5.72602366	-3.76115141	5.50648611
6	4.11032988	-1.09931206	6.89448026
1	4.09056553	-0.49685767	7.80454204
6	3.23154524	-0.80479325	5.84629227
1	2.52551493	0.02190004	5.94727585
7	0.40704691	0.05640458	-1.01741349
7	-1.82145872	-0.15440926	0.74657675
6	-5.95873361	-1.33301651	5.64417809
6	-4.65681293	1.10573014	-4.99577627
6	-2.78741126	-0.35954472	1.72391858
6	-4.11097193	-0.13518284	1.18086408
1	-5.04136205	-0.23194155	1.73118627
6	-3.95198673	0.18115373	-0.13705738
1	-4.72780381	0.41165521	-0.85988736

6	-2.53140077	0.13601759	-0.41383425
6	-1.97720777	0.31598968	-1.69113288
6	-0.59261104	0.24303099	-1.96274846
6	-0.01919260	0.37842637	-3.27946997
1	-0.57640150	0.53130714	-4.19852371
6	1.34358223	0.31537644	-3.13020161
1	2.09788849	0.36606856	-3.90924019
6	1.60235246	0.12984045	-1.72384562
6	-2.55151996	-0.81312136	3.03155726
6	-3.73034200	-0.99683823	3.93666985
6	-4.12986682	-2.27924230	4.35773166
1	-3.57094827	-3.15162329	4.01391880
6	-5.23346033	-2.44613131	5.20194451
1	-5.53023412	-3.44976099	5.51155958
6	-5.57367108	-0.05173533	5.23213769
1	-6.13303583	0.82257222	5.57009959
6	-4.47080407	0.11295363	4.38601525
1	-4.17962387	1.11409024	4.06057030
6	-2.90433655	0.58721167	-2.83607298
6	-2.86933956	1.81944002	-3.51636964
1	-2.15627055	2.58229794	-3.19904863
6	-3.73602952	2.07692632	-4.58445691
1	-3.69551573	3.04161311	-5.09337335
6	-4.70460783	-0.12376815	-4.32810306
1	-5.42202584	-0.88625482	-4.63737202
6	-3.83675733	-0.37905940	-3.25997061
1	-3.88752959	-1.33616513	-2.73652074
1	-5.33393640	1.30699681	-5.82719390
1	7.15608515	0.93584095	-4.38110867
1	-6.81928123	-1.46356704	6.30198963
1	5.69757802	-2.39513464	7.59555163
15	0.28367756	-4.19726671	-1.64417097
6	0.03237845	-6.01232750	-1.83964483
1	-1.01678843	-6.14953299	-2.14881097
1	0.11963402	-6.44760204	-0.83076752
6	1.98050535	-3.85480519	-1.03482206
1	2.65587467	-4.13303741	-1.85985236
1	2.03578323	-2.75893701	-0.91573724
6	-0.93755435	-3.57323993	-0.44517545
1	-0.88844582	-4.17681529	0.47098983
1	-0.69534556	-2.52312884	-0.19117847
1	-1.94810877	-3.63552859	-0.86970559
1	1.57929380	-8.50028116	-4.92352424
6	1.67834929	-8.91082116	-3.90728761
1	2.72790101	-8.79425385	-3.59748876
1	0.82267205	-8.66500371	-1.92795840
6	0.72792885	-8.21110929	-2.92877157
1	-0.31677466	-8.37232038	-3.24382945
6	0.99518590	-6.69975507	-2.82345811
1	2.03827009	-6.53893501	-2.50321050
1	0.89955635	-6.24580938	-3.82407783
1	1.46485231	-9.98721718	-3.96108416
1	2.16275695	-5.64844246	0.20211982

6	2.35467356	-4.56425750	0.28008945
1	1.71676615	-4.17781787	1.08988689
1	3.97366818	-4.76525567	1.67509704
6	3.83268977	-4.35159844	0.66372105
1	4.03828336	-3.27168629	0.73819788
1	5.86548669	-4.86714523	0.07161002
6	4.83734154	-5.01449541	-0.28755057
1	4.66569266	-6.10020005	-0.36097712
1	4.79336871	-4.59607966	-1.30492328
1	0.93977919	-3.69442348	-3.88168025
6	0.08425103	-3.36473373	-3.26837854
1	0.22329261	-2.28463628	-3.08651853
6	-1.24652893	-3.64365906	-3.98953563
1	-1.39908134	-4.72992045	-4.11002369
1	-2.08818147	-3.26923710	-3.38443660
6	-1.29021969	-2.97923756	-5.37662877
1	-0.43078260	-3.33223415	-5.97193604
1	-1.15977842	-1.89186607	-5.25815251
6	-2.59438530	-3.27158928	-6.12684567
1	-3.46610076	-2.89484631	-5.57143702
1	-2.59572763	-2.79071891	-7.11483675
1	-2.73505051	-4.35262783	-6.28085082
15	0.48634389	3.32796922	3.52113540
6	0.68291488	5.08254840	4.04472902
1	1.30667340	5.56898069	3.27707455
1	1.28117997	5.06571163	4.97059187
6	-0.44657407	2.38527844	4.79085882
1	-1.48945390	2.73399756	4.72813397
1	-0.43648572	1.33704301	4.44505781
6	2.14785628	2.60382182	3.31528961
1	2.68182246	2.60982818	4.27446308
1	2.04137994	1.57104143	2.95107311
1	2.71511457	3.19241661	2.58231934
1	-2.30008599	8.11627744	4.00038164
6	-1.69996777	8.07178485	4.92175685
1	-2.31541925	7.59967345	5.70240081
1	0.19939192	7.29624521	5.62910466
6	-0.39448488	7.29926195	4.69959851
1	0.21946420	7.81391888	3.94147073
6	-0.63610679	5.84763510	4.25103258
1	-1.25604443	5.33453202	5.00544689
1	-1.21842414	5.85102226	3.31459633
1	-1.49705540	9.10446765	5.23715772
1	0.06997961	3.56537726	6.55004309
6	0.10800645	2.51223397	6.22265061
1	1.16924476	2.21522216	6.23578085
1	-0.12772727	1.71157161	8.20176495
6	-0.66055841	1.64482991	7.23969567
1	-0.60473355	0.59034113	6.92509076
1	-2.58963045	1.45117119	8.23183407
6	-2.12417054	2.05571111	7.44108003
1	-2.20742880	3.11261660	7.74080933
1	-2.72811248	1.90938829	6.53317569

