

Supporting Information

A fluorescent di-zinc(II) complex of bis-calix[4]arene conjugate as chemosensing-ensemble for the selective recognition of ATP

V.V. Sreenivasu Mummidiwarapu,^a Rakesh Kumar Pathak,^a Vijaya Kumar Hinge,^b Jayaraman Dessingou^a and Chebrolu Pulla Rao^{a,b,*}

^aDepartment of Chemistry, ^bDepartment of Biosciences & Bioengineering, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India. Email:
cprao@iitb.ac.in, cprao@chem.iitb.ac.in

Contents

S1. Characterization of L	2
S6. Characterization of $[Zn_2L]$	4
S11. Fluorescence studies of L with metal ions	6
S13. Determination of the association constant by fluorescence titration	7
S15. Determination of minimum concentration of Zn^{2+} by L	7
S17. Determination of the association constant by absorption titration	7
S19. Fluorescence studies of $[Zn_2L]$ with anions	8
S21. Dilution experiment by maintaining the ratio of $[Zn_2L]:ATP^{2-}$ as 1:2	9
S23. Absorption studies of $[Zn_2L]$ with anions	10
S25. PM3 optimized structure of L' and the molecular mechanics minimized structure of $[Zn_2L']$	12
S27. The metric data of Zn^{2+} coordination sphere of MM minimized $[(Zn)_2L'X]$ complexes	13
S28. Cartesian coordinates for PM3 optimized structure of $[L']$	15
S29. Cartesian coordinates for MM minimized structure of $[Zn_2L']$	19
S30. Cartesian coordinates for MM minimized structure of $[Zn_2L'PPi]^{4-}$	23
S31. Cartesian coordinates for MM minimized structure of $[Zn_2L'ADP]^{2-}$	26
S32. Cartesian coordinates for MM minimized structure of $[Zn_2L'ATP]^{2-}$	30

S1. Characterization of L

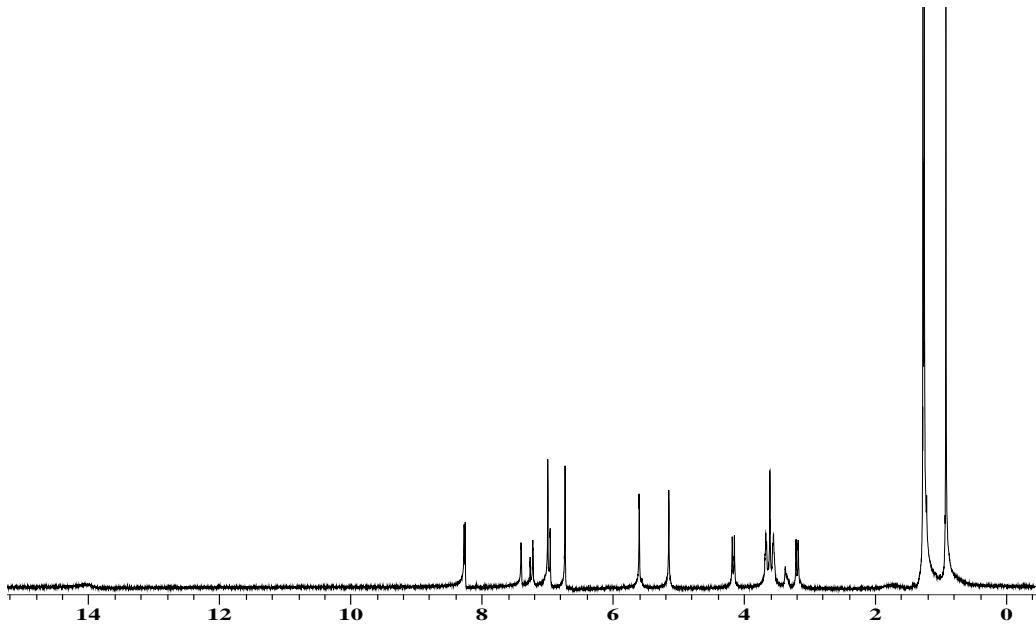


Figure S2. ^1H NMR spectrum (CDCl_3 , 400 MHz) of **L**

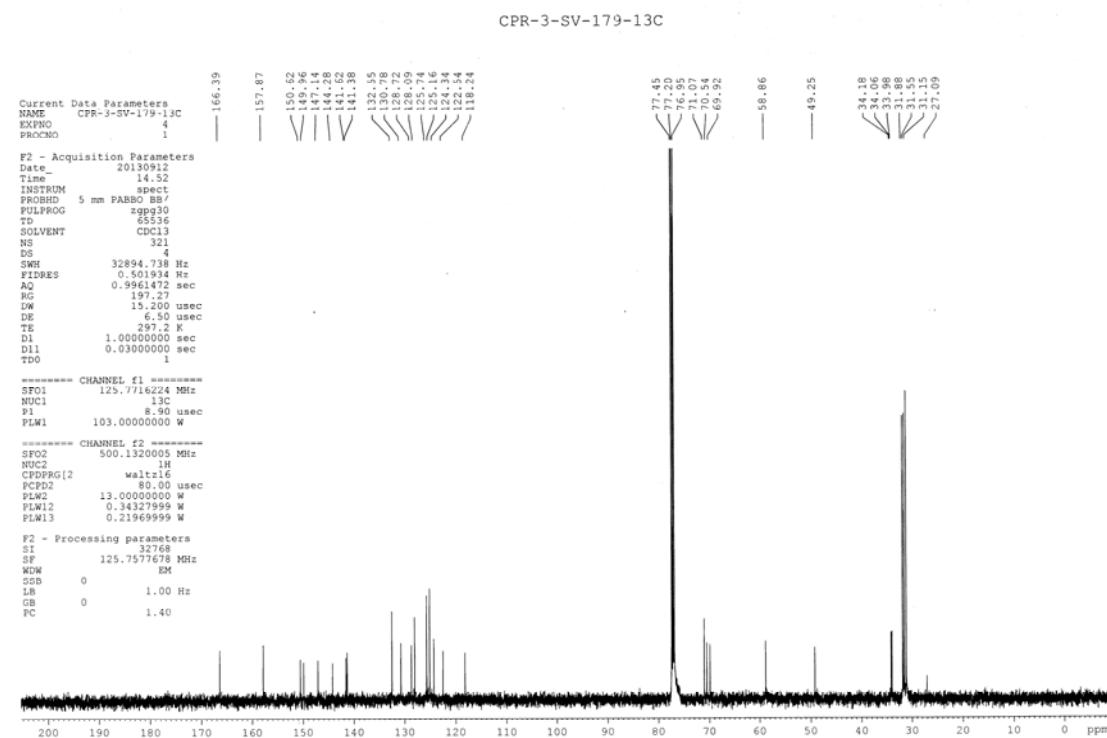


Figure S3. ^{13}C NMR spectrum (CDCl_3 , 100 MHz) of **L**

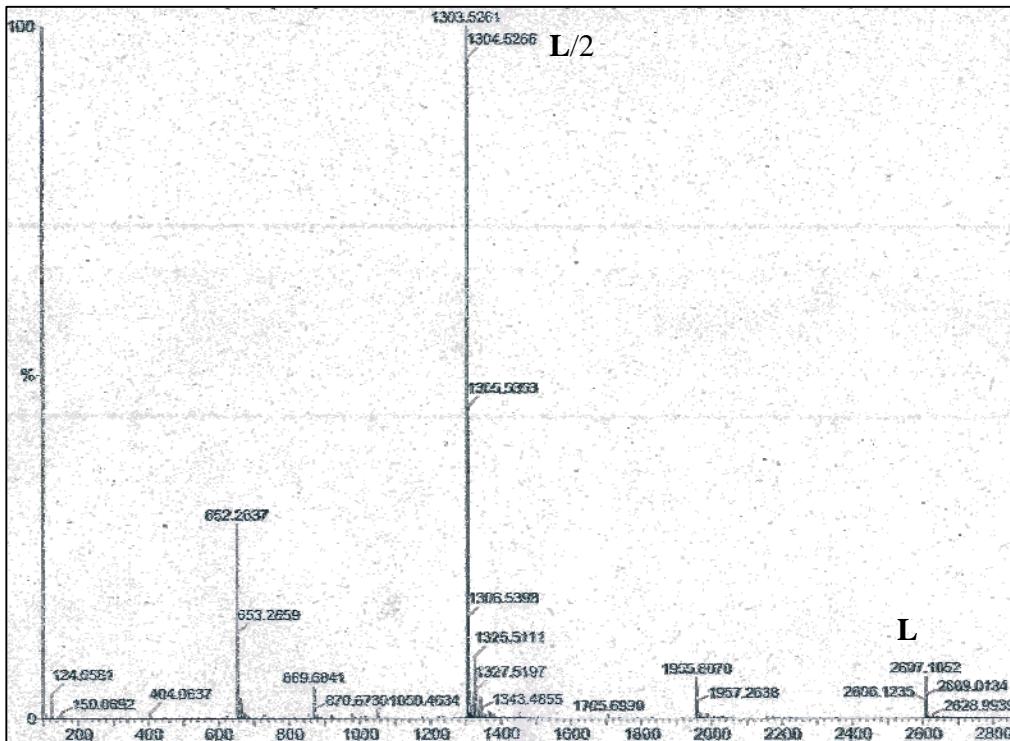


Figure S4. ESI MS of **L**.

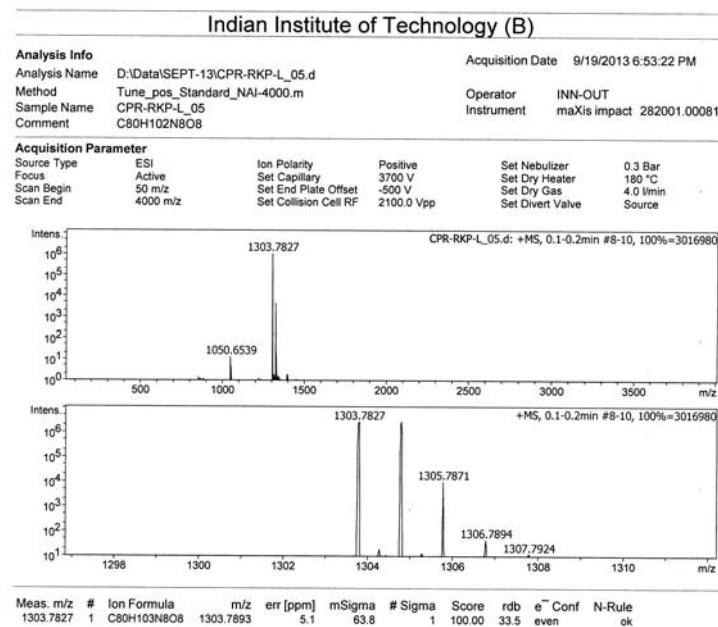


Figure S5. HRMS spectrum of **L**

S6. Characterization of [Zn₂L]

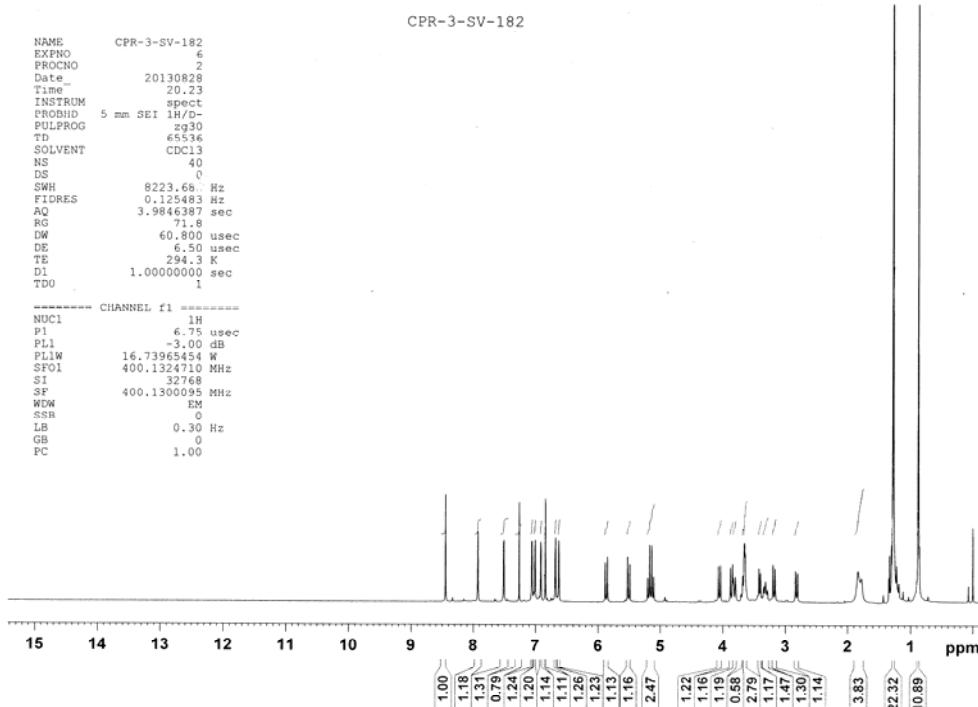


Figure S7. ¹H NMR spectrum (CDCl₃, 400 MHz) of [Zn₂L]

