ELECTRONIC SUPPLEMENTARY INFORMATION

A fluorescent sensor for Zn²⁺ and NO₂⁻ based on the rational control of C=N

isomerization

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Experimental section

Instruments

UV-vis spectra were recorded on a Shimadzu 3100 spectrometer; fluorescence measurements were carried out using an Edinburgh Instruments Ltd-FLS920 fluorescence spectrophotometer. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker AV III 400 MHz NMR spectrometer with tetramethysilane (TMS) as an internal standard. Infrared spectra were recorded using a Bruker Vertex 70 FT-IR spectrometer with KBr pellets.

Sample preparation

All tests described in this paper were carried out at room temperature (25 °C) with distilled water. In the experiments of titration with various metal ions, the sensor was dissolved in HEPES acetonitrile-H₂O (9:1) buffer solution to afford the test solution (1×10^{-5} M). Stock solutions (1×10^{-5} M) of the mental salts of LiCl, NaCl, KCl, MgCl₂, CaCl₂, BaCl₂, NiCl₂, CuCl₂, ZnCl₂, CdCl₂, HgCl₂, PbCl₂, AgNO₃, MnCl₂, FeCl₃, CoCl₂, CrCl₃, SrCl₃ and AlCl₃ were prepared in aquesous solution. Stock solutions (1×10^{-5} M) of the anion salts of CH₃COONa, NaBF₄, NaF, NaCl, NaBr, NaI, NaNO₃, NaNO₂, Na₂S, NaHSO₃, Na₂S₂O₃, NaSO₄, Na₃PO₄, Na₂HPO₄, NaH₂PO₄, Na₄P₂O₇, ATP, ADP and AMP in water were prepared for the sample tests.

Calculation of limit of detection (LOD)

The limit of detection was determined according to the following equation:

LOD= $3\sigma/s$,

where LOD is the limit of detection; σ is the standard deviation of blank measurements; s is the slope between fluorescence intensity versus NO₂⁻ concentration. To testify the accurate detection level of ternary complex L+Zn²⁺+Cl⁻ towards NO₂⁻, the same titration experiment was repeated five times and the average value was applied.

Calculation of the fluorescence quantum yield

The fluorescence quantum yield of L, $L+Zn^{2+}+Cl^{-}$ and $L+Zn^{2+}+NO_{2}^{-}$ was determined according to the following equation:

$$\phi_u = \phi_s \frac{F_u A_s n_u^2}{F_s A_u n_s^2}$$

where ϕ is fluorescence quantum yield; *F* is integrated area under the corrected emission spectra; *A* is the absorbance at the excitation wavelength; *n* is the refractive index of the solution; the subscripts *u* and *s* refer to the unknown and the standard, respectively. 9,10-Diphenylanthracene in hexane solution was used as the standard, which has a quantum yield of 0.95.

Calculation of radiative decay rate constant (K_{τ}) and nonradiative decay rate constant ($K_{n\tau}$)

The fluorescence lifetime of L, L+Zn²⁺+Cl⁻ and L+Zn²⁺+NO₂⁻ in acetonitrile-H₂O (9:1) was measured by single photon counting, and it shows a good single-exponential decay. The radiative decay rate constant (K_{τ}) and nonradiative decay rate constant ($K_{n\tau}$) was determined according to the following equation:

$$\tau = (K_{\tau} + K_{n\tau})^{-1}$$
$$\phi = K_{\tau}\tau$$

Where τ is the lifetime; K_{τ} refers to the radiative decay rate constant; $K_{n\tau}$ refers to the nonradiative decay rate constant; ϕ refers to the emission fluorescence quantum yield.

Theoretical calculation

Structural optimizations from Density functional theory (DFT) were calculated with the Gaussian 09 program. In all cases, the structures were optimized using the B3LYP functional and the mixed basis sets 6-31+G(d) (C, H, O, N and Cl) and LANL2DZ (Zn). For all optimized structures, frequency calculations were carried out to confirm the absence of imaginary frequencies. The molecular structures were visualized and plotted with the GaussView 5.0 program.



