Supplement Information

Table 1 : Analysis of the wave of $HgCl_2$ at different concentrations of the depolizer at 22.°C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$).

**** Effect of concentration for metal($HgCl_2$) at 0.1 scan rate (υ =0.1) at 22.˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$)****

M x10^{-4}	Epa Volt	(-)Epc Volt	(-)ΔEP volt	(-) ipa x10^{-4}	ipc x10^{-4}	(-) ipa/ipc	E^0	Da x 10^{-10}	Dc x10^{-9}	(-) $Ep_{c/2}$	αna	Ksc x10^{-7}	Γc x10^{-7}	Qc x10^{-8}	(-)Γa x10^{-8}	(-)Qa x10^{-5}
3.23	0.0758	0.1074	0.1832	0.42	1.32	0.31	0.0158	2.90	2.94	0.0021	0.0033	3.62	3.62	1.10	0.35	2.10
4.76	0.0910	0.2276	0.3186	0.97	1.75	0.55	0.0683	7.21	2.37	0.0202	0.0034	0.67	0.67	1.46	0.81	4.88
6.25	0.0001	0.3092	0.3091	1.49	2.52	0.59	0.1547	9.94	2.84	0.0393	0.0034	0.29	0.294	2.10	1.24	7.52
7.69	0.1137	0.2963	0.4100	1.74	2.66	0.65	0.0913	9.01	2.10	0.0853	0.0034	2.13	2.13	2.22	1.45	8.81
9.09	0.1255	0.0498	0.0757	1.75	1.18	1.49	0.0877	6.52	2.95	0.1359	0.0034	9.69	0.96	0.98	1.46	8.86

Table 2 Analysis of the wave of $HgCl_2$ at different concentrations of the depolizer at 22.˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$).

**** Effect of concentration for Ligand girnard reagent at 0.1 scan rate (υ =0.1) at 22˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$)****

Table 3 Analysis of the wave of $HgCl_2$ at different concentrations of the depolizer at22˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$).

L x10^{-4}	E_{Pa} Volt	(-)E_{pc} Volt	(-)ΔE_P volt	(-)ip_a x10^{-4}	ipc x10^{-4}	(-)i_{pa}/i_{pc}	E^0	D_a x10^{-9}	Dc x10^{-9}	$Ep_{c/2}$	αna	Ks x10^{-10}	Γc x10^{-8}	Qc x10^{-5}	(-)Γa x10^{-8}	(-)Qa x10^{-4}
1.37	0.2541	0.2371	0.4912	1.79	3.08	0.58	0.0085	0.83	2.45	0.0201	0.0033	7.42	2.56	0.16	1.49	0.904
2.70	0.2582	0.2287	0.4869	2.23	2.24	0.99	0.0147	1.33	1.34	0.0231	0.0033	5.97	1.87	0.11	1.86	1.13
4.00	0.2579	0.2227	0.4806	2.12	1.87	1.13	0.0176	1.23	0.95	0.0161	0.0034	5.72	1.56	9.44	1.77	1.07
5.26	0.2562	0.2185	0.4746	2.08	1.66	1.25	0.0188	1.21	0.77	0.0161	0.0034	5.80	1.38	8.39	1.73	1.05
6.49	0.2554	0.2746	0.5300	2.21	1.48	1.50	0.0096	1.41	6.29	0.0255	0.0034	1.74	1.23	7.45	1.84	1.12
7.69	0.2652	0.2878	0.5530	2.40	1.37	1.76	0.0113	1.71	0.55	0.0091	0.0033	1.04	1.14	6.91	2.00	1.21

(effect of scan rate on metal at22˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$)

υ	Ep_a Volt	(-)Ep_c Volt	(-)ΔEp volt	(-)i_{pa} x10^{-8}	i_{pc} x10 $^{-5}$	(-) I_{PA}/I_{PC}	(-) E^0	D a x1 0^{-9}	Dc x10^{-5}	(-) Epc/2	αna	Ks x10^{-}	Γc x10^{-8}	Qc x10^{-8}	(-)$Γ_a$ x 10^{-8}	(-)Qa x10^{-5}
o.1	0.1259	0.0436	0.0823	18.3	11.8	1.55	0.084	0.71	1.72	0.1370	0.5021	13.8	0.98	0.60	1.53	1.53
0.05	0.1143	0.0579	0.0564	14.0	7.61	1.84	0.086	0.83	1.57	0.1282	0.6670	7.56	1.27	0.77	2.33	2.33
0.02	0.1138	0.1054	0.0084	9.82	7.75	1.27	0.100	1.02	2.52	0.1635	0.8067	1.17	3.23	1.96	4.09	4.09
0.01	0.2803	0.1218	0.1585	9.98	7.39	1.35	0.201	2.11	3.40	0.1781	0.8335	0.27	6.16	3.73	8.32	8.32

Table 4 : Analysis of the wave of $HgCl_2$ at different concentrations of the depolizer at 22.˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$).