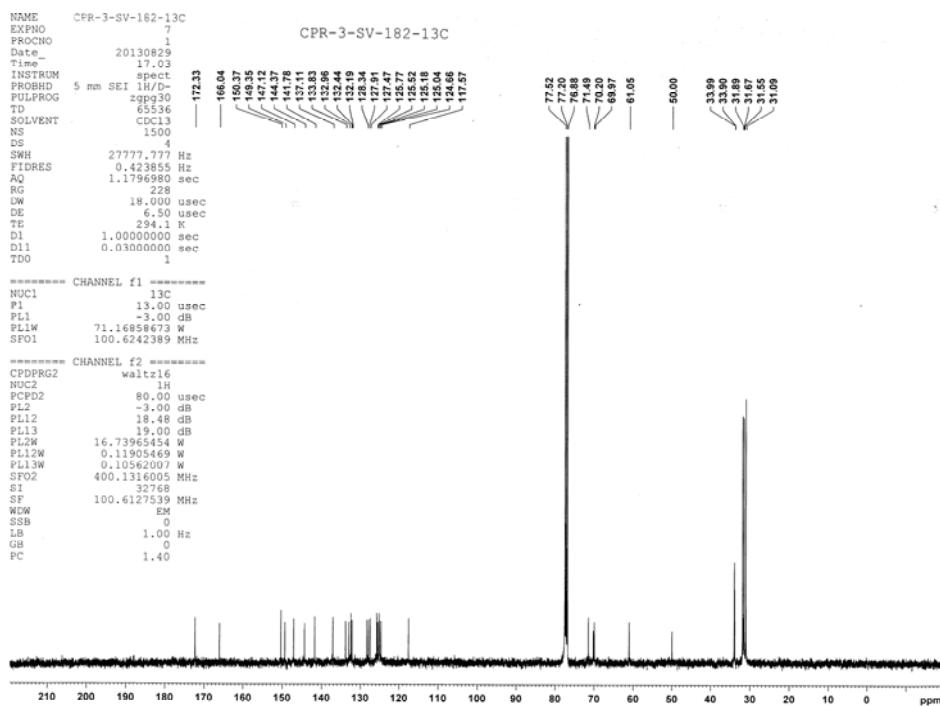


Figure S8. ¹³C NMR spectrum (CDCl₃, 100 MHz) of [Zn₂L]

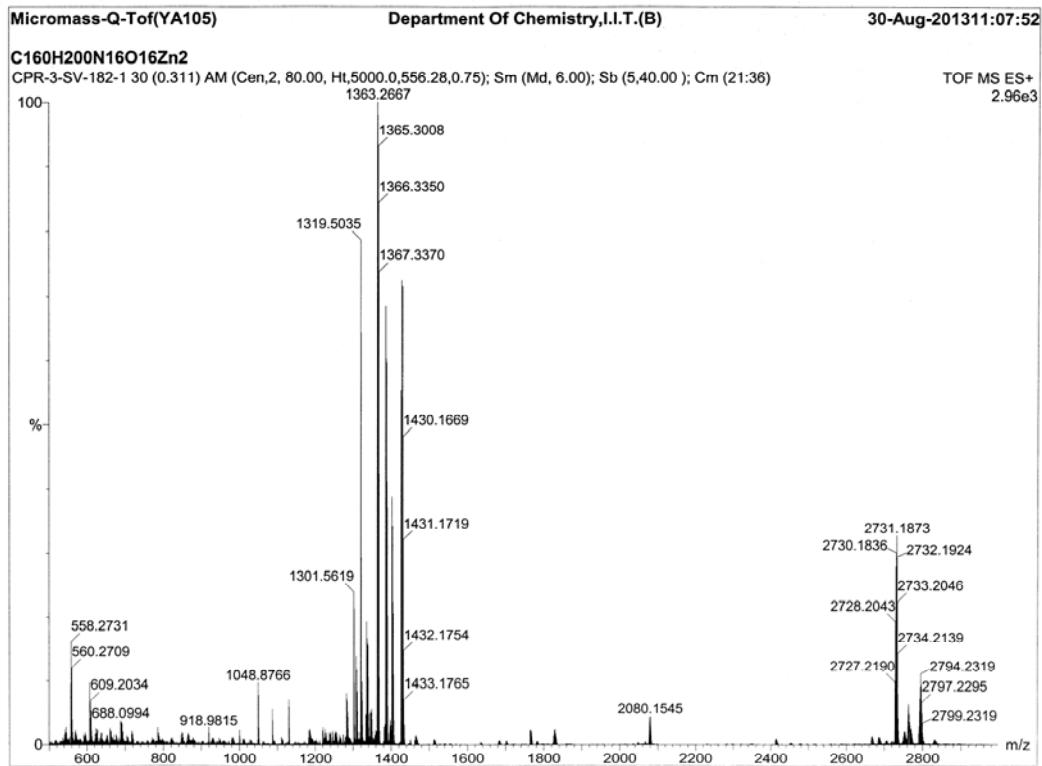


Figure S9. ESI MS of $[Zn_2L]$.

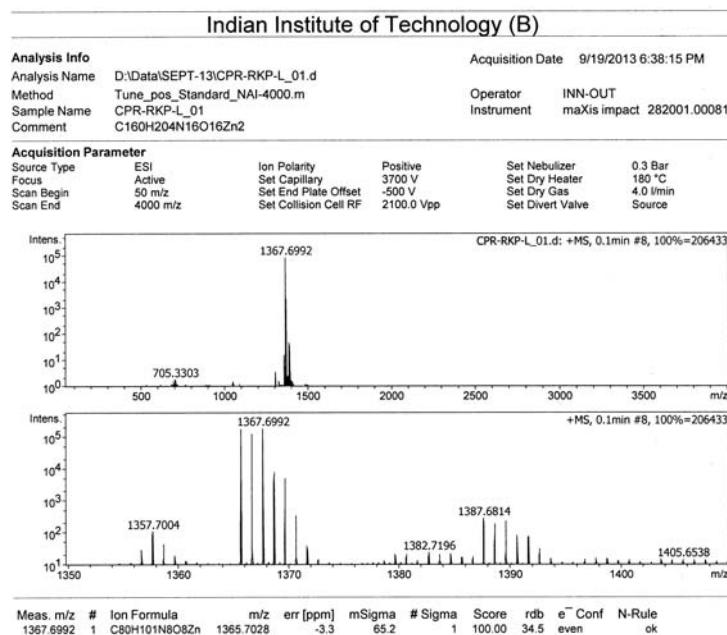


Figure S10. HRMS spectrum of $[Zn_2L]$

S11. Fluorescence studies of L with metal ions

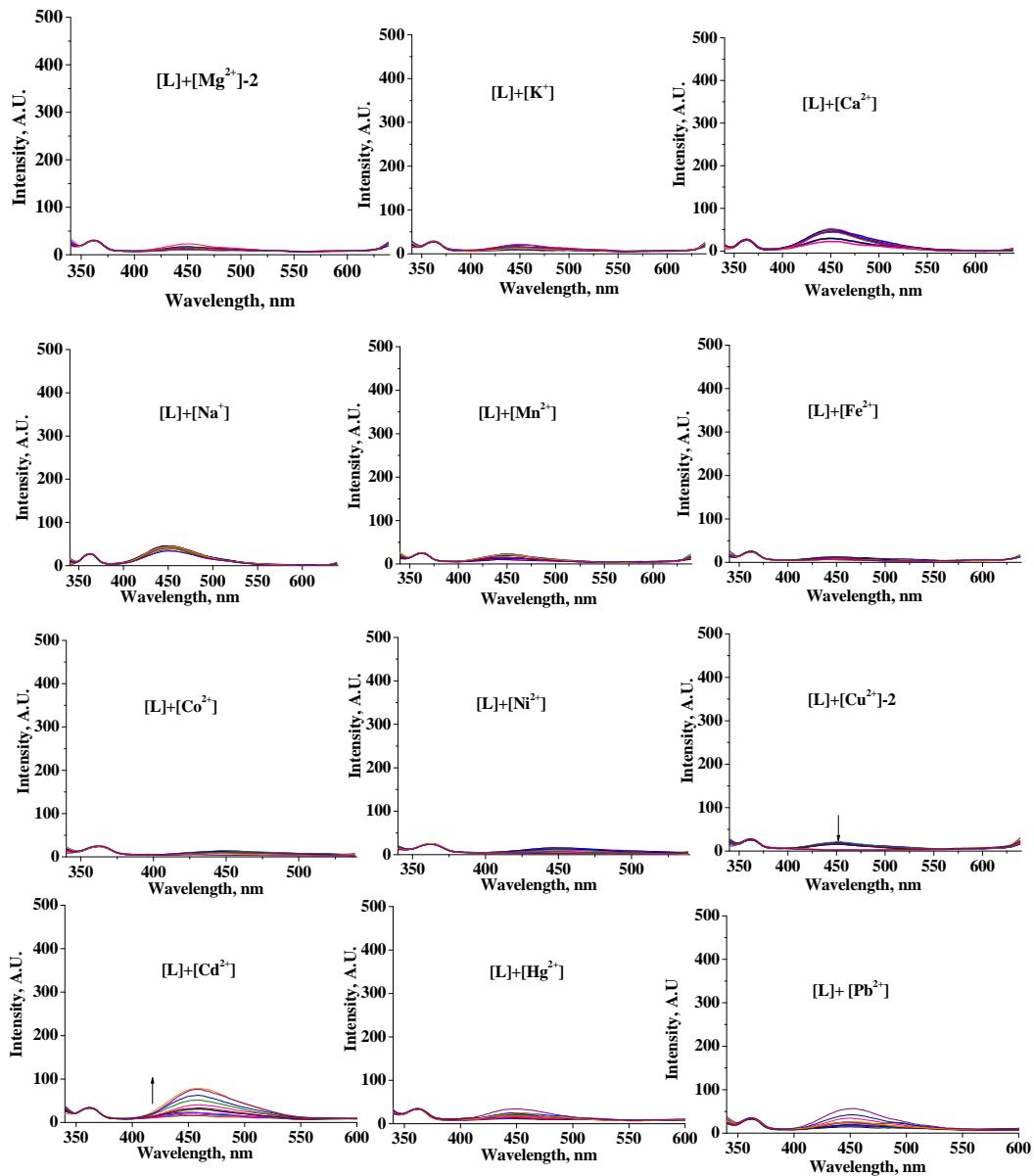


Figure S12. Fluorescence spectral traces for the titration of L with other metal ions.

S13. Determination of the association constant by fluorescence titration

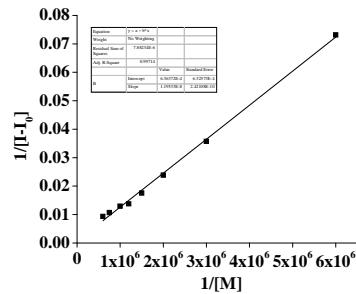


Figure S14. The binding constant of **L** with Zn^{2+} has been derived based on the Benesi – Hildebrand equation using fluorescence emission data

S15. Determination of minimum concentration of Zn^{2+} by **L**

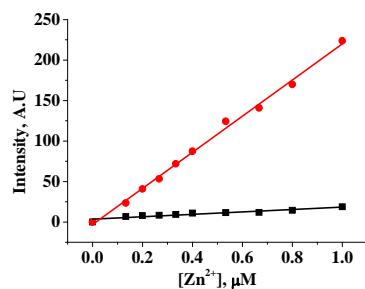


Figure S16. Determination of minimum concentration of Zn^{2+} that can be detected by **L** carried out by maintaining the ratio of **L**: Zn^{2+} as 1:2

S17. Determination of the association constant by absorption titration

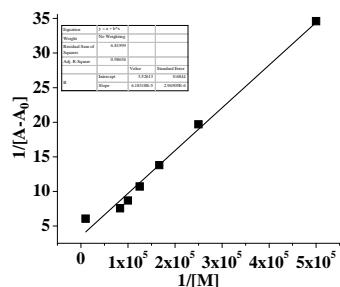
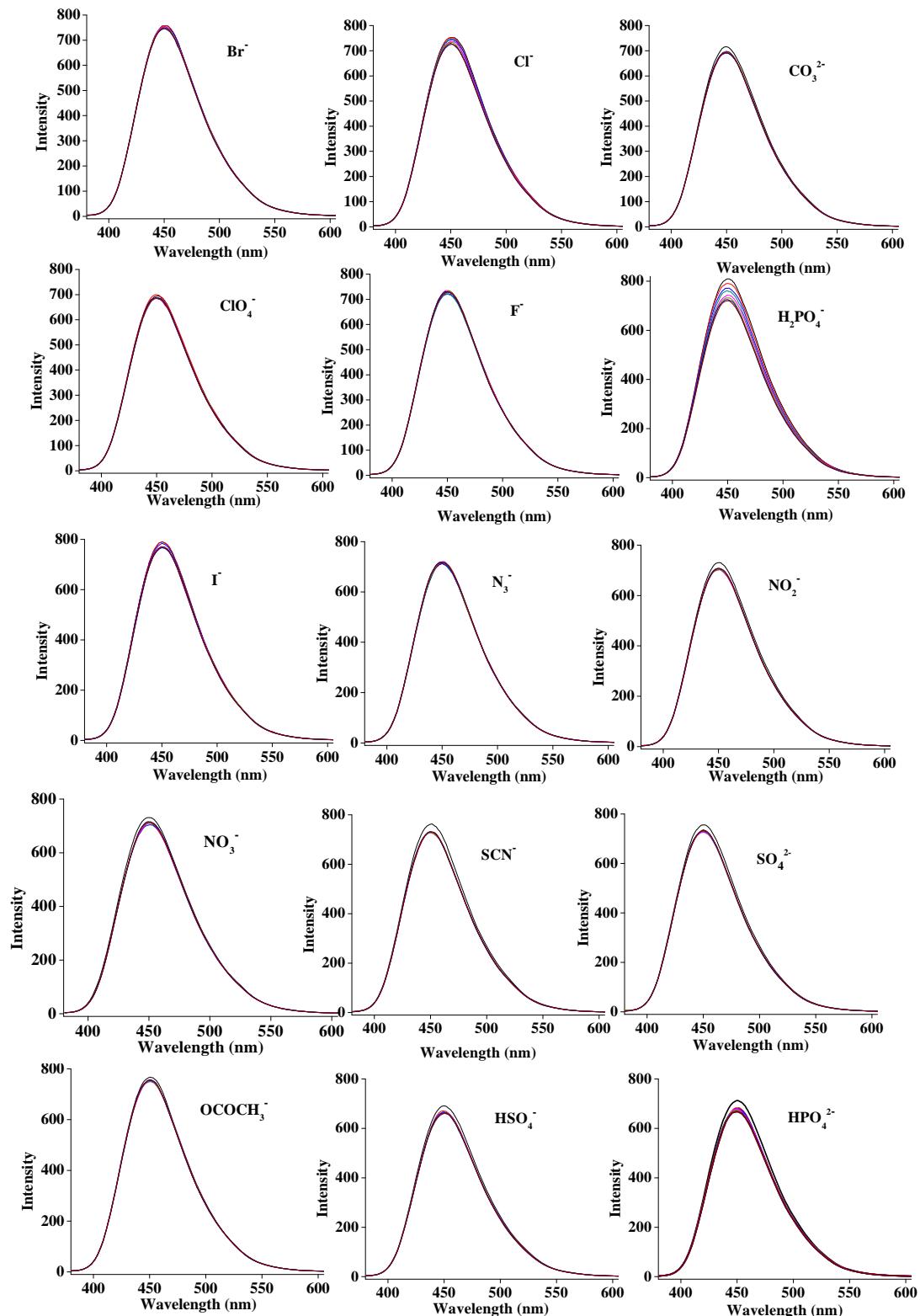