1	-1.42220931	3.64669732	2.11164614
6	-0.41835514	3.22790347	1.92964063
1	-0.54700978	2.14754293	1.71846839
6	0.28234852	3.92986762	0.75198298
1	0.55500644	4.96646635	1.01697678
1	1.21953644	3.39899774	0.51848911
6	-0.60550571	3.95045016	-0.50337009
1	-1.53067017	4.50996616	-0.28286781
1	-0.91039537	2.91848634	-0.73763730
6	0.10717578	4.57578978	-1.70774882
1	1.00019660	3.99605265	-1.98593227
1	-0.55310968	4.60957741	-2.58598365
1	0.42770320	5.60776006	-1.49572408

$[\{Cryp(Cs^{+})\}_2\{Ni^{I}(TPP^{2-})\}^{-}]^{+}$, S =1/2

charge=+1 mult=2

28	0.13900189	0.09302244	0.03114557
7	1.82370428	1.10885981	0.42434727
7	1.14392262	-1.65253576	0.21189595
6	-1.88477445	-7.40421625	0.10969040
6	7.38303787	-1.90394031	2.00073713
6	0.59849630	-2.93050533	0.22122277
6	1.58979460	-3.89816547	0.63302988
1	1.41373054	-4.96718302	0.73569313
6	2.74169879	-3.20871155	0.87713606
1	3.69883625	-3.60269894	1.21286331
6	2.46247653	-1.81448400	0.61750426
6	3.38277605	-0.78166925	0.83998315
6	3.06691099	0.58347608	0.75063155
6	4.01453532	1.64335065	0.98811545
1	5.06405958	1.50089290	1.23480158
6	3.34717155	2.82051172	0.81336099
1	3.73086984	3.83030704	0.93847733
6	1.98985214	2.48620167	0.45939576
6	-0.73900791	-3.25075604	-0.04143115
6	-1.13945077	-4.69047504	0.01058693
6	-0.70379946	-5.59113564	-0.97420465
1	-0.06983384	-5.22463232	-1.78691704
6	-1.07350586	-6.93652234	-0.92634327
1	-0.72862852	-7.62262827	-1.70472776
6	-2.32079183	-6.51824665	1.09771300
1	-2.95301670	-6.87840805	1.91447565
6	-1.95313713	-5.17196655	1.05000538
1	-2.28728597	-4.48565772	1.83566828
6	4.77100267	-1.16244031	1.24391085
6	5.24819640	-0.89628359	2.53798554
1	4.59038901	-0.39755508	3.25668486
6	6.54134227	-1.26416777	2.91361252
1	6.89424711	-1.05087581	3.92667215
6	6.92129803	-2.17471788	0.71096947
1	7.57383256	-2.67290725	-0.01123638
6	5.62721995	-1.80789641	0.33735552
1	5.26802232	-2.02089185	-0.67363638