Figure S1. Absorption spectra of L (1×10^{-5} M) in acetonitrile-H₂O (9:1) containing HEPES (0.01 M, pH=7.4) buffer solution in the presence of various metal ions (Li⁺, Na⁺, K⁺, Mg²⁺, Ca²⁺, Ba²⁺, Ni²⁺, Cu²⁺, Zn²⁺, Cd²⁺, Hg²⁺, Pb²⁺, Ag⁺, Mn²⁺, Fe³⁺, Co²⁺, Cr³⁺, Sr³⁺ and Al³⁺).



Figure S2. Job's plot of the L+Zn²⁺ complex in acetonitrile-H₂O (9:1) containing HEPES (0.01 M, pH=7.4) at 25 °C. The total concentration of L and Zn²⁺ was 0.1 mM. Excitation is at 370 nm, and emission is monitored at 495 nm.



Figure S3. Fluorescence spectra of L (1×10^{-5} M) in acetonitrile–H₂O (9:1) containing HEPES (0.01 M, pH = 7.4) buffer solution in the presence of various metal ions (Li⁺, Na⁺, K⁺, Mg²⁺, Ca²⁺, Ba²⁺, Ni²⁺, Cu²⁺, Zn²⁺, Cd²⁺, Hg²⁺, Pb²⁺, Ag⁺, Mn²⁺, Fe³⁺, Co²⁺, Cr³⁺, Sr³⁺ and Al³⁺). Excitation wavelength is 370 nm.



Figure S4. Change ratio of fluorescence of L (1×10^{-5} M) upon addition of Zn²⁺ (1×10^{-5} M) in acetonitrile-H₂O (9:1) containing HEPES (0.01 M, pH=7.4) at 25 °C. Excitation is at 370 nm, and emission is monitored at 495 nm. F₀ and F are the fluorescence intensities before and after addition of Zn²⁺, respectively.



Figure S5. Partial ¹H NMR spectra of L (DMSO-d₆) and in the presence of ZnCl₂.



Figure S6. Fluorescence spectra of $L+Zn^{2+}+Cl^{-}$ complex $(1 \times 10^{-5} \text{ M})$ in acetonitrile-H₂O (9:1) containing HEPES (0.01 M, pH=7.4) buffer solution in the presence of various anions (Ac⁻, BF₄⁻, F⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, NO₂⁻, S²⁻, HSO₃⁻, S₂O₃²⁻, SO₄²⁻, CrO₄⁻, PO₄³⁻, HPO₄²⁻, H₂PO₄⁻, PPi, ATP). Excitation wavelength is at 370 nm.



Figure S7. Fluorescence spectra of $L+Zn^{2+}+Cl^{-}(1\times10^{-5} \text{ M})$ in acetonitrile-H₂O (9:1, HEPES 0.01 M, pH=7.4) as the concentration of NO₂⁻ (1×10⁻¹¹ M) increased from 0 to 10⁻¹⁰ M. Insert: Change ratio of fluorescence of $L+Zn^{2+}+Cl^{-}(1\times10^{-5} \text{ M})$ upon addition of NO₂⁻ (1×10⁻¹¹ M). Excited at 370 nm.



Figure S8. Changes in the absorption spectra of L (1×10^{-5} M) in acetonitrile-H₂O (9:1) containing HEPES (0.01 M, pH=7.4) upon titration with NO₂⁻ (1×10^{-5} M).



Figure S9. Changes in the absorption spectra of $L+Zn^{2+}+Cl^{-}$ (1×10⁻⁵ M) in acetonitrile-H₂O (9:1) containing HEPES (0.01 M, pH=7.4) upon titration with NO₂⁻ (1×10⁻⁵ M).



Figure S10. The fluorescence photo of L (1×10^{-5} M), L+Zn²⁺ (1×10^{-5} M) and L+Zn²⁺+NO₂⁻ (1×10^{-5} M)

M) in acetonitrile- $H_2O(9:1)$ solution under UV-light. Excitation wavelength is at 365 nm.



Figure S11. The fluorescence lifetime of the ternary complex L+Zn²⁺+Cl⁻.



Figure S12. The fluorescence lifetime of $L+Zn^{2+}+NO_2^{-}$.



Figure S13. Calculated structures of L, $L+Zn^{2+}+Cl^{-}$ and $L+Zn^{2+}+NO_{2}^{-}$ (B3LYP/6-31G(d), LANL2DZ), where the light-gray, red, white, dark-gray and cyan atoms denote C, N, O, H, Zn and Cl atoms, respectively.



Figure S14. ESI mass spectra of the compound 3.