Figure S18. The binding constant of **L** with Zn^{2+} has been derived based on the Benesi – Hildebrand equation using absorption titration

S19. Fluorescence studies of $[Zn_2L]$ with anions



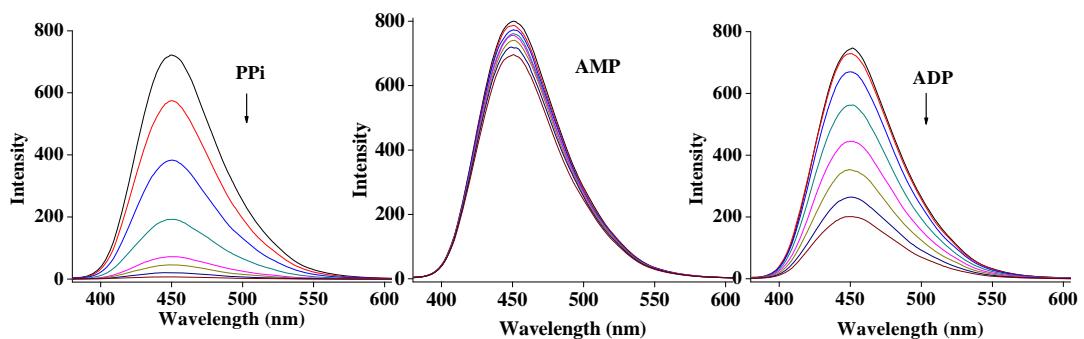


Figure S20. Fluorescence spectral traces for the titration of $[Zn_2L]$ with anions.

S21. Dilution experiment by maintaining the ratio of $[Zn_2L]$:ATP as 1:2

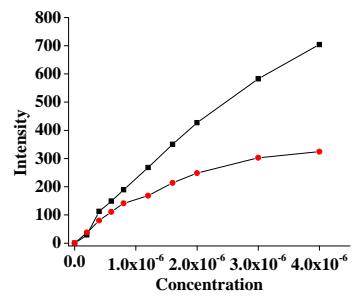
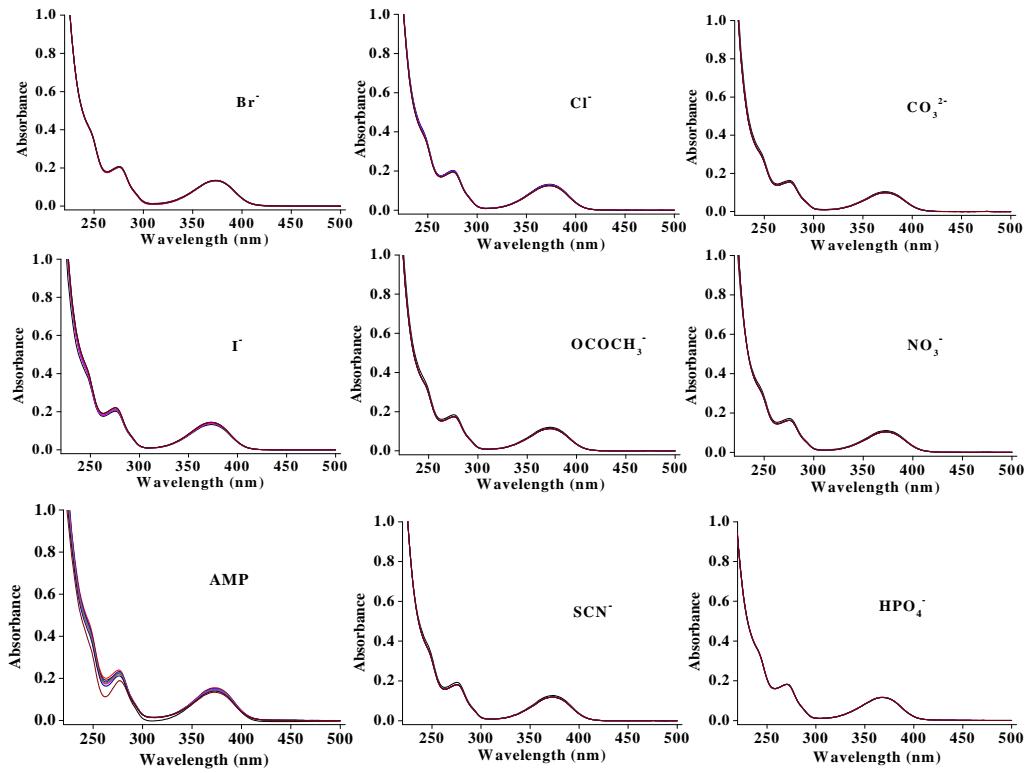


Figure S22. Minimum concentration of ATP that can be detected by $[Zn_2L]$.

S23. Absorption studies of $[\text{Zn}_2\text{L}]$ with anions



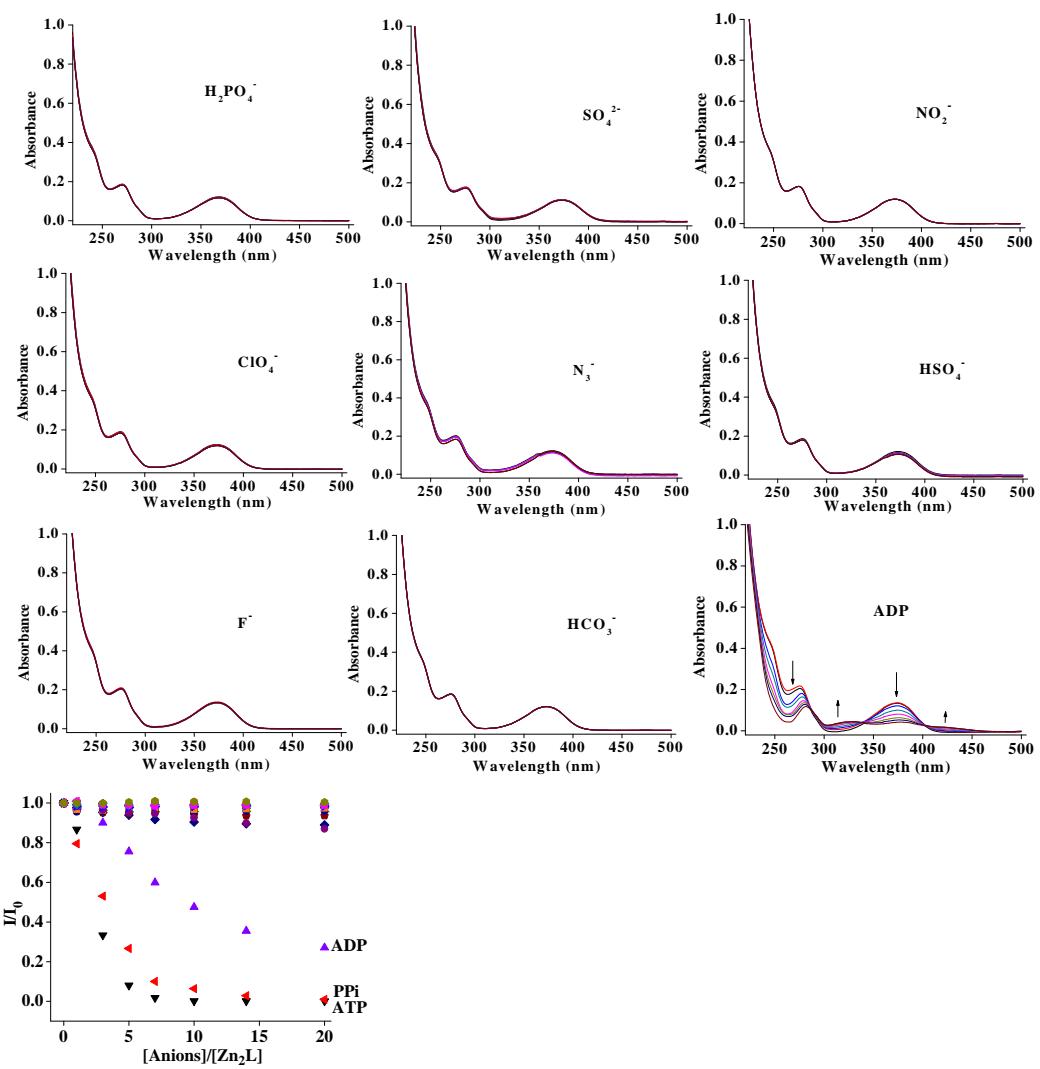


Figure S24. Absorption spectral traces for the titration of $[\text{Zn}_2\text{L}]$ with other anions.

S25. PM3 optimized structure of **L'** and the molecular mechanics minimized structure of $[Zn_2L']$.

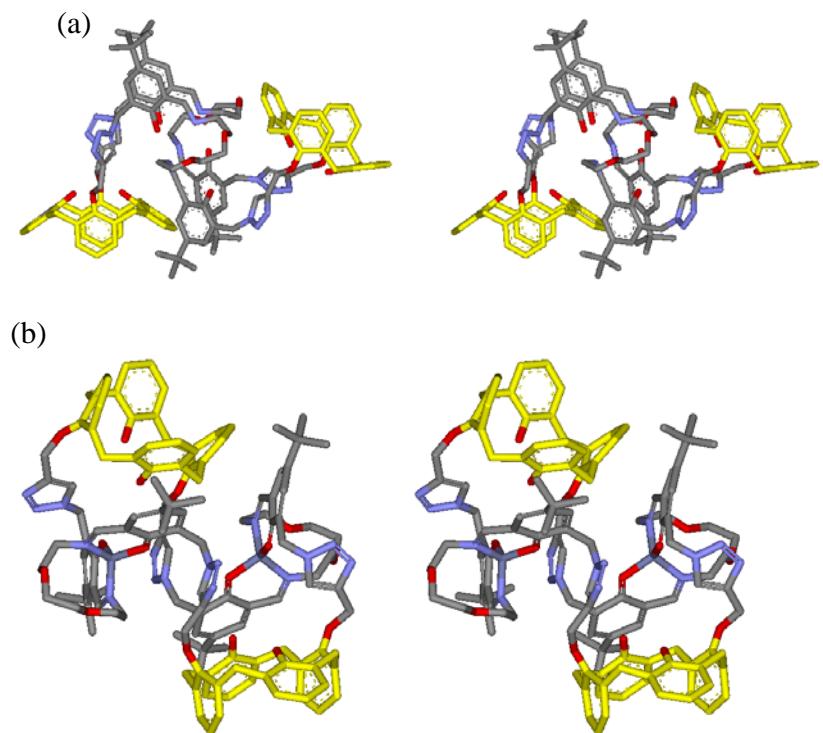


Figure S26. Stereo view representation of (a) **L'**, (b) $[Zn_2L']$.

S27. The metric data of Zn^{2+} coordination sphere of MM minimized $[(\text{Zn})_2\mathbf{L}'\mathbf{X}]$ complexes

Table S01. The metric data {bond distances (\AA)} of Zn^{2+} coordination sphere of MM minimized structures of $[(\text{Zn})_2\mathbf{L}'\mathbf{X}]$ complexes.

Distances (\AA)	$[(\text{Zn})_2\mathbf{L}'\text{PPi}]^{4-}$	$[(\text{Zn})_2\mathbf{L}'\text{ADP}]^{2-}$	$[(\text{Zn})_2\mathbf{L}'\text{ATP}]^{2-}$
O1 – Zn _a	1.908	1.878	1.874
O2 – Zn _a	1.974	1.875	1.850
O3 – Zn _a	1.8513	1.832	1.781
O4 – Zn _a	1.841	1.836	1.841
N1 – Zn _a	2.023	1.977	1.959
N2 – Zn _a	2.035	2.001	1.957
O5 – Zn _b	1.951	1.852	1.874
O6 – Zn _b	1.973	1.799	1.791
O7 – Zn _b	1.852	1.816	1.785
O8 – Zn _b	1.828	1.873	1.861
N3 – Zn _b	2.038	1.961	2.018
N4 – Zn _b	1.949	2.004	1.949

Table S02. The calculated metric data {bond distances (\AA)} of Zn_a coordination sphere of MM minimized structures of $[(\text{Zn})_2\text{L}'\text{X}]$ complexes.

Angle ($^{\circ}$)	$[(\text{Zn})_2\text{L}'\text{PPi}]^{4-}$	$[(\text{Zn})_2\text{L}'\text{ADP}]^{2-}$	$[(\text{Zn})_2\text{L}'\text{ATP}]^{2-}$
O1 – Zn_a - O2	163.4	158.4	161.6
N1 – Zn_a - O3	152.7	150.5	151.1
N2 – Zn_a - O4	150.9	154.9	155.2
O1 – Zn_a - N1	101.1	76.6	79.4
O1 – Zn_a - N2	64.6	86.2	88.9
O1 – Zn_a - O3	87.0	81.5	82.2
O1 – Zn_a - O4	103.4	118.0	114.4
O2 – Zn_a - O3	109.3	111.7	109.6
O2 – Zn_a - O4	80.26	80.2	81.0
O3 – Zn_a - O4	87.5	89.2	86.7
N1 – Zn_a - N2	108.4	109.6	113.1
N1 – Zn_a - O2	79.4	95.2	94.0
N1 – Zn_a - O4	82.2	83.8	80.8
N2 – Zn_a - O2	99.2	83.8	77.7
N2 – Zn_a - O3	92.6	88.1	88.4

Table S03. The calculated metric data {bond distances (\AA)} of Zn_b coordination sphere of MM minimized structures of $[(\text{Zn})_2\text{L}'\text{X}]$ complexes.