7	-1.54831766	-0.92250653	-0.35235135
7	-0.87019771	1.83533108	-0.15370783
6	2.04994213	7.62101345	0.29680516
6	-7.02014108	2.04252644	-2.24952317
6	-0.33398817	3.11544539	-0.12054212
6	-1.31479165	4.08335915	-0.55872898
1	-1.14433376	5.15520886	-0.63651391
6	-2.45057461	3.39062604	-0.86256020
1	-3.39535970	3.78259185	-1.23425601
6	-2.17427069	1.99575040	-0.60805622
6	-3.08373951	0.96283124	-0.86303237
6	-2.77911384	-0.40001470	-0.72529926
6	-3.73492333	-1.45907256	-0.93109077
1	-4.77724292	-1.31470759	-1.20726376
6	-3.08722279	-2.63414473	-0.67686131
1	-3.48021397	-3.64578851	-0.75200444
6	-1.72983329	-2.29765785	-0.32573443
6	0.99134742	3.44011994	0.20089213
6	1.36565578	4.88627890	0.23440701
6	0.81798494	5.74439574	1.20220411
1	0.11920269	5.33729972	1.93869579
6	1.15677125	7.09808826	1.23436293
1	0.72250054	7.74784819	1.99910302
6	2.60126063	6.77997586	-0.67263562
1	3.29945408	7.18167289	-1.41255213
6	2.26306533	5.42606437	-0.70228421
1	2.69513557	4.77097973	-1.46511272
6	-4.45014808	1.33450408	-1.34438568
6	-4.83313250	1.08906653	-2.67365499
1	-4.11841550	0.62883916	-3.36464279
6	-6.10821094	1.44180718	-3.12061469
1	-6.39188171	1.24552529	-4.15865764
6	-6.64835461	2.29271395	-0.92688445
1	-7.35642243	2.76101307	-0.23777085
6	-5.37326881	1.94211199	-0.47909614
1	-5.08233670	2.13691602	0.55732292
1	-8.01876211	2.31517314	-2.60080948
1	-2.17630146	-8.45710433	0.14726046
1	2.31607343	8.68087056	0.32159289
1	8.39623960	-2.19058430	2.29400812
55	-0.16718728	1.88672993	-3.41832680
55	0.36243554	-1.75302524	3.45929132
8	-0.43307418	-3.84704138	5.32284884
8	-2.58622212	-2.73640326	3.83471416
8	-0.94743669	-1.25499977	8.89545989
8	-3.19041820	-0.20846179	7.33202533
8	2.11860175	-0.52377084	5.73460554
8	-0.01392857	1.10681754	4.65964418
7	1.21563087	-2.86116769	7.58639237
7	-2.87065861	0.32784023	4.34614553
6	0.86448086	-4.27085314	7.40104416
1	1.66497790	-4.96528615	7.76151183
1	-0.01628944	-4.47894409	8.02959665

6	0.53484342	-4.67633619	5.96123832
1	0.21635135	-5.73909595	5.96247358
1	1.43577805	-4.62211061	5.32403983
6	-1.79562719	-4.09702426	5.67261932
1	-2.14840922	-5.02568176	5.17816026
1	-1.91722095	-4.21454795	6.76750057
6	-2.65265926	-2.91318894	5.25968330
1	-2.33539756	-1.99951259	5.79691898
1	-3.69513875	-3.14218042	5.56520223
6	-3.60806497	-1.88160057	3.29941490
1	-3.83367999	-2.26129706	2.28635357
1	-4.53254614	-1.99116246	3.89907219
6	-3.22277169	-0.40738802	3.12497130
1	-4.07589209	0.07277526	2.58007917
1	-2.37168452	-0.35500957	2.42268491
6	1.11152504	-2.49458761	9.00495325
1	1.64646822	-3.22291999	9.66139073
1	1.60129206	-1.51905341	9.15208825
6	-0.31296958	-2.35148586	9.52655076
1	-0.25302010	-2.19860573	10.62714490
1	-0.89756434	-3.28518262	9.37463867
6	-2.26712278	-1.06308537	9.38008425
1	-2.89269920	-1.96600880	9.20791995
1	-2.26456352	-0.86367076	10.47404314
6	-2.89821696	0.12178604	8.68201769
1	-2.20224838	0.98566630	8.73741474
1	-3.82495577	0.39955888	9.22999766
6	-3.75484196	0.89649149	6.64393871
1	-4.71277723	1.20494945	7.11836104
1	-3.07620432	1.77344158	6.69881071
6	-4.05436564	0.51904192	5.19904956
1	-4.73956006	1.29321722	4.77722706
1	-4.62588160	-0.42231884	5.22563359
6	2.54432631	-2.54273967	7.05327998
1	3.36059018	-2.94696420	7.70228730
1	2.66489025	-3.03758515	6.07398504
6	2.82321934	-1.05286177	6.86066727
1	3.91742052	-0.92143977	6.72053099
1	2.54462336	-0.48704821	7.77142363
6	2.10790715	0.90707548	5.75561358
1	1.61775018	1.26694085	6.68338195
1	3.14329410	1.30952261	5.73268344
6	1.36194652	1.46153191	4.55713154
1	1.81644804	1.09411423	3.61019808
1	1.48780947	2.56527381	4.55887713
6	-0.81478564	1.63299464	3.59708633
1	-0.53202269	2.68448139	3.38227831
1	-0.64745252	1.07745485	2.64672998
6	-2.28015664	1.63562824	4.01752092
1	-2.85463552	2.15299886	3.21124431
1	-2.34828420	2.27124583	4.91477989
8	-1.67065895	2.55419479	-5.82636553
8	-2.06664435	-0.10758686	-4.90944651