(effect of another scan rate on metal(1:1) at22.˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$)

υ	Ep_a Volt	(-)Ep_c Volt	(-)ΔEp volt	(-)i_{pa} x10^{-8}	i_{pc} x10^{-5}	(-) I_{PA}/I_{PC}	(-) E^0	Da x10^{-9}	Dc x10^{-5}	(-) Epc/2	αna	Ks x10^{-}	Γc x10^{-8}	Qc x10^{-8}	(-)$Γ_a$ x 10^{-8}	(-)Qa x10^{-5}
0.1	0.2627	0.396	0.3957	2.42	1.35	1.79	0.036	1.40	4.37	0.0396	0.1317	0.76	1.13	0.68	2.02	1.22
0.05	0.2436	0.315	0.3146	1.86	0.56	5.40	0.158	1.34	4.61	0.0482	1.1370	3.53	0.52	0.31	2.80	1.70
0.02	0.2290	0.087	0.0865	1.68	0.31	3.34	0.036	4.13	3.70	0.1278	0.1761	9.33	2.32	1.41	7.76	4.70
0.01	0.2192	0.105	0.1050	1.31	0.28	5.40	0.158	6.72	2.31	0.1406	1.1370	0.93	2.59	1.57	14.0	8.48

Table 5 Effect of concentration for Ligand Valproic acid at 0.1 scan rate a t22˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$).

(effect of stability const on complex(1:3) at 0.1 scan rate (υ =0.1) at22˚C for reaction, ($Hg^{+2} \leftrightarrow Hg^{+1}$)

x10^{-4} Mol.L^{-1}	**Lx10^{-4} Mol.L^{-1}**	**ΔEp Volt**	**Bj**	**(+)ΔG (KJ/mol)**
8.96	**1.37**	**0.0792**	**0.0074**	**11.972**
8.82	**2.70**	**0.0730**	**0.0383**	**7.949**
8.70	**4.00**	**0.0701**	**0.1422**	**4.753**
8.57	**5.26**	**0.0688**	**0.4422**	**1.988**
8.45	**6.49**	**0.0973**	**0.1266**	**5.036**
8.33	**7.69**	**0.0990**	**0.2947**	**2.977**

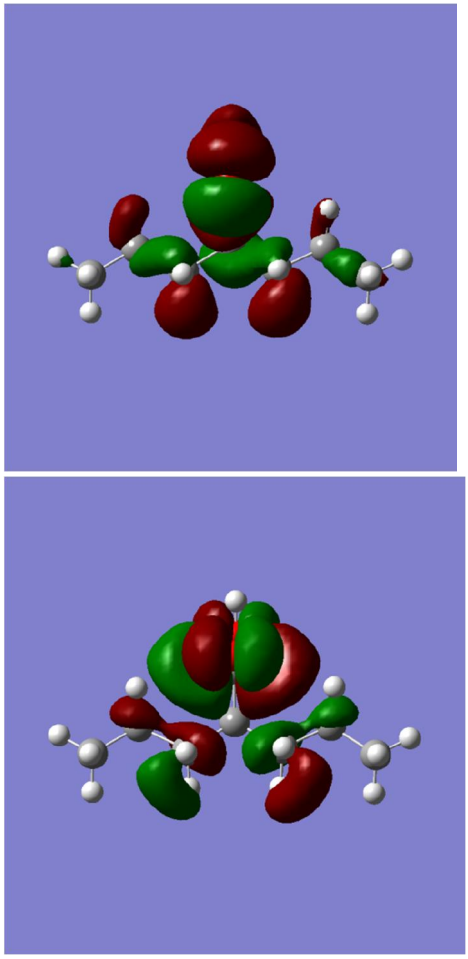

Fig.(8) : HOMO (with energy -0.43306 ev) and LUMO (with energy -0.17474 ev) for the ligand.

Valproic acid in water

Dipole moment (field-independent basis, Debye)