Angle ($^{\circ}$)	$[(\text{Zn})_2\text{L}'\text{PPi}]^{4-}$	$[(\text{Zn})_2\text{L}'\text{ADP}]^{2-}$	$[(\text{Zn})_2\text{L}'\text{ATP}]^{2-}$
O5 – Zn_b - O8	156.1	141.8	140.1
N3 – Zn_b - O6	149.8	140.9	137.1
N4 – Zn_b - O7	155.0	141.8	136.7
O5 – Zn_b - N3	97.4	86.0	72.9
O5 – Zn_b - N4	106.2	88.4	127.9
O5 – Zn_b - O6	87.4	65.9	82.2
O5 – Zn_b - O7	74.6	126.2	92.2
O6 – Zn_b - O7	113.2	98.0	99.3
O6 – Zn_b - O8	77.5	90.9	130.1
O7 – Zn_b - O8	94.1	84.9	63.4
N3 – Zn_b - N4	62.9	92.8	93.5
N3 – Zn_b - O7	95.1	76.4	115.7
N3 – Zn_b - O8	102.2	126.	89.0
N4 – Zn_b - O6	90.8	112.0	74.7
N4 – Zn_b - O8	94.7	71.9	87.4

Table S04. The range and its average values of trans angles are given for Zn²⁺ coordination sphere of [(Zn)₂L'X] complexes.

Angle (°)	[(Zn) ₂ L'PPi] ⁴⁻ Range (average)	[(Zn) ₂ L'ADP] ²⁻ Range (average)	[(Zn) ₂ L'ATP] ²⁻ Range (average)
Zn _a Trans angles	151-163 (156)	151-158 (155)	151-162 (156)
Zn _a other angles	65-109 (91)	77-118 (92)	78-114 (91)
Zn _b Trans angles	150-156 (154)	141-142 (141.5)	137-140 (137.9)
Zn _b other angles	63-113 (91)	66-126 (93)	137-130 (94)

S28. Cartesian coordinates for PM3 optimized structure of [L'].

Z	Coordinates				Coordinates			
	X	Y	Z	X	Y	Z	X	
8	6.43875	-1.52477	2.232743	1	11.73281	-2.32824	-2.61309	
8	5.411696	0.453263	-0.12072	6	-9.43259	-1.34526	1.188343	
8	7.736145	-2.61756	-0.3944	6	-8.65875	-1.41877	2.471728	
8	-5.79428	-0.99239	2.305056	1	-9.34669	-1.57624	3.326393	
8	0.80646	-1.91664	2.318767	1	-8.16126	-0.44164	2.661843	
8	-1.40348	2.982174	2.349037	6	-6.27249	-2.30109	2.290435	
8	1.887083	-1.57836	5.514241	6	-7.65439	-2.5345	2.42433	
8	3.132597	1.151026	4.747121	6	-8.10581	-3.85342	2.480888	
7	4.77953	-4.46821	3.240682	1	-9.17969	-4.04784	2.591866	
7	3.766117	-5.02411	2.706214	6	-7.21181	-4.91331	2.390537	
7	3.109584	-4.08519	1.949363	6	-5.86306	-4.67124	2.167295	
7	-1.15269	-1.3185	5.423566	1	-5.15455	-5.51099	2.071047	
7	1.151821	2.650303	2.987327	6	-5.38056	-3.3649	2.065479	
7	-4.62554	2.970996	3.27988	6	9.093507	-2.74182	2.078002	
7	-5.7003	2.986089	4.134085	1	9.716071	-3.26736	2.831078	
7	-6.08177	1.783961	4.314549	1	8.154766	-3.32699	2.007061	
6	7.555536	-0.75534	2.550219	6	5.892504	-2.18406	3.383545	
6	8.837516	-1.33525	2.539609	1	5.435499	-1.42483	4.062319	
6	9.928248	-0.5499	2.917994	1	6.683406	-2.71827	3.944896	
1	10.9296	-0.99823	2.934263	6	4.841231	-3.10749	2.887781	
6	9.761945	0.789029	3.24572	6	3.76206	-2.85287	2.057351	
6	8.508732	1.378035	3.146337	1	3.44385	-1.92919	1.569704	
1	8.389211	2.450631	3.342894	6	1.820515	-4.33184	1.2625	
6	7.393472	0.623924	2.777143	1	1.871943	-5.31998	0.758245	
6	6.083852	1.333692	2.594362	6	0.20348	-3.06343	2.757653	
1	5.870908	1.946132	3.495924	6	0.657833	-4.27727	2.207889	
1	5.225533	0.622949	2.526572	6	0.003756	-5.45926	2.547821	
6	5.910363	1.714733	0.081981	1	0.337824	-6.41844	2.115655	
6	6.135069	2.214118	1.38005	6	-1.07308	-5.46578	3.436943	
6	6.45648	3.563247	1.532047	6	-1.49047	-4.2604	4.001642	
1	6.620542	3.971551	2.536705	1	-2.33679	-4.26729	4.708712	
6	6.577565	4.39273	0.424669	6	-0.86027	-3.06095	3.676809	
6	6.423197	3.876194	-0.85594	6	-1.3667	-1.8025	4.254136	
1	6.564558	4.529202	-1.7258	6	-0.36188	-1.88614	6.507221	
6	-3.76327	-3.46548	0.21551	1	-0.97879	-2.6657	6.997254	
6	-3.94685	-3.15431	1.673319	1	-0.25836	-1.05548	7.233898	
1	-3.61142	-2.12054	1.895397	6	1.011009	-2.47312	6.162437	
1	-3.2939	-3.81181	2.290563	1	1.473464	-2.89024	7.078521	
6	9.096405	-2.56915	-0.46275	1	0.942094	-3.28454	5.413177	
6	9.797579	-2.71346	0.752616	6	2.459605	-0.58376	6.353272	
6	11.18902	-2.78601	0.712717	1	2.871569	-1.04623	7.271749	

1	11.74989	-2.92629	1.644717	1	1.680298	0.13972	6.661562
6	11.876	-2.67785	-0.49106	6	3.588783	0.097228	5.567928
6	11.18242	-2.45286	-1.67297	1	4.2527	0.637865	6.265852
6	2.729493	0.762921	3.439456	1	4.210879	-0.6349	5.000822
1	1.847895	0.086926	3.485791	6	-6.44096	-3.08849	-4.02948
1	3.559888	0.206421	2.941502	1	-5.79	-3.90259	-4.37431
6	2.443668	2.046636	2.653891	6	-5.86695	-1.95267	-3.45675
1	2.379469	1.807062	1.574552	6	-4.38084	-1.93154	-3.25212
1	3.27942	2.769955	2.774014	1	-3.87007	-2.22433	-4.19733
6	1.012033	3.490846	3.966078	1	-4.00676	-0.90881	-3.03554
6	-1.43511	3.806444	3.424443	6	-4.04217	-2.51734	-0.79121
6	-0.3046	4.075289	4.228166	6	-3.99369	-2.87773	-2.15295
6	-0.43698	4.933392	5.323655	6	-3.59599	-4.17139	-2.49
1	0.437252	5.152185	5.960008	1	-3.54748	-4.46832	-3.55252
6	-1.6572	5.522661	5.638312	6	-3.24871	-5.08677	-1.50638
6	-2.76421	5.263313	4.824295	6	-3.343	-4.73932	-0.16428
1	-3.72546	5.744926	5.074488	1	-3.0899	-5.48661	0.606952
6	-2.67282	4.416646	3.725666	6	6.106118	2.531659	-1.04891
6	-3.88529	4.189088	2.876521	6	6.034756	1.990229	-2.44766
1	-4.57187	5.059186	2.941462	1	5.804939	2.809116	-3.16169
1	-3.60705	4.082917	1.799999	1	5.190149	1.27613	-2.54215
6	-4.31622	1.654679	2.930591	6	-8.94426	-0.63021	0.074477
1	-3.49767	1.359021	2.270593	6	-9.61874	-0.67672	-1.16349
6	-5.26217	0.89298	3.599185	6	-10.8394	-1.34687	-1.22984
6	-5.44018	-0.57957	3.635428	1	-11.3936	-1.3682	-2.17606
1	-4.48867	-1.07429	3.917788	6	-11.3614	-1.99398	-0.11586
1	-6.21645	-0.87944	4.366781	6	-10.6508	-2.01279	1.077203
8	-6.15043	0.272301	-2.5426	1	-11.0496	-2.55805	1.940936
8	-4.28972	-1.23884	-0.37802	6	9.790625	-2.38028	-1.676
8	-7.81827	0.13566	0.12994	6	9.062399	-2.07288	-2.95119
8	6.430907	-0.87569	-2.67118	1	9.654799	-2.4115	-3.82453
8	-1.31184	3.36906	-1.25012	1	8.114284	-2.65472	-2.98537
8	-0.02517	-0.32182	-3.11217	6	7.520915	-0.03829	-2.88965
8	3.049844	2.903455	-4.68288	6	8.800672	-0.59775	-3.06351
8	0.573886	3.162572	-7.0055	6	9.876	0.258935	-3.30213
7	-5.88028	3.738213	-3.32277	1	10.87594	-0.16612	-3.45384
7	-5.332	4.652308	-2.62494	6	9.694289	1.635857	-3.3259
7	-4.48157	4.056039	-1.729	6	8.444046	2.179913	-3.06263
7	1.197768	3.337087	-2.11725	1	8.315505	3.268716	-3.02739
7	-1.01967	0.676255	-6.00827	6	7.343839	1.355366	-2.82023
7	2.630486	-2.7547	-2.78237	6	-9.04044	-0.07398	-2.41129
7	3.460902	-3.84141	-2.91501	1	-9.85203	0.181966	-3.12315
7	4.595526	-3.42853	-3.31708	1	-8.53074	0.883534	-2.1846
6	-6.70867	-0.90117	-3.04844	6	-5.87831	1.220102	-3.58543
6	-8.10639	-1.05825	-3.05572	1	-5.08703	0.819292	-4.25346
6	-8.64465	-2.20957	-3.6349	1	-6.78722	1.391313	-4.19484

1	-9.73449	-2.33246	-3.66672	6	-5.41191	2.47017	-2.93349
6	-7.81993	-3.20271	-4.14571	6	-4.5027	2.669571	-1.90568
6	-3.67171	4.811922	-0.74503	1	-3.91421	1.956844	-1.32419
1	-4.31542	5.597231	-0.29398	1	5.454032	-0.33081	-4.44354
1	-3.39277	4.119696	0.085289	1	6.454682	-1.8183	-4.54076
6	-1.27252	4.683499	-1.57486	1	-12.3277	-2.50325	-0.18387
6	-2.45144	5.430413	-1.35453	1	-7.57565	-5.94262	2.472279
6	-2.47103	6.780962	-1.68168	1	-8.25756	-4.09024	-4.61407
1	-3.38658	7.376976	-1.5229	1	-2.913	-6.08941	-1.79265
6	-1.34802	7.418053	-2.22	1	10.6246	1.387822	3.555479
6	-0.18591	6.680545	-2.41703	1	6.815848	5.452542	0.560355
1	0.701995	7.189667	-2.82877	1	12.96769	-2.75403	-0.50473
6	-0.12828	5.317573	-2.11006	1	10.54477	2.294916	-3.5287
6	1.120567	4.604175	-2.38457	6	-1.7766	6.477532	6.810627
6	2.386292	2.537816	-2.42292	6	-0.77375	6.129117	7.911906
1	2.361191	1.696565	-1.70252	6	-3.18172	6.435072	7.41394
6	2.343059	1.989076	-3.85535	1	-3.9524	6.604009	6.644015
1	1.300345	1.836055	-4.217	1	-3.39127	5.461706	7.876361
1	2.857433	1.00149	-3.89536	1	-3.30412	7.205185	8.186218
6	2.819975	2.756247	-6.07135	1	-1.00901	5.163575	8.378351
1	3.81788	2.985921	-6.48529	1	-0.77409	6.890399	8.702445
1	2.565533	1.715852	-6.35228	1	0.251004	6.0586	7.512002
6	1.784514	3.766177	-6.60448	6	-1.48954	7.88949	6.292765
1	2.135312	4.196699	-7.55904	1	-0.47989	7.959601	5.867746
1	1.618405	4.600171	-5.89464	1	-2.20163	8.176892	5.508252
6	-0.40286	3.04556	-5.97925	1	-1.56395	8.632944	7.097485
1	0.065038	2.762912	-5.00918	6	-1.80904	-6.7559	3.747446
1	-0.87675	4.036624	-5.84338	6	-2.95355	-6.90008	2.740256
6	-1.44218	2.010986	-6.42908	6	-2.38638	-6.73495	5.16389
1	-2.44051	2.293578	-6.03062	1	-1.59262	-6.74774	5.92205
1	-1.53531	1.97487	-7.53276	1	-2.99092	-5.82931	5.336661
6	-1.7536	-0.08685	-5.27716	1	-3.0299	-7.60645	5.33932
6	-0.3128	-1.48451	-3.77321	1	-3.7534	-6.15701	2.912406
6	-1.20983	-1.3916	-4.85389	1	-3.41481	-7.89448	2.799369
6	-1.59716	-2.54861	-5.51837	1	-2.60446	-6.75209	1.704161
1	-2.32056	-2.49889	-6.3489	6	-0.87511	-7.96213	3.630556
6	-1.09717	-3.79841	-5.13768	1	-0.08673	-7.93448	4.39428
6	-0.15282	-3.87009	-4.11701	1	-1.42498	-8.904	3.753805
1	0.272255	-4.85295	-3.85177	1	-0.37692	-7.98801	2.647737
6	0.245525	-2.72655	-3.42409	6	-1.57561	-5.0457	-5.85524
6	1.230525	-2.85273	-2.30547	6	-3.06872	-4.91937	-6.16837
1	1.097049	-3.8212	-1.77744	6	-1.36787	-6.29821	-5.0025
1	1.073134	-2.05117	-1.54649	1	-0.32729	-6.37062	-4.64646
6	3.312275	-1.59028	-3.14873	1	-2.01522	-6.29177	-4.11317
1	2.896181	-0.57316	-3.16056	1	-1.59323	-7.2077	-5.57356
6	4.582464	-2.03225	-3.48367	1	-3.66273	-4.83185	-5.24142