8	1.50382712	1.56543514	-8.78011003
8	0.99286596	-1.15737010	-7.83169417
8	2.32871755	3.24433719	-4.72892895
8	2.52233442	0.43387217	-4.07921102
7	0.56647085	3.93485738	-7.20446128
7	0.60839219	-1.71036516	-4.85605619
6	-0.84224829	4.26755850	-7.42698832
1	-0.99911831	5.35416935	-7.64526894
1	-1.17141056	3.73117295	-8.33144868
6	-1.78726172	3.90095040	-6.27855618
1	-2.82564630	4.13140704	-6.59414766
1	-1.58502548	4.52787211	-5.39160970
6	-2.31055935	1.56779864	-6.63808225
1	-3.40924900	1.60969881	-6.48799266
1	-2.09732079	1.72829795	-7.71331006
6	-1.77458121	0.19162091	-6.28472720
1	-0.68903062	0.13452851	-6.49038413
1	-2.28442608	-0.53801114	-6.94825796
6	-1.91971744	-1.49387762	-4.56544163
1	-2.66383065	-1.69941338	-3.77471239
1	-2.19161620	-2.12087785	-5.43682768
6	-0.55883244	-1.89812728	-3.98523849
1	-0.66707342	-2.96374087	-3.65671261
1	-0.39938802	-1.32806769	-3.05249380
6	1.29793151	3.94329715	-8.47818470
1	1.09966572	4.87358915	-9.06360445
1	2.37803007	3.93074812	-8.26260429
6	1.01943350	2.75021206	-9.38418107
1	1.52886385	2.94036258	-10.35503584
1	-0.06449345	2.65922198	-9.61529443
6	1.29671265	0.43238417	-9.60874066
1	0.21654172	0.29006616	-9.83054353
1	1.82374210	0.54831893	-10.58100599
6	1.83193117	-0.80517588	-8.92204218
1	2.86876025	-0.60640210	-8.57676185
1	1.87692170	-1.62880329	-9.66763242
6	1.48850771	-2.29894850	-7.15034607
1	1.52282727	-3.17721646	-7.83252346
1	2.52950558	-2.12242312	-6.80719824
6	0.57481292	-2.65399547	-5.98450994
1	0.82605002	-3.69112409	-5.65576283
1	-0.45189452	-2.69265089	-6.38188031
6	1.20027578	4.82196821	-6.22358288
1	1.39340907	5.83915639	-6.64648698
1	0.50719101	4.97361320	-5.37803932
6	2.52509254	4.31514484	-5.65597163
1	3.03342993	5.16511674	-5.15267442
1	3.19218605	3.97899777	-6.47406459
6	3.55689680	2.56157899	-4.45953248
1	3.97266252	2.14687774	-5.40070991
1	4.30778001	3.25696303	-4.02689437
6	3.34268986	1.42857434	-3.47425744
1	2.90027672	1.81291967	-2.52817386

1	4.33899875	1.01426605	-3.20983817
6	2.30581467	-0.70724827	-3.24357549
1	3.24927740	-1.00437986	-2.74026726
1	1.58641569	-0.48237221	-2.42408267
6	1.85864492	-1.88681944	-4.09939745
1	1.81021991	-2.78066729	-3.43129702
1	2.66757397	-2.07406159	-4.82350486

$\{Fe^{II}(TPP^{2-})\}^{0}$, *S* =1
charge=0 mult=3

26	2.62169542	10.51978338	18.39681507
7	2.84261667	8.56293369	18.69058876
7	3.53676914	10.35192922	16.63655501
6	4.60864611	15.47229830	12.74616149
6	5.89360745	4.68929080	14.41718787
6	3.83083409	11.37072310	15.73697108
6	4.57930402	10.85922005	14.61854440
1	4.94869643	11.45832438	13.79261795
6	4.73850219	9.51794752	14.82223761
1	5.26228475	8.80230667	14.19746075
6	4.08799336	9.20607245	16.06762658
6	4.05944030	7.92016454	16.61886297
6	3.46505150	7.63911544	17.85418946
6	3.41401437	6.31924053	18.42570624
1	3.82059544	5.42520151	17.96511358
6	2.76999720	6.43274310	19.62501470
1	2.55436795	5.64952195	20.34443010
6	2.41092856	7.81794334	19.78257425
6	3.49399435	12.72158867	15.88326017
6	3.88022519	13.67634132	14.79626826
6	4.91097115	14.61282002	14.99584614
1	5.43422097	14.63452610	15.95364814
6	5.27421488	15.50177116	13.97766181
1	6.08141943	16.21666650	14.14712414
6	3.57983527	14.54575628	12.53808149
1	3.05197672	14.51837318	11.58306185
6	3.22064401	13.65252836	13.55398411
1	2.41605216	12.93303319	13.39088182
6	4.69542010	6.79917815	15.85604886
6	4.09330616	6.29407866	14.68947794
1	3.15070426	6.72458903	14.34612742
6	4.68666258	5.24573054	13.97681217
1	4.20217523	4.86159659	13.07727165
6	6.50252275	5.18648915	15.57582779
1	7.44613497	4.76243929	15.92390073
6	5.90700886	6.23194318	16.29093789
1	6.38527154	6.62056546	17.19202412
7	2.39784079	12.47616347	18.10153897
7	1.71017207	10.68808727	20.15889968
6	0.59230075	5.55716065	24.02329352
6	-0.60719557	16.35746258	22.40098888
6	1.41148538	9.66866268	21.05626197
6	0.67319092	10.18272099	22.18030675