X= 0.0684 Y= -0.7033 Z= -1.9251 Tot= 2.0506

)Quadrupole moment (field-independent basis, Debye-Ang

XX= -61.9139 YY= -58.1158 ZZ= -70.8949

XY= 0.1467 XZ= 0.2696 YZ= -2.4717

) Traceless Quadrupole moment (field-independent basis, Debye-Ang

XX= 1.7276 YY= 5.5258 ZZ= -7.2534

XY= 0.1467 XZ= 0.2696 YZ= -2.4717

Octapole moment (field-independent basis, Debye-Ang**2

XXX= -0.6049 YYY= 46.7787 ZZZ= -4.1941 XYY= 0.4980

XXY= 7.9242 XXZ= -0.9904 XZZ= 0.2941 YZZ= -7.3268

YYZ= -7.9259 XYZ= 0.3236

Hexadecapole moment field-independent basis, Debye

XXXX= -2124.9242 YYYY= -454.5984 ZZZZ= -219.7961 XXXY= -0.1389

XXXZ= -0.0220 YYYX= 1.8779 YYYZ= -15.4397 ZZZX= 0.0715

ZZZY= -9.8846 XXYY= -457.0605 XXZZ= -389.3507 YYZZ= -157.8004

XXYZ= 2.5481 YYXZ= 0.6131 ZZXY= 0.3586

N-N= 5.581834043076D+02 E-N=-2.190638163843D+03 KE= 4.583149118585D+02

Exact polarizability: 100.017 0.109 100.337 -0.231 1.027 99.759

Approx polarizability: 62.289 0.062 69.868 -0.292 1.406 76.852

This molecule is an asymmetric top

Rotational symmetry number 1

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.08861 0.03244 0.02687

Rotational constants (GHZ): 1.84638 0.67603 0.55986

Zero-point vibrational energy 650934.4 (Joules/Mol(

Zero-point correction= 0.247928 (Hartree/Particle(

Thermal correction to Energy= 0.258998

Thermal correction to Enthalpy= 0.259942

Thermal correction to Gibbs Free Energy= 0.210866

Sum of electronic and zero-point Energies= -459.209184

Sum of electronic and thermal Energies= -459.198114

Sum of electronic and thermal Enthalpies= -459.197170

Sum of electronic and thermal Free Energies= -459.246246

	E(Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	162.524	39.896	103.290

Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.807
Rotational	0.889	2.981	30.510
Vibrational	160.746	33.935	31.973

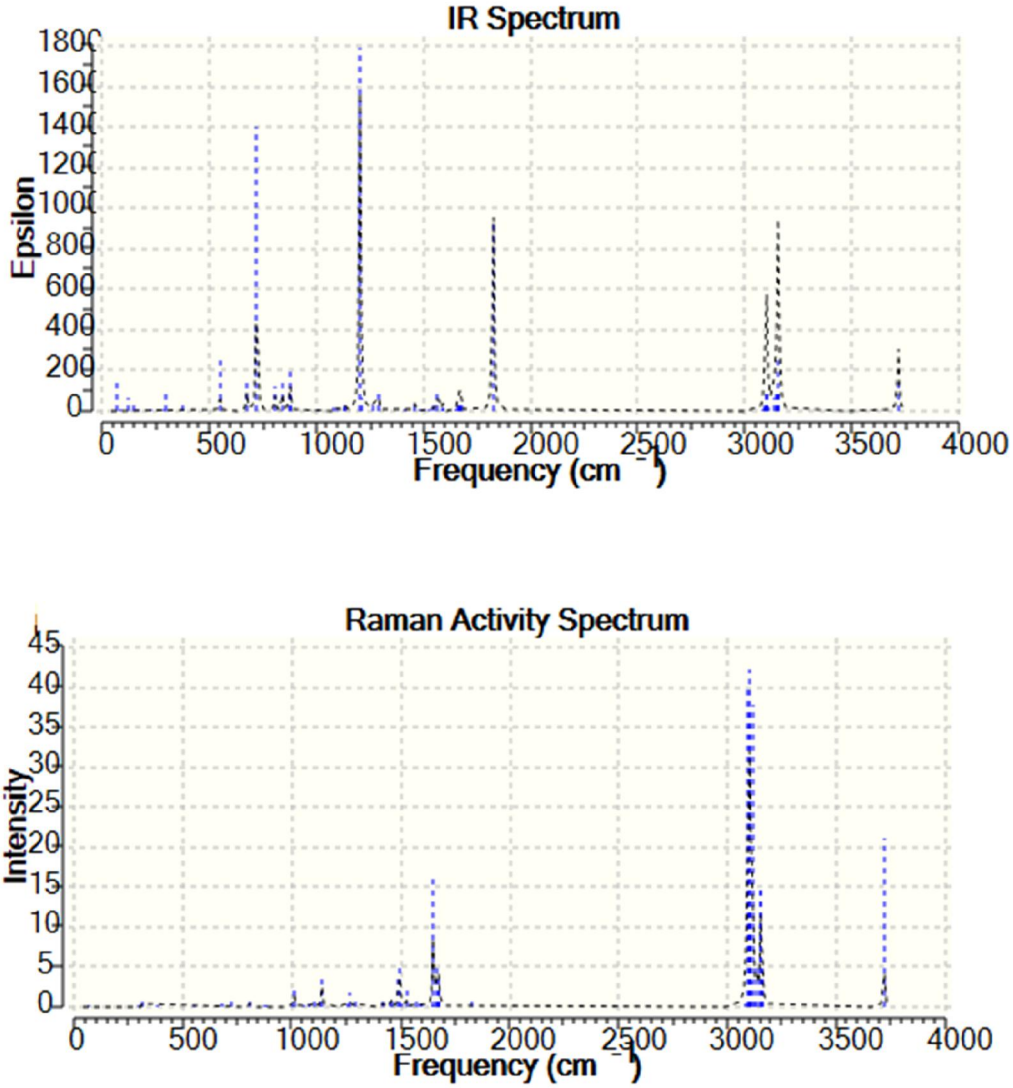

Fig. (9) Valproic acid Gaussian spectrums and statistical thermodynamic calculations index in water.