6	5.769149	-1.23882	-3.89242	1	-3.43577	-5.78969	-6.72555
6	-0.78516	-5.18201	-7.15745	1	-3.27063	-4.01798	-6.77009
1	0.287717	-5.30261	-6.95963	1	7.398874	-2.60002	-1.28695
1	-1.11776	-6.05428	-7.73556	1	5.993022	-0.15072	0.328538
1	-0.90906	-4.29479	-7.79246	1	1.707186	-3.56925	0.462511
6	-1.38616	8.902375	-2.52942	1	-3.08407	8.88828	-3.90494
6	-0.41846	9.257431	-3.65965	1	-0.50097	2.643284	2.256227
1	-0.73704	8.818174	-4.61399	1	-0.44558	2.984767	-1.44921
1	-0.35373	10.34426	-3.79801	1	0.745001	-1.25358	3.003983
1	0.596846	8.883268	-3.44952	1	0.391166	-0.5543	-2.2864
6	-2.79056	9.340654	-2.94869	1	1.950379	5.177763	-2.83007
1	-3.54265	9.040613	-2.20065	1	1.844081	3.79343	4.623309
1	-2.84712	10.43068	-3.06321	1	-2.76927	0.161776	-4.91848
6	-0.97819	9.653622	-1.25923	1	-2.04355	-1.21149	3.613372
1	-1.66132	9.430373	-0.42938	1	3.331356	3.092862	-2.23029
1	0.034686	9.375326	-0.94052	1	-4.90134	-0.84521	-0.9905
1	-0.99056	10.74034	-1.4165	1	-7.48908	0.104354	1.025001

S29. Cartesian coordinates for MM minimized structure of [Zn₂L']

Z	Coordinates			Coordinates			X
	X	Y	Z	X	Y	Z	
8	6.778	-1.513	0.38	6	-6.993	-3.394	-4.739
8	-3.732	0.192	1.329	6	-6.524	-2.024	-4.476
8	1.375	-2.103	2.592	6	-5.033	-1.753	-4.433
8	1.067	0.961	2.262	6	-3.957	-1.991	-2.028
8	-0.531	-0.032	6.606	6	-4.363	-2.562	-3.337
8	1.844	-0.523	7.724	6	-4.061	-3.977	-3.611
7	4.542	-4.854	4.327	6	-3.62	-4.869	-2.541
7	3.58	-5.217	3.425	6	-3.342	-4.328	-1.213
7	3.552	-4.329	2.388	6	4.879	3.254	0.164
7	-0.866	-0.725	3.999	6	4.79	3.061	-1.332
7	2.151	-0.045	4.827	6	-7.811	-0.568	0.198
7	-0.628	2.98	0.467	6	-9.005	-1.089	-0.499
7	-1.249	4.055	1.041	6	-10.023	-1.83	0.259
7	-2.488	3.706	1.5	6	-9.882	-2.009	1.703
6	7.032	-0.95	3.5	6	-8.767	-1.382	2.412
6	8.314	-1.568	3.089	6	8.239	-1.782	-1.48
6	9.503	-0.702	3.031	6	7.26	-1.277	-2.519
6	9.333	0.744	2.892	6	5.967	1.029	-2.47
6	7.987	1.32	2.881	6	7.218	0.238	-2.579
6	6.814	0.478	3.18	6	8.495	0.974	-2.608
6	5.457	1.105	3.421	6	8.552	2.376	-2.193
6	4.808	2.099	1.083	6	7.334	3.052	-1.75
6	5.183	2.277	2.504	6	6.037	2.367	-1.843
6	5.38	3.638	3.03	6	-9.25	-0.767	-1.957

6	5.38	4.789	2.128	6	-7.046	0.828	-5.206
6	5.123	4.6	0.702	6	-6.285	1.965	-4.586
6	-3.462	-2.886	-0.96	6	-5.776	1.983	-3.218
6	-2.854	-2.322	0.305	6	-5.336	3.84	-1.566
6	7.848	-1.943	-0.061	6	-2.779	3.95	-2.082
6	8.759	-2.631	0.877	6	-3.992	4.528	-1.466
6	10.07	-3.104	0.41	6	-3.924	5.833	-0.799
6	10.469	-2.915	-0.984	6	-2.696	6.643	-0.833
6	9.548	-2.284	-1.929	6	-1.613	6.185	-1.719
6	-7.732	-0.638	1.676	6	-1.602	4.83	-2.3
6	-6.71	0.152	2.468	6	-0.356	4.452	-3
6	-4.36	-0.779	1.771	6	1.339	2.723	-3.606
6	-5.479	-0.689	2.738	6	1.52	1.916	-4.912
6	-5.614	-1.778	3.722	6	0.966	1.893	-7.224
6	-5.096	-3.106	3.389	6	-0.12	2.409	-8.202
6	-4.347	-3.296	2.147	6	-2.02	2.975	-6.831
6	-3.914	-2.129	1.362	6	-2.905	2.212	-5.818
6	8.351	-2.869	2.315	6	-1.973	-0.058	-5.314
6	6.094	-2.819	4.664	6	-0.891	-0.811	-3.027
6	5.186	-3.692	3.844	6	-1.295	-1.038	-4.44
6	4.541	-3.343	2.58	6	-1.049	-2.358	-5.048
6	2.547	-4.312	1.345	6	-0.611	-3.517	-4.251
6	0.649	-3.1	2.632	6	-0.514	-3.322	-2.798
6	1.158	-4.301	1.944	6	-0.409	-1.967	-2.243
6	0.346	-5.523	1.893	6	0.425	-1.791	-0.993
6	-0.857	-5.671	2.73	6	2.629	-0.776	-1.657
6	-1.327	-4.479	3.456	6	3.661	-1.276	-2.561
6	-0.66	-3.171	3.332	6	4.386	-0.424	-3.561
6	-1.403	-2.021	3.89	6	1.72	6.299	3.912
6	-1.638	0.403	4.495	6	1.764	6.449	5.465
6	-1.784	0.364	6.035	6	0.313	6.773	3.432
6	-0.536	0.019	8.041	6	2.82	7.223	3.308
6	0.707	-0.731	8.584	6	-1.547	-7.035	2.844
6	1.994	-1.585	6.759	6	-2.112	-7.446	1.45
6	2.849	-1.077	5.576	6	-2.733	-7.035	3.859
6	2.45	1.326	4.965	6	-0.514	-8.1	3.328
6	1.519	2.052	2.619	6	-0.121	-4.792	-4.943
6	2.014	2.345	3.987	6	-1.247	-5.376	-5.85
6	2.19	3.751	4.388	6	0.296	-5.905	-3.932
6	1.944	4.857	3.448	6	1.126	-4.442	-5.813
6	1.81	4.509	2.022	6	-2.597	7.923	0.003
6	1.493	3.134	1.617	6	-1.168	8.55	-0.026
6	0.811	2.913	0.284	6	-3.602	8.977	-0.553
6	-1.487	1.859	0.533	6	-2.942	7.601	1.491
6	-2.677	2.334	1.232	3	0.941	-0.493	3.412
6	-3.902	1.551	1.6	3	-1.467	1.859	-3.283

8	-7.681	0.071	-4.215	1	10.455	-1.125	2.886
8	-3.97	-0.782	-1.788	1	7.878	2.355	2.735
8	-6.905	-0.099	-0.495	1	5.418	1.439	4.46
8	4.852	0.709	-2.899	1	4.676	0.357	3.284
8	-2.836	2.76	-2.402	1	5.605	3.783	4.046
8	-0.921	0.282	-2.454	1	5.158	5.429	0.057
8	0.861	2.608	-5.983	1	-2.358	-1.376	0.085
8	-1.429	2.026	-7.741	1	-2.096	-3.01	0.683
7	-6.403	3.317	-4.987	1	10.73	-3.577	1.077
7	-5.964	4.113	-3.962	1	9.83	-2.193	-2.937
7	-5.577	3.341	-2.905	1	-7.146	0.454	3.423
7	-0.041	3.135	-3.392	1	-6.459	1.062	1.929
7	-2.11	1.308	-5	1	-6.272	-1.672	4.535
7	1.831	-1.894	-1.338	1	-4.026	-4.26	1.88
7	2.364	-3.001	-1.942	1	9.055	-3.547	2.8
7	3.453	-2.666	-2.697	1	7.372	-3.344	2.309
6	-7.499	-1.1	-3.861	1	5.694	-2.762	5.679
6	-8.423	-1.662	-2.854	1	7.084	-3.272	4.72
6	-8.719	-3.105	-2.908	1	4.483	-2.37	2.196
6	-8.073	-3.947	-3.919	1	2.678	-5.192	0.712
1	0.688	-6.336	1.322	1	1.089	0.922	-4.78
1	-2.189	-4.539	4.053	1	2.585	1.822	-5.128
1	-2.632	0.392	4.047	1	1.955	2.056	-7.657
1	-1.139	1.33	4.205	1	0.812	0.822	-7.075
1	-2.078	1.353	6.392	1	0.043	1.932	-9.171
1	-2.556	-0.36	6.304	1	-0.04	3.49	-8.334
1	-1.435	-0.448	8.449	1	-1.276	3.549	-6.28
1	-0.497	1.063	8.361	1	-2.64	3.67	-7.401
1	0.946	-0.332	9.572	1	-3.407	2.932	-5.171
1	0.484	-1.794	8.693	1	-3.668	1.65	-6.362
1	1.032	-1.926	6.373	1	-1.191	-2.471	-6.084
1	2.501	-2.429	7.232	1	-0.326	-4.138	-2.164
1	3.065	-1.911	4.906	1	0.176	-2.574	-0.277
1	3.796	-0.69	5.958	1	0.224	-0.826	-0.528
1	2.518	3.957	5.365	1	2.265	0.204	-1.682
1	1.761	5.274	1.302	1	3.678	-0.112	-4.329
1	1.119	3.685	-0.423	1	5.183	-0.981	-4.049
1	1.097	1.943	-0.123	1	-10.616	-2.536	2.241
1	-1.158	0.866	0.553	1	-5.316	-3.928	4.005
1	-4.109	1.71	2.66	1	-8.336	-4.96	-4.007
1	-4.731	1.937	1.01	1	-3.45	-5.886	-2.74
1	-9.452	-3.519	-2.28	1	10.169	1.359	2.73
1	-6.454	-4.025	-5.383	1	5.614	5.744	2.496
1	-4.6	-2.031	-5.397	1	11.406	-3.259	-1.313
1	-4.848	-0.692	-4.286	1	9.475	2.877	-2.156
1	-4.204	-4.368	-4.576	1	0.259	6.768	2.344

1	-2.944	-4.96	-0.475	1	-0.459	6.109	3.826
1	4.694	4.027	-1.832	1	0.115	7.788	3.782
1	3.898	2.476	-1.558	1	1.01	5.81	5.929
1	-10.864	-2.226	-0.232	1	1.561	7.484	5.748
1	-8.723	-1.45	3.46	1	2.749	6.176	5.846
1	7.542	-1.655	-3.504	1	3.803	6.91	3.662
1	6.282	-1.682	-2.271	1	2.808	7.179	2.218
1	9.387	0.477	-2.857	1	2.652	8.257	3.614
1	7.39	4.035	-1.382	1	-2.382	-6.754	4.854
1	-10.306	-0.907	-2.196	1	-3.508	-6.336	3.541
1	-9.003	0.281	-2.133	1	-3.176	-8.032	3.919
1	-6.37	0.228	-5.813	1	-2.853	-6.716	1.12
1	-7.818	1.237	-5.861	1	-2.591	-8.425	1.511
1	-6.03	1.264	-2.503	1	-1.314	-7.497	0.708
1	-6.133	4.54	-1.309	1	-0.077	-7.79	4.28
1	-5.363	3.015	-0.854	1	-1.004	-9.066	3.466
1	-4.774	6.195	-0.299	1	0.287	-8.224	2.598
1	-0.796	6.816	-1.911	1	1.121	-5.562	-3.304
1	1.658	2.111	-2.762	1	-0.549	-6.178	-3.297
1	0.625	-6.797	-4.469	1	-3.979	7.277	1.587
1	-2.121	-5.624	-5.247	1	-2.292	6.806	1.86
1	-0.897	-6.284	-6.346	1	-2.801	8.487	2.112
1	-1.541	-4.659	-6.617	1	-4.24	-0.137	-2.408
1	1.908	-4.006	-5.187	1	-6.111	0.246	-0.139
1	1.519	-5.342	-6.289	1	6.148	-1.06	-0.146
1	0.862	-3.726	-6.593	1	4.349	0.239	1.144
1	-0.92	8.891	-1.033	1	2.678	-3.425	0.725
1	-1.12	9.409	0.646	1	-3.379	9.189	-1.601
1	-0.425	7.818	0.295	1	0.388	5.189	-3.112
1	-4.626	8.607	-0.481	1	2.991	1.638	5.813
1	-3.528	9.905	0.016	1	-2.332	-0.389	-6.247
1	1.985	3.603	-3.652	1	-2.367	-2.189	4.275
8	6.149	-1.52	4.153				
8	4.428	1.017	0.626				

S30. Cartesian coordinates for MM minimized structure of $[\text{Zn}_2\text{L}'\text{PPi}]^{4-}$