Figure S15. ESI mass spectrum of the compound 4.



Figure S16. ESI mass spectrum of L.



Figure S17. ESI mass spectra of L+Zn²⁺+Cl⁻



Figure S18. The mass spectra of $L+Zn^{2+}+NO_2^{-}$.



Figure S19. ¹H NMR spectra of compound 3 in CDCl₃.



Figure S20. ¹³C NMR spectra of compound 3 in CDCl₃.



Figure S21. ¹H NMR spectra of compound 4 in CDCl₃.



Figure S22. ¹H NMR spectra of L in DMSO.



Figure S23. ¹H NMR spectra of L+Zn²⁺+Cl⁻ in d6-DMSO.



Figure S24. ¹³C NMR spectra of L in d6-DMSO.

Table S1. XYZ coordination of the optimized structure of L.



Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Ŷ	Z
1	6	0	4.517509	2.663613	0.276041
2	6	0	5.030255	1.376838	0.213606
3	6	0	6.411332	1.138860	0.468512
4	6	0	7.260538	2.240343	0.793921
5	6	0	6.700027	3.543989	0.851018
6	6	0	5.358887	3.747578	0.596498
7	1	0	3.462655	2.816500	0.071855
8	6	0	6.964045	-0.173342	0.404609
9	6	0	8.634647	1.989490	1.047387
10	1	0	7.346931	4.381982	1.097931
11	1	0	4.942264	4.749421	0.640849
12	6	0	9.148612	0.710324	0.982055
13	6	0	8.310919	-0.375361	0.658668
14	1	0	9.280982	2.827868	1.295549
15	1	0	10.202070	0.534814	1.178481
16	1	0	8.702492	-1.385784	0.601522
17	6	0	4.194341	0.237391	-0.111892
18	6	0	6.122454	-1.348044	0.065625
19	7	0	4.772585	-1.042645	-0.178669
20	7	0	2.912192	0.234070	-0.366300
21	6	0	2.591142	-1.089351	-0.627034
22	6	0	3.732984	-1.918101	-0.510507
23	6	0	1.341872	-1.657796	-0.938243
24	6	0	3.694191	-3.297549	-0.701542
25	6	0	1.301472	-3.044294	-1.125323

26	6	0	2.450617	-3.844671	-1.014864
27	1	0	0.360089	-3.512617	-1.399951
28	1	0	2.369231	-4.914150	-1.185693
29	1	0	4.587400	-3.901566	-0.610688
30	6	0	0.123574	-0.793511	-1.118212
31	8	0	0.115749	0.243892	-1.745507
32	8	0	6.533154	-2.495551	-0.003340
33	7	0	-1.001541	-1.333661	-0.491780
34	7	0	-2.213574	-0.735492	-0.565500
35	6	0	-3.146016	-1.274321	0.138323
36	6	0	-6.766222	-1.134161	1.166521
37	6	0	-7.637283	-1.844890	2.017494
38	6	0	-8.960266	-1.468157	2.164707
39	6	0	-9.432284	-0.352903	1.455926
40	6	0	-8.600068	0.367355	0.609562
41	6	0	-7.252165	-0.013250	0.438642
42	1	0	-7.242910	-2.700539	2.560408
43	1	0	-9.622470	-2.022133	2.822840
44	1	0	-10.465989	-0.037881	1.569340
45	1	0	-8.998393	1.231016	0.092865
46	6	0	-5.396301	-1.501897	1.013971
47	1	0	-5.037619	-2.364508	1.573948
48	7	0	-6.383969	0.661738	-0.409654
49	6	0	-5.004541	0.359032	-0.545707
50	6	0	-4.527468	-0.817237	0.211172
51	8	0	-4.298096	1.052963	-1.262799
52	6	0	-6.848471	1.802470	-1.217439
53	1	0	-6.200270	1.836636	-2.093710
54	1	0	-7.866195	1.592615	-1.558532
55	6	0	-6.770113	3.140990	-0.473241
56	1	0	-7.363804	3.091326	0.448844
57	1	0	-5.728207	3.301291	-0.174294
58	6	0	-7.249930	4.305276	-1.345249
59	1	0	-8.295743	4.175071	-1.651457
60	1	0	-7.178391	5.255383	-0.805187
61	1	0	-6.644568	4.392849	-2.255011
62	1	0	-0.872365	-2.132628	0.129575
63	1	0	-2.933235	-2.161752	0.756986

Table S2. XYZ coordination of the optimized structure of $L+Zn^{2+}+Cl^{-}$.



Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Туре	Х	Y	Ζ
1		0	4 697594	2 443233	-0 314749
2	6	0	5 301586	1 210679	-0.075809
3	6	0	6.721439	1.099819	-0.000974
4	6	0	7.516987	2.272358	-0.170485
5	6	0	6.866432	3.511988	-0.411214
6	6	0	5.486521	3.593710	-0.482616
7	1	0	3.615223	2.495222	-0.371270
8	6	0	7.361637	-0.148881	0.235551
9	6	0	8.929311	2.157517	-0.094181
10	1	0	7.473236	4.404000	-0.541576
11	1	0	5.006971	4.548898	-0.670481
12	6	0	9.532599	0.935071	0.138723
13	6	0	8.748388	-0.220794	0.303296
14	1	0	9.535181	3.050436	-0.223091
15	1	0	10.613979	0.862387	0.194183
16	1	0	9.210272	-1.185942	0.484434
17	6	0	4.528590	0.009498	0.097805
18	6	0	6.578759	-1.389835	0.409401
19	7	0	5.173627	-1.201197	0.319936
20	7	0	3.205924	-0.109456	0.068405
21	6	0	2.957391	-1.437317	0.268695
22	6	0	4.168646	-2.165732	0.430881
23	6	0	1.714556	-2.137381	0.311555
24	6	0	4.209738	-3.533589	0.638314
25	6	0	1.767543	-3.538202	0.516674
26	6	0	2.973101	-4.209296	0.678380