1	0.30268956	9.58384887	23.00591204
6	0.52589224	11.52626806	21.98276084
1	0.01197544	12.24442839	22.61285067
6	1.17114580	11.83648907	20.73419269
6	1.19851272	13.12208792	20.18234450
6	1.77926227	13.40066898	18.94009903
6	1.82017741	14.71862963	18.36343984
1	1.41460291	15.61292463	18.82444389
6	2.45311253	14.60304206	17.15843129
1	2.65899555	15.38449341	16.43428346
6	2.81754928	13.21892952	17.00340886
6	1.73542295	8.31546229	20.90313809
6	1.33936956	7.35843029	21.98468687
6	0.29672203	6.43634619	21.78035839
1	-0.22768308	6.42725720	20.82297597
6	-0.07558485	5.54453050	22.79278258
1	-0.89149248	4.84051779	22.61950228
6	1.63291641	6.46939558	24.23606922
1	2.16233573	6.48369665	25.19047112
6	2.00170201	7.36501489	23.22569211
1	2.81515067	8.07362029	23.39256982
6	0.57225652	14.24476232	20.95086048
6	1.19254060	14.75622506	22.10497932
1	2.14175261	14.32939830	22.43443797
6	0.60855985	15.80613359	22.82312595
1	1.10711058	16.19521303	23.71279776
6	-1.23434125	15.85361954	21.25501692
1	-2.18491723	16.27360264	20.92124177
6	-0.64810696	14.80681008	20.53423132
1	-1.14057937	14.41321728	19.64301064
1	-1.06347001	17.17478403	22.96195812
1	4.89038373	16.16705916	11.95318471
1	0.30333057	4.86035214	24.81185605
1	6.35712410	3.87305640	13.86058659

{$Fe^{I}(TPP^{2-})$}$^{-}$, S = 1/2
charge=-1 mult=2

26	2.62156030	10.51987325	18.39664580
7	2.84402596	8.56587274	18.69479925
7	3.53977574	10.35643104	16.64013841
6	4.58866005	15.47746034	12.72325551
6	5.88683346	4.68179979	14.41094253
6	3.83281482	11.37501113	15.72869633
6	4.58081929	10.86291275	14.61185345
1	4.95003452	11.45781405	13.78242267
6	4.74212989	9.51965961	14.82110554
1	5.26782786	8.80564607	14.19486785
6	4.09208844	9.20776027	16.06589229
6	4.06014033	7.92277588	16.62102066
6	3.46825054	7.63671714	17.85730546
6	3.41132707	6.31646754	18.42543537
1	3.81354049	5.41987109	17.96438187
6	2.76466337	6.42602652	19.62712578

1	2.54928537	5.63843456	20.34236338
6	2.40856704	7.81043465	19.78761622
6	3.48960411	12.72449132	15.87572341
6	3.86966169	13.67641596	14.78695486
6	4.86007465	14.65614758	14.99268828
1	5.35077893	14.71183241	15.96613036
6	5.21591697	15.54779908	13.97368483
1	5.98946258	16.29718552	14.15653152
6	3.60261837	14.50723947	12.50340005
1	3.10362469	14.44394599	11.53365535
6	3.24767207	13.61809107	13.52490878
1	2.47919560	12.86242667	13.35180736
6	4.69178759	6.80296904	15.85748405
6	4.12637796	6.33693558	14.65493061
1	3.21421890	6.80889628	14.28511264
6	4.71648439	5.28903996	13.93817796
1	4.25731535	4.94330438	13.00918053
6	6.46051603	5.13430834	15.60597633
1	7.37533225	4.67172149	15.98347883
6	5.86918685	6.18374378	16.31945087
1	6.31794126	6.53519701	17.25036789
7	2.39348687	12.47302175	18.09563925
7	1.70928737	10.68430024	20.15614278
6	0.59787645	5.54903445	24.03809092
6	-0.58670390	16.36649040	22.41580967
6	1.41213992	9.66520197	21.06579259
6	0.68147989	10.18151494	22.19225627
1	0.31453657	9.58809412	23.02384833
6	0.53450138	11.52749976	21.99018621
1	0.02371010	12.24521602	22.62449678
6	1.17296357	11.83632067	20.73868037
6	1.20071589	13.12044336	20.18141032
6	1.77333040	13.40299221	18.93537538
6	1.81415939	14.72015956	18.35873226
1	1.41104989	15.61664403	18.81924404
6	2.44731935	14.60789355	17.15020533
1	2.64875935	15.39266187	16.42785600
6	2.81392513	13.22563864	16.99500219
6	1.73651104	8.31226481	20.90875166
6	1.34314848	7.35706942	21.98997599
6	0.33593475	6.39624887	21.77710541
1	-0.15715381	6.35778902	20.80401575
6	-0.03278083	5.50095503	22.78832540
1	-0.81910261	4.76637969	22.59997645
6	1.60062025	6.50033131	24.26497757
1	2.10255031	6.54600659	25.23419735
6	1.96866552	7.39284640	23.25105090
1	2.75047260	8.13345457	23.42947406
6	0.58254541	14.24260710	20.95272706
6	1.17171687	14.71395913	22.14163596
1	2.09214563	14.24492295	22.49432005
6	0.59439490	15.76337409	22.86658506
1	1.07183512	16.11345411	23.78468252

6	-1.18416761	15.90834993	21.23465685
1	-2.10763145	16.36766195	20.87460687
6	-0.60553406	14.85744050	20.51294189
1	-1.07298014	14.50119950	19.59310977
1	-1.03755839	17.18574794	22.97990762
1	4.86597709	16.17202846	11.92743827
1	0.31043483	4.85176415	24.82792690
1	6.34762200	3.86370580	13.85322432