Z	Coordinates				Coordinates			
	X	Y	Z	X	Y	Z	X	
30	-1.30997	-2.4801	2.06842	6	-5.29999	0.388151	-4.47118	
8	5.559882	-3.01122	0.799962	1	-5.03441	-0.5577	-4.92535	
8	5.987501	0.120233	0.256955	6	-4.67483	0.809399	-3.28425	
8	8.02878	-2.10952	-0.90747	6	-3.67585	-0.11425	-2.61346	
8	-8.33397	-0.81216	1.174788	1	-2.81556	-0.24113	-3.3026	
8	-1.27193	-2.29812	0.102865	1	-3.24366	0.320728	-1.68818	
8	-2.39976	-0.86154	2.10929	6	-5.37202	-1.61472	-1.36171	
8	-4.19007	-4.59272	4.255872	6	-4.31479	-1.46074	-2.30685	
8	-2.17996	-4.6009	6.329903	6	-3.92457	-2.57146	-3.07305	
7	2.690951	-5.22355	0.197149	1	-3.12485	-2.48701	-3.79609	
7	1.618486	-4.87529	-0.61025	6	-4.5896	-3.78901	-2.95289	
7	1.873106	-3.71361	-1.04453	6	-5.65255	-3.92736	-2.06714	
7	-2.83679	-3.8295	2.094825	1	-6.16693	-4.87867	-2.01111	
7	-1.64492	-3.40515	3.751106	6	6.315502	2.252283	1.288537	
7	-5.32461	1.80709	2.073811	6	7.015263	2.753685	0.043193	
7	-5.92905	2.908665	1.934802	1	7.078351	3.864006	0.045732	
7	-7.27625	2.583068	1.826407	1	6.393067	2.49702	-0.83777	
6	6.393837	-2.77203	1.880621	6	-8.43029	2.617225	-1.32343	
6	7.652417	-3.41889	1.981488	6	-8.11347	3.73963	-2.1197	
6	8.445423	-3.20967	3.122255	6	-9.13483	4.629415	-2.48532	
1	9.397037	-3.7159	3.228126	1	-8.91698	5.495586	-3.0977	
6	8.03625	-2.33114	4.120931	6	-10.4457	4.414889	-2.05759	
6	6.842491	-1.62911	3.986497	6	-10.7558	3.31115	-1.26148	
1	6.559813	-0.92228	4.757107	1	-11.7808	3.165201	-0.94397	
6	6.021104	-1.82088	2.863729	6	10.46348	-1.86957	-1.0627	
6	4.776482	-0.97241	2.734004	6	10.39201	-0.58654	-1.86635	
1	4.177204	-1.09657	3.661856	1	11.37154	-0.37125	-2.34715	
1	4.114643	-1.31462	1.915242	1	9.694782	-0.71564	-2.71456	
6	5.811592	0.934662	1.352474	6	8.748119	1.186971	-1.0123	
6	5.156639	0.482706	2.531977	6	10.03312	0.593077	-0.98524	
6	4.948275	1.388402	3.584924	6	11.00055	1.089974	-0.09752	
1	4.449513	1.07217	4.492675	1	11.99424	0.65953	-0.07545	
6	5.421811	2.696314	3.501199	6	10.69112	2.125951	0.782386	
6	6.113695	3.122888	2.369226	6	9.406484	2.66616	0.805651	
1	6.488331	4.138152	2.333709	1	9.174948	3.446228	1.520685	
6	-6.06536	-2.84533	-1.27896	6	8.417352	2.191373	-0.06897	
6	-7.27292	-3.0036	-0.3761	6	-6.6891	3.999605	-2.56964	
1	-6.97422	-2.74507	0.66101	1	-6.63774	4.876343	-3.25112	
1	-7.61196	-4.06192	-0.34357	1	-6.0987	4.263269	-1.66779	
6	9.29891	-2.52754	-0.57737	6	-3.36075	3.468866	-2.09101	
6	9.428498	-3.64633	0.271331	1	-2.55241	2.919976	-2.62226	

6	10.70335	-4.1524	0.564954	1	-3.78917	4.228582	-2.78631
1	10.81715	-5.01761	1.206213	6	-2.76168	4.198487	-0.9304
6	11.84251	-3.53599	0.050947	6	-2.05231	3.64717	0.057853
6	11.72644	-2.39902	-0.74763	1	-1.84331	2.590807	0.163436
1	12.629	-1.9202	-1.10692	6	-0.88988	4.365542	2.120788
6	-9.7578	2.398089	-0.88792	1	-1.3561	4.987064	2.914569
6	-10.1331	1.195285	-0.03714	1	-0.98264	3.31026	2.451864
1	-11.2008	1.219072	0.28137	6	1.355164	4.05606	1.065218
1	-9.45926	1.001188	0.816462	6	0.582811	4.696321	1.969763
6	-8.87588	-1.037	-0.12864	6	1.216503	5.679269	2.9
6	-9.83078	-0.13764	-0.74849	1	0.568206	6.159881	3.620812
6	-10.3815	-0.44525	-1.99498	6	2.547813	5.967969	2.835052
1	-11.101	0.220571	-2.45458	6	3.371195	5.2522	1.807856
6	-9.97489	-1.5963	-2.66848	1	4.427429	5.469061	1.692131
6	-8.99579	-2.42962	-2.1215	6	2.794438	4.350381	1.005721
1	-8.66339	-3.28991	-2.68952	6	3.441542	3.663287	-0.04379
6	-8.42324	-2.14969	-0.86779	6	3.778112	3.662849	-2.25223
6	8.203144	-4.29228	0.87707	1	3.43814	4.697824	-2.30773
1	8.448665	-5.28952	1.303217	6	3.798368	3.193303	-3.7014
1	7.462842	-4.47133	0.070643	1	2.97819	2.494389	-3.91771
6	4.772444	-4.15305	1.081724	1	4.752942	2.671849	-3.86711
1	4.395849	-4.15598	2.132833	6	2.51961	5.048927	-4.4605
1	5.368921	-5.07565	0.917351	1	2.242348	5.576353	-5.39735
6	3.565659	-4.21243	0.192447	1	1.66884	4.453988	-4.02959
6	3.073322	-3.27817	-0.59535	6	2.67829	6.044559	-3.25678
1	3.49466	-2.2981	-0.77511	1	3.331926	6.905286	-3.51093
6	0.925759	-2.92183	-1.85345	1	3.165941	5.311417	-2.55932
1	1.308541	-2.85591	-2.89016	6	0.772914	5.491608	-1.95917
6	-1.30051	-3.42658	-0.7398	1	1.444508	5.270206	-1.12394
6	-0.44149	-3.55907	-1.85754	1	-0.14376	5.930138	-1.51818
6	-0.64196	-4.61937	-2.76196	6	0.388034	4.215466	-2.76436
1	0.036471	-4.72227	-3.59843	1	-0.61216	4.39687	-3.22247
6	-1.60667	-5.61703	-2.51444	1	1.138943	4.240702	-3.59325
6	-2.31285	-5.53599	-1.29393	6	0.176222	1.970938	-2.90781
1	-2.99393	-6.31121	-0.97433	6	1.723978	0.303111	-3.39742
6	-2.12271	-4.43578	-0.45208	6	0.481482	0.852824	-3.6853
6	-2.63905	-4.35181	0.837354	6	-0.32585	0.389812	-4.72588
6	-4.25094	-3.38476	2.154028	1	-1.27758	0.879414	-4.87061
1	-4.90349	-3.98809	1.474916	6	0.087799	-0.63115	-5.5189
1	-4.34373	-2.33273	1.817243	6	1.382512	-1.16296	-5.30282
6	-4.85222	-3.55245	3.559915	1	1.746162	-1.95859	-5.93863
1	-4.78204	-2.57433	4.081458	6	2.209567	-0.7039	-4.25885
1	-5.93486	-3.79515	3.470439	6	3.531202	-1.39173	-4.0311
6	-4.49892	-4.55044	5.634709	1	3.687275	-2.22099	-4.75483
1	-5.4781	-5.04802	5.807069	1	3.514911	-1.85603	-3.02671
1	-4.55013	-3.51243	6.039225	6	5.516725	-0.23139	-3.14301

6	-3.41621	-5.2897	6.424148	1	5.467444	-0.64236	-2.14608
1	-3.71859	-5.29286	7.492809	6	6.442806	0.588892	-3.69045
1	-3.36729	-6.36198	6.121955	6	7.628763	1.200842	-3.01636
6	-1.30838	-5.19184	5.379481	1	7.46467	2.298804	-2.93755
1	-1.81174	-5.88637	4.66542	1	8.530921	1.009337	-3.63565
1	-0.529	-5.76799	5.922134	30	1.723527	1.916068	-0.8882
6	-0.63066	-4.0993	4.549136	1	-11.2258	5.108748	-2.34344
1	0.08812	-4.59849	3.868888	1	-10.3947	-1.82642	-3.63918
1	-0.05573	-3.40554	5.205816	1	-6.77576	0.817635	-5.97254
6	-2.13352	-2.29653	4.420221	1	-4.29611	-4.62684	-3.56632
6	-2.8358	-0.31606	3.335153	1	8.661325	-2.17235	4.990234
6	-2.6476	-0.99927	4.545739	1	5.270132	3.375974	4.328658
6	-3.01459	-0.46097	5.777494	1	12.82228	-3.92946	0.289421
1	-2.84329	-1.05891	6.661096	1	11.44391	2.495321	1.466796
6	-3.59781	0.8207	5.844922	15	1.116864	0.330757	0.731421
6	-3.82322	1.501168	4.629314	15	0.983176	-2.14079	2.212259
1	-4.2985	2.473424	4.636723	8	1.694127	-1.31802	0.831515
6	-3.4746	0.940231	3.386678	8	2.462654	1.409018	0.73246
6	-3.86983	1.685416	2.142341	8	-0.20859	0.989767	1.674111
1	-3.41249	2.694852	2.176239	8	0.118917	-3.52182	1.60291
1	-3.50953	1.170809	1.227053	8	-0.27569	-1.21432	2.93887
6	-6.17967	0.767433	2.082494	8	0.624634	0.444262	-0.75759
1	-5.8963	-0.27583	2.151078	8	2.008293	-2.76713	3.493566
6	-7.38824	1.250621	1.918628	6	-4.01531	1.478969	7.176
6	-8.60931	0.467339	1.68017	6	-3.69024	0.60666	8.412663
1	-9.07547	0.375403	2.652564	6	-5.53836	1.734038	7.168642
1	-9.12769	0.850323	1.199331	1	-5.83042	2.446731	6.369352
8	-4.3409	2.557959	-1.6328	1	-6.08834	0.782076	7.004577
8	-5.77443	-0.59635	-0.52523	1	-5.87011	2.167024	8.137304
8	-7.44027	1.731965	-0.99189	1	-4.24007	-0.35861	8.373002
8	7.747197	0.597345	-1.7479	1	-3.993	1.122469	9.349865
8	0.777521	3.263326	0.077555	1	-2.59892	0.406073	8.479325
8	2.485485	0.803248	-2.33007	6	-3.26998	2.821537	7.341685
8	3.716202	4.280342	-4.63184	1	-2.17081	2.660143	7.304089
8	1.395417	6.479328	-2.78948	1	-3.54344	3.54296	6.543685
7	-2.82045	5.53447	-0.75673	1	-3.5208	3.294526	8.315952
7	-2.10072	5.789946	0.406317	6	-1.74186	-6.80914	-3.48295
7	-1.62632	4.566216	0.872269	6	-1.91492	-6.30307	-4.93541
7	3.53016	2.79695	-1.1244	6	-2.95634	-7.71062	-3.15476
7	0.351891	2.962452	-1.96933	1	-2.82497	-8.22091	-2.17654
7	4.655085	-0.4687	-4.13782	1	-3.89403	-7.11461	-3.13368
7	4.998082	0.115256	-5.20927	1	-3.07527	-8.50763	-3.92061
7	6.061858	0.760398	-4.96555	1	-2.78116	-5.61505	-5.0138
6	-5.01812	2.0693	-2.73671	1	-2.08481	-7.15283	-5.63157
6	-6.10523	2.798274	-3.28472	1	-1.01314	-5.76776	-5.29725
6	-6.71154	2.348094	-4.46673	6	-0.46566	-7.67115	-3.39856

1	-7.52914	2.90491	-4.90796	1	-0.31016	-8.03212	-2.35873
6	-6.29561	1.161266	-5.06545	1	-0.54291	-8.55512	-4.06827
1	0.066941	0.083742	-8.17842	1	0.432497	-7.09228	-3.70193
6	3.234989	7.001371	3.754345	6	-0.79067	-1.22619	-6.64335
6	3.836056	8.12874	2.888648	6	-2.20307	-0.59606	-6.72001
1	3.042685	8.611301	2.277654	6	-0.97417	-2.74359	-6.40516
1	4.307962	8.90707	3.526891	1	-0.01468	-3.29421	-6.49097
1	4.617996	7.742879	2.201755	1	-1.38817	-2.92956	-5.39178
6	2.272883	7.652956	4.777474	1	-1.67038	-3.18196	-7.15259
1	1.829431	6.885327	5.44803	1	-2.74584	-0.73901	-5.76274
1	2.814253	8.383101	5.417749	1	-2.80718	-1.07375	-7.52177
6	4.363702	6.308677	4.546165	1	-2.14512	0.489017	-6.95314
1	3.956016	5.459616	5.136241	6	-0.10164	-1.00137	-8.00597
1	5.154639	5.920095	3.871659	1	0.879388	-1.51813	-8.05771
1	4.848356	7.021222	5.24836	1	-0.73015	-1.39394	-8.83466
1	-5.11496	0.13645	-0.54088	1	1.458431	8.204853	4.260244
1	-7.56239	0.96464	-1.60678	1	-3.2594	-5.22294	0.87208
1	8.033919	-1.85791	-1.86313	1	-2.09757	-2.6198	5.439587
1	5.26222	-0.54778	0.233748	1	4.448457	4.014013	0.045724
1	0.85129	-1.89421	-1.46365	1	-0.80707	2.200392	-3.26191

S31. Cartesian coordinates for MM minimized structure of $[\text{Zn}_2\text{L}'\text{ADP}]^{2-}$