28 1 0 2.967113 -5.282330 0.839280 29 1 0 5.151196 -4.053771 0.760615 30 6 0 0.446517 -1.447424 0.140813 31 8 0 7.038553 -2.49383 0.611692 33 7 0 -0.671998 -2.290388 0.096124 34 7 0 -1.769569 -1.577898 -0.106858 35 6 0 -2.920374 -2.219167 -0.058716 36 6 0 -7.789342 -2.567705 -0.316148 38 6 0 -9.046002 -1.993061 -0.332313 39 6 0 -9.046002 -1.993061 -0.323213 40 6 0 -8.033985 0.226841 -0.163375 41 6 0 -5.746177 -0.340578 -0.156845 42 1 0 -7.670109 -3.645970 -0.371663	27	1	0	0.835998	-4.088372	0.551061
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34	7	0	-1.769569	-1.577898	-0.106858
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37	6	0	-7.789342	-2.567705	-0.316148
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38	6	0	-9.040602	-1.993061	-0.332313
4060 -8.033985 0.226841 -0.163375 41 60 -6.746177 -0.340678 -0.156845 42 10 -7.670109 -3.645970 -0.371663 43 10 -9.931417 -2.608097 -0.401545 44 10 -10.135985 -0.131277 -0.253285 45 10 -8.173981 1.296338 -0.086684 46 60 -5.336413 -2.330789 -0.199203 47 10 -5.242282 -3.413009 -0.252547 48 70 -5.590867 0.437300 -0.079019 49 60 -4.323622 -0.098905 -0.000209 50 60 -4.189256 -1.557449 -0.109626 51 80 -3.357256 0.683789 0.178312 52 60 -5.678727 1.924072 -0.058876 53 10 -4.752617 2.291201 -0.499556 54 10 -6.765302 2.069275 1.813918 57 10 -5.013709 2.180337 1.970663 58 60 -5.959140 4.026205 1.336247 59 10 -6.802552 4.334255 0.702302 60 10 -5.056244 4.440228 0.867834 61 300 -1.440620 0.534527 -0.588531 62 <	39	6	0	-9.152263	-0.590920	-0.251233
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	40	6	0	-8.033985	0.226841	-0.163375
4210 -7.670109 -3.645970 -0.371663 43 10 -9.931417 -2.608097 -0.401545 44 10 -10.135985 -0.131277 -0.253285 45 10 -8.173981 1.296338 -0.086684 46 60 -5.336413 -2.330789 -0.199203 47 10 -5.242282 -3.413009 -0.252547 48 70 -5.590867 0.437300 -0.079019 49 60 -4.323622 -0.098905 -0.000209 50 60 -4.189256 -1.557449 -0.109626 51 80 -3.357256 0.683789 0.178312 52 60 -5.678727 1.924072 -0.058876 53 10 -4.752617 2.291201 -0.499556 54 10 -6.494319 2.210470 -0.725145 55 60 -5.863645 2.493365 1.351948 56 10 -5.013709 2.180337 1.970663 58 60 -5.959140 4.026205 1.336247 59 10 -6.802552 4.334255 0.702302 60 10 -5.056244 4.440228 0.867834 61 300 -1.440620 0.534527 -0.588531 62 10 -6.129733 4.619276 2.738674 64 <td>41</td> <td>6</td> <td>0</td> <td>-6.746177</td> <td>-0.340678</td> <td>-0.156845</td>	41	6	0	-6.746177	-0.340678	-0.156845
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	42	1	0	-7.670109	-3.645970	-0.371663
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	43	1	0	-9.931417	-2.608097	-0.401545
4510 -8.173981 1.296338 -0.086684 46 60 -5.336413 -2.330789 -0.199203 47 10 -5.242282 -3.413009 -0.252547 48 70 -5.590867 0.437300 -0.079019 49 60 -4.323622 -0.098905 -0.000209 50 60 -4.189256 -1.557449 -0.109626 51 80 -3.357256 0.683789 0.178312 52 60 -5.678727 1.924072 -0.058876 53 10 -4.752617 2.291201 -0.499556 54 10 -6.494319 2.210470 -0.725145 55 60 -5.863645 2.493365 1.351948 56 10 -5.013709 2.180337 1.970663 58 60 -5.959140 4.026205 1.336247 59 10 -6.802552 4.334255 0.702302 60 10 -5.056244 4.440228 0.867834 61 300 -1.440620 0.534527 -0.588531 62 10 -6.129733 4.619276 2.738674 64 10 -6.193816 5.711327 2.696608 65 10 -7.043369 4.249705 3.219354 66 10 -5.283262 4.359098 3.385013 67 1	44	1	0	-10.135985	-0.131277	-0.253285
46 6 0 -5.336413 -2.330789 -0.199203 47 1 0 -5.242282 -3.413009 -0.252547 48 7 0 -5.590867 0.437300 -0.079019 49 6 0 -4.323622 -0.098905 -0.000209 50 6 0 -4.189256 -1.557449 -0.109626 51 8 0 -3.357256 0.683789 0.178312 52 6 0 -5.678727 1.924072 -0.058876 53 1 0 -4.752617 2.291201 -0.499556 54 1 0 -6.494319 2.210470 -0.725145 55 6 0 -5.863645 2.493365 1.351948 56 1 0 -5.013709 2.180337 1.970663 58 6 0 -5.056244 4.440228 0.867834 61 30 0 -1.440620 0.534527 -0.588531 62 1 0 -2.902597 -3.305387 0.049189 63 6 0 -7.043369 4.249705 3.219354 66 1 0 -5.283262 4.359098 3.385013 67 17 0 -1.460530 1.848475 -2.433522	45	1	0	-8.173981	1.296338	-0.086684