$\{Cu^{II}(TPP^{2-})\}^{0}$, *S* = 1/2

charge=0 mult=2

29	2.62377004	10.52047566	18.39812275
7	2.85422772	8.53457963	18.70304648
7	3.54448942	10.35169140	16.60553280
6	4.59943048	15.47517884	12.73230164
6	5.88524831	4.68698370	14.41240573
6	3.83502172	11.37309721	15.72013882
6	4.58808306	10.86066550	14.59896127
1	4.95899313	11.45599694	13.77101357
6	4.74754568	9.51970570	14.80697476
1	5.27572873	8.80618910	14.18296604
6	4.09178501	9.20726395	16.05564160
6	4.06042981	7.92049481	16.61905933
6	3.47243591	7.62849089	17.86135753
6	3.41924991	6.30263083	18.43240604
1	3.82031719	5.40641029	17.97057440
6	2.77574458	6.41246601	19.63275394
1	2.56096906	5.62598240	20.34876622
6	2.41951737	7.80320172	19.79288054
6	3.49285528	12.72694443	15.87560483
6	3.87731269	13.68122108	14.78703092
6	4.89787733	14.62875288	14.98748825
1	5.41338662	14.66279381	15.94908807
6	5.25674087	15.51768842	13.96776385
1	6.05372571	16.24342065	14.13968145
6	3.58213676	14.53638550	12.52240192
1	3.06228259	14.49704980	11.56345546
6	3.22512870	13.64528759	13.54090164
1	2.43111246	12.91481972	13.37496772
6	4.69362084	6.79910464	15.85449271
6	4.10462731	6.31580828	14.67170848
1	3.17525544	6.76463229	14.31620739
6	4.69459238	5.26653900	13.95772906
1	4.22078479	4.90060348	13.04505721
6	6.48114898	5.16217826	15.58689377
1	7.41160734	4.71953424	15.94697939
6	5.88902437	6.20839899	16.30357951
1	6.35694854	6.57864836	17.21764207
7	2.39252745	12.50622541	18.09274954
7	1.70356506	10.68906533	20.19099990
6	0.59988138	5.55259288	24.03491317
6	-0.60627927	16.35857454	22.40265092
6	1.40606077	9.66641648	21.07274364

6	0.65692656	10.18007480	22.19600591
1	0.28143338	9.58422879	23.02151005
6	0.50753941	11.52300307	21.99332711
1	-0.01442610	12.23819044	22.62063764
6	1.16413335	11.83517640	20.74501165
6	1.19894346	13.12269468	20.18341412
6	1.78055241	13.41344333	18.93779073
6	1.82916091	14.73836248	18.36422151
1	1.43191925	15.63530628	18.82792530
6	2.46176249	14.62652660	17.15832629
1	2.66996646	15.41207954	16.43936732
6	2.81803472	13.23582648	16.99804654
6	1.74045819	8.31114720	20.91308849
6	1.34483066	7.35390307	21.99516051
6	0.31787978	6.41572524	21.78400180
1	-0.19398837	6.39241744	20.82013419
6	-0.05272397	5.52340484	22.79653862
1	-0.85490024	4.80537381	22.61679163
6	1.62411107	6.48146485	24.25498215
1	2.14062612	6.50993371	25.21612155
6	1.99256154	7.37628711	23.24380915
1	2.79232864	8.09864687	23.41739851
6	0.57288299	14.24520786	20.95223350
6	1.16874143	14.72529422	22.13289555
1	2.09849665	14.27331644	22.48339921
6	0.58495668	15.77511944	22.85094870
1	1.06389693	16.13847900	23.76196622
6	-1.20904526	15.88648301	21.23044236
1	-2.14007079	16.33199218	20.87538427
6	-0.62315026	14.83957077	20.50971604
1	-1.09661155	14.47138299	19.59768022
1	-1.06232075	17.17594703	22.96372519
1	4.87855459	16.16921264	11.93777290
1	0.31175825	4.85584638	24.82383633
1	6.34618814	3.87008856	13.85464967

{$Cu^{II}(TPP^{\bullet 3-})$}$^{-}$, $S = 1$

charge=-1 mult=3

29	2.61944440	10.51859764	18.39606602
7	2.85933747	8.51129878	18.70704451
7	3.31997848	10.30025257	16.44871505
6	4.63931916	15.45080286	12.70783988
6	5.86868020	4.70215203	14.34500251
6	3.71006624	11.34546834	15.62943653
6	4.58640464	10.85600109	14.57921065
1	5.06401684	11.46659379	13.81831741
6	4.73989646	9.51418051	14.78339304
1	5.36757898	8.82896334	14.22098486
6	3.95851636	9.17397894	15.96058398
6	3.95452531	7.89637353	16.55219127
6	3.43236731	7.60044953	17.84001895
6	3.40012156	6.28130250	18.42014130
1	3.73842344	5.36727731	17.94143611