Z	Coordinates			Coordinates			X
	X	Y	Z	X	Y	Z	
30	1.66	2.593	1.961	6	1.314	-3.873	-0.054
8	-6.204	1.326	1.201	1	1.557	-4.377	0.905
8	-6.28	-0.782	-1.421	1	1.359	-2.78	0.141
8	-7.602	2.133	-1.457	6	-0.7	-3.584	-1.521
8	9.056	0.366	1.82	6	-0.082	-4.241	-0.509
8	0.849	3.603	0.607	6	-0.846	-5.247	0.278
8	3.066	1.425	2.265	1	-0.315	-5.762	1.068
8	4.701	4.452	3.316	6	-2.148	-5.518	0.006
8	3.143	4.666	5.805	6	-2.801	-4.756	-1.105
7	-3.714	3.135	3.221	1	-3.842	-4.95	-1.348
7	-2.701	3.87	2.611	6	-2.121	-3.832	-1.807
7	-2.823	3.753	1.301	6	-2.732	-3.103	-2.814
7	2.992	3.943	1.311	6	-2.869	-1.446	-4.441
7	1.88	3.132	3.834	1	-3.741	-0.978	-3.998
7	5.427	-1.591	1.84	6	-2.482	-1.055	-5.829
7	5.915	-2.798	1.621	1	-1.643	-0.328	-5.765
7	7.294	-2.76	1.815	1	-3.352	-0.561	-6.314
6	-7.442	0.757	1.452	6	-1.449	-1.842	-7.751
6	-8.607	1.564	1.454	1	-1.575	-0.773	-8.048
6	-9.845	0.992	1.79	1	-1.867	-2.443	-8.586
1	-10.739	1.602	1.821	6	0.037	-2.171	-7.623

6	-9.946	-0.368	2.062	1	0.162	-3.281	-7.605
6	-8.821	-1.183	1.97	1	0.552	-1.818	-8.541
1	-8.929	-2.246	2.147	6	0.869	-2.404	-5.462
6	-7.568	-0.641	1.637	1	-0.068	-2.834	-5.061
6	-6.403	-1.588	1.46	1	1.508	-3.244	-5.822
1	-6.307	-2.171	2.4	6	1.652	-1.715	-4.351
1	-5.433	-1.064	1.34	1	2.603	-1.35	-4.802
6	-6.659	-2.061	-1.066	1	1.954	-2.468	-3.608
6	-6.656	-2.516	0.285	6	1.544	0.565	-3.586
6	-7.011	-3.848	0.555	6	-0.518	1.727	-3.2
1	-7.025	-4.219	1.572	6	0.873	1.732	-3.277
6	-7.386	-4.71	-0.473	6	1.583	2.95	-3.257
6	-7.425	-4.258	-1.788	1	2.658	2.899	-3.35
1	-7.738	-4.941	-2.568	6	0.948	4.148	-3.206
6	7.206	2.351	-1.188	6	-0.458	4.148	-3.09
6	8.122	2.399	0.018	1	-0.99	5.087	-3.015
1	7.557	2.026	0.896	6	-1.195	2.954	-3.088
1	8.419	3.444	0.252	6	-2.677	3.022	-2.848
6	-8.851	2.714	-1.458	1	-3.026	4.073	-2.758
6	-9.349	3.213	-0.235	1	-2.886	2.523	-1.879
6	-10.586	3.874	-0.206	6	-4.511	1.589	-3.685
1	-10.977	4.27	0.723	1	-4.836	1.237	-2.714
6	-11.34	4.013	-1.37	6	-5.104	1.383	-4.857
6	-10.879	3.481	-2.573	6	-6.376	0.624	-5.069
1	-11.499	3.577	-3.455	1	-6.141	-0.336	-5.58
6	10.91	-2.905	-0.387	1	-7.047	1.229	-5.718
6	11.045	-1.806	0.661	30	-0.727	-1.001	-2.589
1	12.032	-1.841	1.174	1	12.927	-5.208	-1.896
1	10.248	-1.788	1.425	1	11.92	1.481	-2.52
6	9.712	0.483	0.572	1	9.414	-0.774	-5.905
6	10.84	-0.418	0.079	1	6.029	4.402	-3.636
6	11.625	0.004	-0.997	1	-10.906	-0.8	2.313
1	12.452	-0.603	-1.342	1	-7.662	-5.732	-0.245
6	11.314	1.179	-1.675	1	-12.296	4.519	-1.335
6	10.198	1.939	-1.324	1	-11.758	-1.711	-3.751
1	9.961	2.812	-1.92	15	-1.098	-0.461	-0.355
6	9.38	1.591	-0.236	15	0.048	1.015	1.658
6	-8.572	3.02	1.048	8	-1.037	1.145	0.302
1	-9.004	3.627	1.873	8	-2.24	-0.552	-1.649
1	-7.535	3.389	0.9	8	-1.286	-1.848	0.703
6	-5.638	1.725	2.435	8	-0.018	2.456	2.644
1	-5.326	0.831	3.017	8	1.63	1.122	0.925
1	-6.358	2.322	3.043	8	0.277	-0.648	-1.097
6	-4.426	2.585	2.219	8	0.091	-0.442	2.672
6	-3.889	2.958	1.054	6	2.804	-2.591	6.381
1	-4.242	2.685	0.068	6	2.183	-2.114	7.717

6	-1.945	4.355	0.296	6	4.231	-3.096	6.682
1	-2.558	4.945	-0.419	1	4.7	-3.557	5.787
6	0.444	4.847	1.024	1	4.876	-2.256	7.018
6	-0.898	5.256	0.904	1	4.216	-3.868	7.482
6	-1.254	6.555	1.293	1	2.783	-1.29	8.161
1	-2.291	6.853	1.218	1	2.158	-2.942	8.458
6	-0.277	7.471	1.738	1	1.136	-1.77	7.567
6	1.065	7.027	1.766	6	1.942	-3.761	5.859
1	1.868	7.684	2.07	1	0.934	-3.393	5.575
6	1.39	5.704	1.424	1	2.399	-4.243	4.97
6	2.707	5.272	1.413	1	1.824	-4.545	6.638
6	4.398	3.57	1.077	6	-0.697	8.896	2.151
1	4.87	4.303	0.384	6	-1.353	9.608	0.948
1	4.445	2.591	0.556	6	0.493	9.767	2.623
6	5.213	3.52	2.385	1	0.992	9.311	3.505
1	5.191	2.482	2.781	1	1.235	9.899	1.807
1	6.272	3.768	2.158	1	0.145	10.78	2.922
6	5.203	4.199	4.609	1	-0.654	9.629	0.084
1	6.292	4.427	4.641	1	-1.621	10.655	1.207
1	5.041	3.139	4.915	1	-2.285	9.096	0.629
6	4.48	5.096	5.618	6	-1.708	8.815	3.315
1	5.002	4.999	6.593	1	-1.265	8.267	4.174
1	4.562	6.17	5.33	1	-1.995	9.832	3.66
6	2.246	5.323	4.924	1	-2.639	8.293	3.012
1	2.739	5.808	4.055	6	1.691	5.501	-3.339
1	1.718	6.123	5.484	6	3.225	5.352	-3.486
6	1.212	4.323	4.399	6	1.435	6.368	-2.091
1	0.574	4.806	3.645	1	0.354	6.555	-1.921
1	0.502	4.066	5.218	1	1.851	5.861	-1.202
6	1.918	2.069	4.805	1	1.934	7.357	-2.186
6	2.966	0.485	3.266	1	3.656	4.846	-2.594
6	2.425	0.805	4.52	1	3.713	6.347	-3.571
6	2.395	-0.172	5.533	1	3.483	4.776	-4.401
1	1.98	0.103	6.491	6	1.174	6.245	-4.589
6	2.864	-1.484	5.308	1	0.098	6.502	-4.497
6	3.391	-1.78	4.039	1	1.73	7.196	-4.741
1	3.759	-2.774	3.823	1	1.307	5.615	-5.496
6	3.457	-0.813	3.028	6	-2.963	-6.583	0.773
6	4.027	-1.216	1.69	6	-3.247	-7.766	-0.172
1	3.448	-2.079	1.299	1	-2.294	-8.222	-0.518
1	3.952	-0.406	0.935	1	-3.843	-8.549	0.346
6	6.45	-0.777	2.171	1	-3.817	-7.437	-1.067
1	6.358	0.281	2.379	6	-2.236	-7.128	2.028
6	7.579	-1.487	2.149	1	-1.973	-6.299	2.718
6	8.962	-0.952	2.355	1	-2.885	-7.84	2.584
1	9.178	-0.916	3.444	6	-4.301	-5.973	1.238

1	9.725	-1.57	1.85	1	-4.129	-4.991	1.726
8	5.977	-2.924	-2.534	1	-4.988	-5.82	0.384
8	6.837	0.014	-0.834	1	-4.826	-6.642	1.953
8	8.521	-2.507	-0.883	1	6.187	-0.687	-1.076
8	-6.945	0.393	-3.799	1	8.669	-1.75	-0.283
8	-0.004	-2.715	-2.33	1	-7.157	2.362	-2.308
8	-1.209	0.571	-3.492	1	-5.738	-0.38	-0.702
8	-2.131	-2.206	-6.564	1	-1.461	3.55	-0.286
8	0.606	-1.495	-6.512	1	-1.313	-7.68	1.748
7	3.602	-5.495	-2.392	1	3.508	6.004	1.446
7	2.537	-5.554	-1.5	1	1.59	2.259	5.824
7	2.317	-4.258	-1.039	1	-3.771	-3.313	-3.063
7	-1.959	-2.174	-3.597	1	2.589	0.642	-3.867
7	0.9	-0.626	-3.692	6	-3.363	-2.575	3.84
7	-3.445	2.373	-3.898	8	-2.103	-2.136	3.39
7	-3.415	2.663	-5.188	6	-2.027	-0.771	3.719
7	-4.415	2.052	-5.803	6	-2.77	-0.584	5.039
6	6.891	-2.347	-3.398	8	-3.34	0.697	5.109
6	8.094	-3.026	-3.714	6	-3.811	-1.688	5.01
6	8.985	-2.454	-4.635	8	-5.097	-1.174	4.776
1	9.902	-2.967	-4.899	6	-0.584	-0.346	3.808
6	8.717	-1.208	-5.199	7	-3.284	-3.978	4.239
6	7.573	-0.503	-4.83	6	-2.288	-4.557	5.099
1	7.401	0.478	-5.256	7	-2.741	-5.645	5.769
6	6.664	-1.045	-3.906	6	-4.026	-5.787	5.407
6	5.466	-0.216	-3.486	6	-4.393	-4.812	4.538
1	4.864	-0.021	-4.399	7	-5.66	-4.697	4.072
1	4.788	-0.759	-2.796	6	-6.586	-5.613	4.485
6	6.633	1.131	-1.617	7	-6.234	-6.614	5.355
6	5.907	1.088	-2.843	6	-4.959	-6.721	5.835
6	5.676	2.286	-3.54	7	-4.603	-7.755	6.753
1	5.121	2.284	-4.471	1	-4.073	-2.492	2.99
6	6.194	3.492	-3.075	1	-2.529	-0.18	2.917
6	6.961	3.526	-1.914	1	-3.79	-2.236	5.983
1	7.383	4.47	-1.592	1	-2.08	-0.75	5.901
6	-7.081	-2.934	-2.096	1	-1.294	-4.153	5.226
6	-7.161	-2.463	-3.532	1	-7.603	-5.549	4.123
1	-7.253	-3.325	-4.229	1	-5.734	-1.912	4.964
1	-6.204	-1.969	-3.797	1	-3.642	0.82	6.047
6	9.711	-3.158	-1.125	1	-0.128	-0.977	4.561
6	9.716	-4.113	-2.165	1	-0.573	0.648	4.239
6	10.879	-4.849	-2.43	1	-4.822	-8.669	6.297
1	10.895	-5.586	-3.224	1	-5.228	-7.664	7.586
6	12.033	-4.636	-1.682	1	-2.258	-1.857	1.099
6	12.052	-3.67	-0.677	6	-8.354	-1.552	-3.736
1	12.976	-3.507	-0.136	6	8.483	-4.317	-3.023

6	-9.643	2.815	-2.638	1	8.657	-5.095	-3.799
6	-9.221	2.196	-3.957	1	7.669	-4.697	-2.372
1	-9.862	2.567	-4.786	6	5.045	-3.651	-3.306
1	-8.204	2.544	-4.218	1	4.55	-2.999	-4.062
6	-8.198	-0.158	-3.915	1	5.543	-4.497	-3.833
6	-9.337	0.684	-3.924	6	3.978	-4.201	-2.417
6	-10.616	0.105	-3.885	6	3.202	-3.487	-1.591
1	-11.5	0.731	-3.915	1	3.277	-2.421	-1.416
6	-10.767	-1.278	-3.787	1	-9.781	-3.169	-3.581
6	-9.645	-2.101	-3.7				

S32. Cartesian coordinates for MM minimized structure of $[\text{Zn}_2\text{L}'\text{ATP}]^{2-}$

Z	Coordinates				Coordinates			
	X	Y	Z	X	Y	Z	X	
30	1.8131	-2.3326	-2.3164	6	7.6111	-0.2696	4.9106	
8	-5.8979	-1.7566	-1.3614	1	7.4061	-1.2946	5.1956	
8	-5.8899	-0.9096	1.9826	6	6.6921	0.4454	4.1236	
8	-7.9339	-2.9636	0.5296	6	5.4421	-0.2566	3.6346	
8	9.0611	-0.4166	-2.1874	1	4.8711	-0.5836	4.5306	
8	1.2071	-3.5926	-1.0674	1	4.7591	0.4134	3.0746	
8	3.0831	-0.9816	-2.4814	6	6.4731	-1.2976	1.5226	
8	5.3961	-4.1226	-4.0454	6	5.8051	-1.4466	2.7686	
8	3.5451	-3.6316	-6.1264	6	5.5831	-2.7386	3.2736	
7	-3.9609	-3.9586	-3.2844	1	5.0681	-2.8826	4.2156	
7	-2.9039	-4.7286	-2.8054	6	6.0651	-3.8586	2.5976	
7	-2.4139	-4.1086	-1.6574	6	6.7951	-3.7066	1.4206	
7	3.3001	-3.6596	-2.0094	1	7.1951	-4.5876	0.9346	
7	1.8621	-2.4956	-4.2574	6	-6.2939	1.0144	3.3776	
7	5.4561	1.7724	-1.8064	6	-6.7979	0.1044	4.4736	
7	6.1471	2.9754	-1.6904	1	-6.8339	0.6384	5.4486	
7	7.4601	2.7434	-2.0924	1	-6.0639	-0.7066	4.6056	
6	-6.8399	-0.7226	-1.4184	6	9.6401	2.9734	1.4976	
6	-8.1519	-0.9876	-1.8754	6	9.7731	3.6634	2.7226	
6	-9.0589	0.0734	-2.0234	6	10.9961	4.2644	3.0526	
1	-10.0609	-0.1096	-2.3894	1	11.1121	4.8014	3.9856	
6	-8.6859	1.3734	-1.6904	6	12.0831	4.1754	2.1846	
6	-7.4199	1.6244	-1.1664	6	11.9701	3.4704	0.9876	
1	-7.1649	2.6374	-0.8804	1	12.8381	3.3944	0.3446	
6	-6.4959	0.5804	-0.9914	6	-10.2889	-3.3576	1.1656	
6	-5.1789	0.8824	-0.3054	6	-9.9889	-3.4586	2.6506	
1	-4.6539	1.6704	-0.8854	1	-10.8559	-3.8926	3.1956	
1	-4.4799	0.0224	-0.3044	1	-9.1629	-4.1776	2.8246	
6	-5.8669	0.4814	2.1416	6	-8.4389	-1.7426	3.7466	
6	-5.4409	1.3604	1.1076	6	-9.7129	-2.0906	3.2416	