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	46	6	0	-5.336413	-2.330789	-0.199203
4870 -5.590867 0.437300 -0.079019 49 60 -4.323622 -0.098905 -0.000209 50 60 -4.189256 -1.557449 -0.109626 51 80 -3.357256 0.683789 0.178312 52 60 -5.678727 1.924072 -0.058876 53 10 -4.752617 2.291201 -0.499556 54 10 -6.494319 2.210470 -0.725145 55 60 -5.863645 2.493365 1.351948 56 10 -6.765302 2.069275 1.813918 57 10 -5.013709 2.180337 1.970663 58 60 -5.959140 4.026205 1.336247 59 10 -6.802552 4.334255 0.702302 60 10 -5.056244 4.440228 0.867834 61 300 -1.440620 0.534527 -0.588531 62 10 -2.902597 -3.305387 0.049189 63 60 -6.129733 4.619276 2.738674 64 10 -6.193816 5.711327 2.696608 65 10 -7.043369 4.249705 3.219354 66 10 -5.283262 4.359098 3.385013 67 170 -1.460530 1.848475 -2.433522	47	1	0	-5.242282	-3.413009	-0.252547
4960 -4.323622 -0.098905 -0.000209 5060 -4.189256 -1.557449 -0.109626 5180 -3.357256 0.683789 0.178312 5260 -5.678727 1.924072 -0.058876 5310 -4.752617 2.291201 -0.499556 5410 -6.494319 2.210470 -0.725145 5560 -5.863645 2.493365 1.351948 5610 -6.765302 2.069275 1.813918 5710 -5.013709 2.180337 1.970663 5860 -5.959140 4.026205 1.336247 5910 -6.802552 4.334255 0.702302 6010 -5.056244 4.440228 0.867834 61300 -1.440620 0.534527 -0.588531 6210 -6.193816 5.711327 2.696608 6510 -7.043369 4.249705 3.219354 6610 -5.283262 4.359098 3.385013 67170 -1.460530 1.848475 -2.433522	48	7	0	-5.590867	0.437300	-0.079019
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	49	6	0	-4.323622	-0.098905	-0.000209
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	50	6	0	-4.189256	-1.557449	-0.109626
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	51	8	0	-3.357256	0.683789	0.178312
5310 -4.752617 2.291201 -0.499556 54 10 -6.494319 2.210470 -0.725145 55 60 -5.863645 2.493365 1.351948 56 10 -6.765302 2.069275 1.813918 57 10 -5.013709 2.180337 1.970663 58 60 -5.959140 4.026205 1.336247 59 10 -6.802552 4.334255 0.702302 60 10 -5.056244 4.440228 0.867834 61 300 -1.440620 0.534527 -0.588531 62 10 -2.902597 -3.305387 0.049189 63 60 -6.129733 4.619276 2.738674 64 10 -6.193816 5.711327 2.696608 65 10 -7.043369 4.249705 3.219354 66 10 -5.283262 4.359098 3.385013 67 170 -1.460530 1.848475 -2.433522	52	6	0	-5.678727	1.924072	-0.058876
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	53	1	0	-4.752617	2.291201	-0.499556
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	54	1	0	-6.494319	2.210470	-0.725145
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	55	6	0	-5.863645	2.493365	1.351948
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	56	1	0	-6.765302	2.069275	1.813918
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	57	1	0	-5.013709	2.180337	1.970663
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	58	6	0	-5.959140	4.026205	1.336247
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	59	1	0	-6.802552	4.334255	0.702302
	60	1	0	-5.056244	4.440228	0.867834
62 1 0 -2.902597 -3.305387 0.049189 63 6 0 -6.129733 4.619276 2.738674 64 1 0 -6.193816 5.711327 2.696608 65 1 0 -7.043369 4.249705 3.219354 66 1 0 -5.283262 4.359098 3.385013 67 17 0 -1.460530 1.848475 -2.433522	61	30	0	-1.440620	0.534527	-0.588531
63 6 0 -6.129733 4.619276 2.738674 64 1 0 -6.193816 5.711327 2.696608 65 1 0 -7.043369 4.249705 3.219354 66 1 0 -5.283262 4.359098 3.385013 67 17 0 -1.460530 1.848475 -2.433522	62	1	0	-2.902597	-3.305387	0.049189
64 1 0 -6.193816 5.711327 2.696608 65 1 0 -7.043369 4.249705 3.219354 66 1 0 -5.283262 4.359098 3.385013 67 17 0 -1.460530 1.848475 -2.433522	63	6	0	-6.129733	4.619276	2.738674
65 1 0 -7.043369 4.249705 3.219354 66 1 0 -5.283262 4.359098 3.385013 67 17 0 -1.460530 1.848475 -2.433522	64	1	0	-6.193816	5.711327	2.696608
66 1 0 -5.283262 4.359098 3.385013 67 17 0 -1.460530 1.848475 -2.433522	65	1	0	-7.043369	4.249705	3.219354
67 17 0 -1.460530 1.848475 -2.433522	66	1	0	-5.283262	4.359098	3.385013
	67	17	0	-1.460530	1.848475	-2.433522