6	2.79623956	6.40096860	19.65071518
1	2.64207225	5.61596653	20.38496246
6	2.46403778	7.79284094	19.82009401
6	3.40134575	12.70570646	15.81735864
6	3.82708293	13.65985973	14.74997162
6	4.75423065	14.68933620	15.01212494
1	5.16507308	14.78397799	16.01859388
6	5.15628404	15.57299485	14.00470568
1	5.88180606	16.35723771	14.23269652
6	3.71842119	14.43275635	12.43104387
1	3.30560583	14.32669221	11.42519545
6	3.31808804	13.54897888	13.43996478
1	2.59775042	12.75870419	13.22119384
6	4.61407668	6.78908357	15.79872022
6	4.14700868	6.40587625	14.52454513
1	3.28510934	6.92583831	14.10269623
6	4.76558659	5.37613861	13.80626371
1	4.38026718	5.09706321	12.82286173
6	6.34601152	5.07182990	15.60978577
1	7.21106807	4.56078252	16.03865609
6	5.72591546	6.10066406	16.32679895
1	6.10657694	6.38962924	17.30778125
7	2.38030063	12.52646204	18.08554558
7	1.91891279	10.73795144	20.34301848
6	0.62167017	5.59127469	24.09649037
6	-0.63674583	16.33730904	22.43900919
6	1.53442949	9.69334709	21.16554578
6	0.66032122	10.18262066	22.21778667
1	0.18696960	9.57238379	22.98161696
6	0.50229648	11.52356408	22.01120860
1	-0.12523394	12.20829603	22.57436235
6	1.27875920	11.86344786	20.83072837
6	1.28085647	13.14066753	20.23836619
6	1.80444049	13.43683940	18.95121921
6	1.83921840	14.75642008	18.37239887
1	1.50060250	15.67029866	18.85120234
6	2.44641849	14.63743926	17.14335921
1	2.60252527	15.42275953	16.40983903
6	2.77898117	13.24562298	16.97421620
6	1.84477105	8.33335506	20.97833589
6	1.42426984	7.38007638	22.04860031
6	0.49683715	6.34951044	21.79170347
1	0.08228889	6.25297739	20.78691004
6	0.09987612	5.46666033	22.80179504
1	-0.62616583	4.68173084	22.57787230
6	1.54306679	6.61026689	24.36808854
1	1.96017159	6.71782468	25.37201578
6	1.93899164	7.49270570	23.35620106
1	2.65955536	8.28382472	23.57103286
6	0.62000603	14.24833261	20.99028356
6	1.08713950	14.63541807	22.26320376
1	1.95014501	14.11790944	22.68584703
6	0.46747551	15.66624847	22.97900986

1	0.85281924	15.94841186	23.96151461
6	-1.11404370	15.96388899	21.17529736
1	-1.97985504	16.47282649	20.74543026
6	-0.49270696	14.93415230	20.46065973
1	-0.87290376	14.64254834	19.48028579
1	-1.12102570	17.14190180	22.99646744
1	4.95208919	16.14118257	11.92166865
1	0.31233977	4.90194025	24.88493753
1	6.35211910	3.89833132	13.78570898

$\{Cu^{II}(TPP^{4-})\}^{2-}$, S = 1/2

charge=-2 mult=2

29	2.62316608	10.52096486	18.39742391
7	2.89019046	8.50162239	18.72674071
7	3.39067806	10.32227431	16.47879027
6	4.53362223	15.44570420	12.60433790
6	5.88484365	4.68066136	14.34535668
6	3.74629005	11.36479131	15.63871346
6	4.61213062	10.87630924	14.59458502
1	5.07133994	11.47984198	13.81687893
6	4.77797126	9.52514386	14.80343461
1	5.41169531	8.84656024	14.23919047
6	4.02067923	9.18575361	15.97937817
6	4.01154253	7.89912422	16.57154498
6	3.45938289	7.59171451	17.84210164
6	3.37046587	6.26637308	18.38835445
1	3.69617993	5.35262834	17.89934882
6	2.75142575	6.37585088	19.61661866
1	2.56038083	5.57420222	20.32354872
6	2.44074920	7.76728004	19.81208200
6	3.40637211	12.73656548	15.80658009
6	3.79410738	13.66914474	14.72178618
6	4.59487856	14.81577920	14.95621301
1	4.94579427	15.00713268	15.97132509
6	4.95375090	15.68571458	13.92216262
1	5.58126381	16.55368975	14.14536185
6	3.74724541	14.31057702	12.34700740
1	3.40189934	14.10440387	11.32966856
6	3.38676638	13.44382594	13.38252173
1	2.76923892	12.56948431	13.16942218
6	4.65403051	6.79473838	15.81206282
6	4.25055256	6.47775856	14.49343021
1	3.44517032	7.06015303	14.04283032
6	4.85377529	5.44112830	13.77280610
1	4.50853042	5.21848539	12.75916960
6	6.30126155	4.98077901	15.65143051
1	7.11200773	4.40869688	16.11145368
6	5.69787237	6.01902696	16.36958493
1	6.03521188	6.25173021	17.38080503
7	2.35430284	12.53979327	18.06824756
7	1.85740520	10.71655705	20.31762608
6	0.60110951	5.56612079	24.12608759
6	-0.53703617	16.37548030	22.50918635