6	-5.4029	2.7434	1.3586	6	-10.7529	-1.1486	3.2816
1	-5.0909	3.4344	0.5846	1	-11.7419	-1.4106	2.9266
6	-5.8269	3.2564	2.5816	6	-10.5239	0.1384	3.7596
6	-6.2659	2.4004	3.5876	6	-9.2489	0.5144	4.1756
1	-6.5949	2.8204	4.5296	1	-9.0819	1.5354	4.4966
6	7.0231	-2.4306	0.8856	6	-8.1869	-0.4036	4.1486
6	7.8891	-2.2786	-0.3464	6	8.6101	3.7484	3.6866
1	7.2791	-1.7996	-1.1364	1	8.8671	4.3654	4.5746
1	8.2071	-3.2706	-0.7354	1	7.7741	4.2704	3.1746
6	-9.2909	-3.0446	0.2006	6	5.0921	3.2044	3.8966
6	-9.6599	-2.8156	-1.1434	1	4.5781	2.4734	4.5596
6	-10.9979	-2.9736	-1.5324	1	5.6001	3.9644	4.5306
1	-11.2939	-2.8106	-2.5614	6	4.0591	3.8664	3.0476
6	-11.9669	-3.3306	-0.5984	6	3.3011	3.2594	2.1266
6	-11.6199	-3.5126	0.7396	1	3.3711	2.2184	1.8346
1	-12.4009	-3.7546	1.4506	6	1.3761	3.8044	0.6876
6	10.7621	2.8464	0.6336	1	1.5631	4.4114	-0.2244
6	10.7111	2.0234	-0.6414	1	1.4111	2.7384	0.3746
1	9.8781	2.4254	-1.2304	6	-0.5829	3.3154	2.1626
1	11.6321	2.1704	-1.2464	6	0.0191	4.1264	1.2676
6	9.4581	-0.3366	-0.8334	6	-0.6779	5.3524	0.8096
6	10.5811	0.5414	-0.3394	1	-0.1669	5.9664	0.0846
6	11.4611	0.0004	0.6116	6	-1.8859	5.6974	1.3066
1	12.3311	0.5594	0.9346	6	-2.5199	4.7774	2.2916
6	11.1671	-1.1956	1.2566	1	-3.4909	5.0324	2.6926
6	9.9901	-1.8826	0.9766	6	-1.9189	3.6344	2.6726
1	9.7651	-2.7796	1.5416	6	-2.5069	2.8154	3.5466
6	9.1281	-1.4606	-0.0464	6	-2.8769	0.7334	4.7186
6	-8.6249	-2.3946	-2.1634	1	-3.3179	-0.1096	4.1476
1	-9.0439	-2.4226	-3.1934	6	-2.2229	0.2684	6.0086
1	-7.7909	-3.1266	-2.1494	1	-1.2869	-0.2826	5.7746
6	-5.1169	-1.8466	-2.5534	1	-2.9309	-0.4236	6.5166
1	-4.5769	-0.8896	-2.7324	6	-1.2449	0.9914	7.9846
1	-5.7699	-2.0566	-3.4304	1	-1.2919	-0.1016	8.2106
6	-4.1069	-2.9386	-2.4134	1	-1.6829	1.5094	8.8636
6	-3.2079	-3.0386	-1.4334	6	0.2121	1.4274	7.8526
1	-3.1419	-2.3866	-0.5734	1	0.2611	2.5424	7.8096
6	-1.4779	-4.6926	-0.7024	1	0.7491	1.1294	8.7776
1	-2.0269	-5.3936	-0.0394	6	1.0141	1.6644	5.6826
6	0.9101	-4.8606	-1.5674	1	0.0471	2.0584	5.3146
6	-0.3649	-5.4336	-1.3964	1	1.6431	2.5264	6.0046
6	-0.5869	-6.7496	-1.8234	6	1.7661	0.9684	4.5546
1	-1.5709	-7.1806	-1.6894	1	2.6851	0.5264	5.0006
6	0.4561	-7.5176	-2.3784	1	2.1241	1.7204	3.8366
6	1.7221	-6.9016	-2.4944	6	1.5421	-1.2546	3.6546
1	2.5661	-7.4416	-2.9004	6	-0.5079	-2.2676	3.0686

6	1.9151	-5.5636	-2.1024	6	0.8731	-2.3206	3.2126
6	3.1241	-5.0026	-2.1814	6	1.5451	-3.5476	3.0306
6	4.6891	-3.1836	-1.9234	1	2.6161	-3.5746	3.1866
1	5.3241	-3.9276	-1.3914	6	0.8871	-4.6916	2.7126
1	4.7311	-2.2646	-1.3044	6	-0.5199	-4.6316	2.5606
6	5.2851	-2.9186	-3.3144	1	-1.0949	-5.5096	2.3096
1	4.6491	-2.1916	-3.8604	6	-1.2179	-3.4276	2.7346
1	6.2961	-2.4756	-3.1824	6	-2.6959	-3.3656	2.4616
6	5.8341	-3.8616	-5.3704	1	-2.9769	-4.1396	1.7166
1	6.7551	-4.4546	-5.5534	1	-2.9619	-2.3846	2.0116
1	6.1011	-2.7956	-5.5724	6	-4.8069	-3.8146	3.6266
6	4.7691	-4.3016	-6.3764	1	-5.3209	-4.2036	2.7566
1	5.1151	-4.0166	-7.3934	6	-5.4039	-3.3276	4.7156
1	4.6901	-5.4156	-6.3804	6	-6.8849	-3.2006	4.8766
6	2.6151	-4.5096	-5.5224	1	-7.1319	-2.5626	5.7546
1	3.0841	-5.1116	-4.7214	1	-7.3099	-4.2126	5.0456
1	2.2231	-5.2186	-6.2844	30	-0.6519	0.5384	2.7766
6	1.4341	-3.7316	-4.9324	1	13.0231	4.6434	2.4486
1	0.8711	-4.3746	-4.2334	1	11.8311	-1.5646	2.0276
1	0.7201	-3.4926	-5.7514	1	9.5111	-0.2456	5.9146
6	1.8891	-1.3036	-5.0614	1	5.9011	-4.8466	3.0066
6	2.8991	0.1064	-3.3324	1	-9.3909	2.1854	-1.8114
6	2.2991	-0.0556	-4.5884	1	-5.8249	4.3254	2.7496
6	2.1291	1.0684	-5.4194	1	-12.9979	-3.4456	-0.9084
1	1.6721	0.9174	-6.3864	1	-11.3319	0.8584	3.7786
6	2.4991	2.3634	-4.9964	15	-0.9639	0.2624	0.4506
6	3.1281	2.4884	-3.7434	15	0.0971	-0.9946	-1.7534
1	3.4491	3.4594	-3.3904	8	-0.8809	-1.2846	-0.3444
6	3.3371	1.3774	-2.9174	8	-2.1399	0.2794	1.7206
6	4.0281	1.5834	-1.5904	8	-1.0169	1.7684	-0.4104
1	3.6041	2.4794	-1.0864	8	0.0961	-2.3746	-2.8274
1	3.8751	0.7274	-0.9004	8	1.7271	-1.0066	-1.1224
6	6.3341	0.8594	-2.2694	8	0.3131	0.3294	1.2936
1	6.0871	-0.1666	-2.4964	8	-0.0989	0.4894	-2.6644
6	7.5291	1.4374	-2.4254	6	2.2221	3.6294	-5.8354
6	8.7571	0.7534	-2.9484	6	1.5181	3.3284	-7.1804
1	9.6331	1.4184	-3.0564	6	3.5541	4.3434	-6.1524
1	8.5251	0.4214	-3.9824	1	4.0591	4.6974	-5.2294
8	6.0401	2.5414	3.0626	1	4.2441	3.6534	-6.6854
8	6.6291	-0.0526	0.9036	1	3.3811	5.2324	-6.7964
8	8.3881	2.4294	1.1846	1	2.1491	2.6724	-7.8194
8	-7.4079	-2.6816	3.6506	1	1.3351	4.2664	-7.7484
8	0.1001	2.2504	2.7326	1	0.5321	2.8434	-7.0124
8	-1.1839	-1.1156	3.4496	6	1.3051	4.5804	-5.0344
8	-1.9769	1.3834	6.8376	1	0.3571	4.0654	-4.7614
8	0.8281	0.7694	6.7586	1	1.7921	4.9284	-4.0994

7	3.6841	5.1544	3.1736	1	1.0521	5.4834	-5.6324
7	2.6351	5.3224	2.2766	6	0.1871	-8.9746	-2.8064
7	2.4271	4.0924	1.6556	6	-0.2619	-9.7946	-1.5774
7	-1.9749	1.5224	3.8766	6	1.4311	-9.6706	-3.4084
7	0.9501	-0.0396	3.8466	1	1.7871	-9.1316	-4.3134
7	-3.4799	-3.5676	3.6736	1	2.2551	-9.7246	-2.6634
7	-3.2699	-2.8676	4.8636	1	1.1911	-10.7126	-3.7134
7	-4.4949	-2.7366	5.5136	1	0.5111	-9.7476	-0.7784
6	6.9681	1.7934	3.7966	1	-0.4189	-10.8606	-1.8504
6	8.2081	2.3684	4.1596	1	-1.2169	-9.4146	-1.1584
6	9.1121	1.6244	4.9346	6	-0.9259	-8.9996	-3.8764
1	10.0611	2.0544	5.2306	1	-0.6379	-8.3746	-4.7484
6	8.8071	0.3194	5.3176	1	-1.1069	-10.0366	-4.2344
6	-6.1209	4.2854	-4.1034	1	-1.8879	-8.6166	-3.4764
8	-7.2889	3.8894	-3.4304	6	1.6771	-6.0156	2.5796
6	-3.3639	1.8564	-4.4084	6	2.2591	-6.3986	3.9566
8	-2.5419	1.3394	-3.4264	6	2.8371	-5.8486	1.5706
15	-1.3909	0.3084	-3.7734	1	2.4511	-5.4686	0.6086
8	-1.9939	-1.0786	-3.7774	1	3.6051	-5.1396	1.9346
8	-0.8669	0.6014	-5.1604	1	3.3501	-6.8176	1.3856
7	-4.2309	5.7634	-3.6194	1	2.9711	-5.6296	4.3226
6	-2.8199	5.7674	-3.8844	1	2.8071	-7.3646	3.8976
7	-2.2889	7.0074	-3.7884	1	1.4441	-6.5026	4.7046
6	-3.3059	7.8124	-3.4404	6	0.8051	-7.1966	2.0856
6	-4.4279	7.1374	-3.3134	1	0.3461	-6.9616	1.1006
7	-5.5869	7.7194	-2.9134	1	1.4171	-8.1156	1.9596
6	-5.5839	9.0574	-2.6424	1	0.0051	-7.4356	2.8186
7	-4.4289	9.7804	-2.7694	6	-2.6369	6.9774	0.8866
6	-3.2699	9.1784	-3.1674	6	-2.9309	7.8364	2.1356
7	-2.0619	9.9324	-3.2744	1	-1.9859	8.0824	2.6666
1	-5.4839	4.9504	-2.1304	1	-3.4299	8.7884	1.8506
1	-5.1529	1.7394	-3.2124	1	-3.6039	7.3124	2.8456
1	-6.3479	5.1164	-4.8124	6	-1.8429	7.8604	-0.1084
1	-4.9179	3.4974	-5.7034	1	-1.6399	7.3104	-1.0514
1	-2.2349	4.8844	-4.1024	1	-2.4199	8.7734	-0.3704
1	-6.4939	9.5464	-2.3234	6	-3.9649	6.5814	0.2116
1	-7.7389	4.7224	-3.1314	1	-3.7659	5.9174	-0.6554
1	-6.9359	2.6024	-6.0354	1	-4.6359	6.0454	0.9136
1	-2.7949	2.6014	-5.0064	1	-4.5089	7.4814	-0.1494
1	-3.7109	1.0424	-5.0854	1	6.0441	0.6824	1.2726
1	-2.0589	10.9524	-3.0494	1	8.3311	1.9394	0.3086
1	-1.1669	9.4784	-3.5614	1	-7.6769	-3.4576	1.3686
1	0.093	0.5985	-5.147	1	-5.4569	-1.2626	1.1446
1	-0.122	2.07	-0.5829	1	-1.0609	-3.8906	-0.0624
1	2.5851	-1.3866	3.9226	1	-0.8799	8.1894	0.3376
6	-5.0279	4.6504	-3.1004	1	3.9841	-5.6326	-2.3904

8	-4.1999	3.5264	-2.8794	1	1.5451	-1.3716	-6.0884
6	-4.5929	2.5134	-3.7794	1	-3.4439	3.1164	4.0046
6	-5.5099	3.1204	-4.8344	8	-6.4729	2.1904	-5.2594