6	1.48455581	9.67355142	21.15005647
6	0.62716936	10.16858249	22.19822626
1	0.15748724	9.56743384	22.97148627
6	0.48870780	11.52494658	22.00256283
1	-0.13247392	12.20998560	22.57293620
6	1.24782803	11.85956032	20.82645050
6	1.26665295	13.14823695	20.23878946
6	1.80054716	13.45260861	18.95993435
6	1.87902362	14.77604756	18.40760376
1	1.56204535	15.69141854	18.89924565
6	2.47364993	14.66232870	17.16775458
1	2.65015664	15.46172631	16.45460742
6	2.78381726	13.27081709	16.97241570
6	1.80630766	8.29885965	20.97278121
6	1.39228539	7.35967306	22.04208795
6	0.58050915	6.22651372	21.78190682
1	0.24160489	6.05269621	20.75952773
6	0.19609169	5.34832255	22.79964459
1	-0.43922325	4.49138819	22.55677534
6	1.39879999	6.68718161	24.40864956
1	1.73294038	6.87569304	25.43313214
6	1.78469544	7.56230344	23.38938268
1	2.41158777	8.42490209	23.62196634
6	0.64736187	14.25641439	21.01217411
6	1.07837547	14.56490669	22.32399041
1	1.88653085	13.97331121	22.75739185
6	0.49797161	15.60409218	23.05956129
1	0.86399385	15.81987433	24.06736808
6	-0.98113728	16.08334877	21.21047323
1	-1.79582856	16.66375514	20.76817977
6	-0.40071990	15.04232403	20.47744008
1	-0.75991375	14.81545504	19.47244775
1	-0.99013100	17.18833811	23.08227983
1	4.81437081	16.12556385	11.79619003
1	0.30059108	4.87968987	24.92147420
1	6.35584193	3.86993067	13.78380195

$\{Cu^{II}(TPP^{4-})\}^{2-}$, S = 3/2
charge=-2 mult=4

29	2.62130472	10.52042424	18.39636370
7	2.85301243	8.50704862	18.70500395
7	3.48180875	10.33498953	16.54422151
6	4.53594071	15.47184020	12.63740316
6	5.87615497	4.65569783	14.35258567
6	3.78674934	11.36968020	15.66449440
6	4.57844777	10.86448140	14.58108307
1	4.99532148	11.45942724	13.77426033
6	4.74495624	9.51140859	14.79400680
1	5.31909746	8.81640170	14.18902613
6	4.05357956	9.18510294	16.00698230
6	4.03751839	7.89160196	16.58612516
6	3.46678952	7.59651594	17.84925968
6	3.40991727	6.28349109	18.42196859

1	3.78873599	5.37636653	17.96166517
6	2.78771181	6.39979284	19.64822541
1	2.60169858	5.60834318	20.36742697
6	2.42544428	7.77734321	19.81080514
6	3.45236598	12.73716914	15.82931365
6	3.82428171	13.67490716	14.74113387
6	4.64366056	14.80592957	14.97677402
1	5.01546080	14.97682682	15.98834470
6	4.99033796	15.68776349	13.94778897
1	5.63361232	16.54464024	14.16828487
6	3.72683842	14.35342488	12.38064366
1	3.35274419	14.17066738	11.36908993
6	3.37820755	13.47529715	13.41174650
1	2.74057037	12.61465499	13.20262269
6	4.66703896	6.78444245	15.82476084
6	4.25259318	6.46291421	14.50917313
1	3.44474060	7.04534104	14.06292132
6	4.84483033	5.42208192	13.78673958
1	4.48895795	5.19795184	12.77692073
6	6.30269898	4.95772100	15.65540336
1	7.11406534	4.38283378	16.11128032
6	5.71199896	6.00203258	16.37433463
1	6.06155953	6.23581407	17.38127475
7	2.38937145	12.53422322	18.08772981
7	1.76098978	10.70479257	20.24848625
6	0.61586237	5.54501840	24.10283964
6	-0.53706290	16.39800052	22.49870701
6	1.44303144	9.66872501	21.12211813
6	0.65917598	10.17780760	22.20941008
1	0.23547074	9.58387007	23.01338972
6	0.51392340	11.53492310	22.00703444
1	-0.04920232	12.23415978	22.61749426
6	1.20651408	11.85902846	20.79412501
6	1.23229333	13.15473154	20.22014946
6	1.78805255	13.44735179	18.94978674
6	1.83643868	14.75862217	18.37228640
1	1.46499946	15.66738056	18.83527083
6	2.43790762	14.63815352	17.13617249
1	2.61154587	15.42738571	16.41149612
6	2.79971643	13.26058292	16.97315002
6	1.76314686	8.29882704	20.94996038
6	1.37008502	7.35563364	22.02598642
6	0.54056873	6.23657588	21.76978333
1	0.17871830	6.08024075	20.75224326
6	0.17318809	5.34779226	22.78542341
1	-0.47716701	4.50056301	22.54906094
6	1.43492475	6.65115184	24.37984617
1	1.80043757	6.81888469	25.39712912
6	1.80483453	7.53586244	23.36177812
1	2.45027831	8.38665282	23.58676647
6	0.62547572	14.26504434	20.99532760
6	1.06282368	14.57325416	22.30672247
1	1.86997221	13.97809812	22.73736314

6	0.49353969	15.61610100	23.04446502
1	0.86673017	15.82941250	24.05035867
6	-0.98637072	16.10913181	21.20064331
1	-1.79791165	16.69599649	20.76060360
6	-0.41851787	15.06276916	20.46637708
1	-0.78656010	14.83912294	19.46375856
1	-0.98116424	17.21465316	23.07331048
1	4.80729809	16.16002293	11.83298302
1	0.32812373	4.85171964	24.89710763
1	6.33808352	3.84070970	13.78979198