Table S3. XYZ coordination of the optimized structure of $L+Zn^{2+}+NO_2^{-}$.



Standard orientation:

Center	ter Atomic Atomic Coordinates (Angstroms)				roms)
Number	Number	Туре	Х	Y	Z
1	6	0	4.808019	2.394412	-0.124675
2	6	0	5.391614	1.140822	-0.017279
3	6	0	6.808010	1.010567	0.064395
4	6	0	7.620119	2.185724	0.036665
5	6	0	6.987775	3.452924	-0.073749
6	6	0	5.613031	3.551148	-0.153054
7	1	0	3.726663	2.463939	-0.185716
8	6	0	7.430600	-0.267040	0.173331
9	6	0	9.030006	2.041272	0.121162
10	1	0	7.605946	4.346895	-0.095187
11	1	0	5.140732	4.525341	-0.238080
12	6	0	9.612387	0.794325	0.227404
13	6	0	8.810325	-0.364366	0.253270
14	1	0	9.648475	2.935350	0.100747
15	1	0	10.692425	0.700355	0.291142
16	1	0	9.255400	-1.350610	0.335892
17	6	0	4.595698	-0.071142	0.017923
18	6	0	6.627837	-1.518130	0.204316
19	7	0	5.239075	-1.315794	0.118104
20	7	0	3.292853	-0.169334	-0.032360
21	6	0	3.014536	-1.526879	0.034180
22	6	0	4.217916	-2.274049	0.130789
23	6	0	1.774134	-2.205653	0.026128
24	6	0	4.253919	-3.662171	0.217000
25	6	0	1.815997	-3.605894	0.116680
26	6	0	3.019279	-4.314803	0.207703
27	1	0	0.873024	-4.139135	0.113728

29 1 0 5.193320 -4.194537 0.287966 30 6 0 0.471893 -1.497932 -0.072519 31 8 0 0.456759 -0.236729 -0.231941 32 8 0 7.109555 -2.652806 0.296742 33 7 0 -0.621877 -2.287604 0.018608 34 7 0 -1.755558 -1.566536 -0.074159 35 6 0 -2.868872 -2.25559 0.007644 36 6 0 -7.730237 -2.864927 0.250385 38 6 0 -9.231970 -0.994192 0.084873 40 6 0 -8.168217 -0.122128 -0.097112 41 6 0 -6.847325 -0.611879 -0.12040 42 1 0 -1.52452 -3.548236 0.39291 43 1 0 -8.370011 0.935622 -0.204151 <t< th=""><th>28</th><th>1</th><th>0</th><th>2.991891</th><th>-5.398739</th><th>0.272522</th></t<>	28	1	0	2.991891	-5.398739	0.272522
3060 0.471893 -1.497932 -0.072519 31 80 0.456759 -0.236729 -0.231941 32 80 7.109555 2.2652806 0.296742 33 70 -0.621877 -2.287604 0.018608 34 70 -1.75558 -1.566336 -0.074159 35 60 -2.868872 -2.25559 0.007644 36 60 -6.623612 -2.00349 0.071038 37 60 -7.730237 -2.864927 0.250385 38 60 -9.020942 -2.373615 0.253757 39 60 -9.231970 -0.994192 0.084873 40 60 -8.168217 -0.122128 -0.097112 41 60 -6.847325 -0.611879 0.120040 42 10 -7.540351 -3.925895 0.389703 43 10 -9.864268 -3.042709 0.393048 44 10 -10.242225 -0.595814 0.100927 45 10 -5.287220 -2.483071 0.090213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.287220 -2.483071 0.09207 51 80 -3.52377 0.620665 -0.389097 52 60 -5.921304 1.6675559 -0.526979 50 <t< td=""><td>29</td><td>1</td><td>0</td><td>5.193320</td><td>-4.194537</td><td>0.287966</td></t<>	29	1	0	5.193320	-4.194537	0.287966
31 8 0 0.456759 -0.236729 -0.231941 32 8 0 7.109555 -2.652806 0.296742 33 7 0 -0.621877 -2.287604 0.018608 34 7 0 -1.75558 -1.566336 -0.074159 35 6 0 -2.868872 -2.225559 0.007644 36 6 0 -6.623612 -0.03049 0.071038 37 6 0 -9.020942 -2.373615 0.253757 39 6 0 -9.231970 -0.994192 0.084873 40 6 0 -8.168217 -0.122128 -0.097112 41 6 0 -6.847325 -0.611879 -0.120040 42 1 0 -7.540351 -3.925895 0.389703 43 1 0 -8.37011 0.935622 -0.204151 44 1 0 -5.28720 -2.483071 0.009213 <	30	6	0	0.471893	-1.497932	-0.072519
32807.109555 -2.652806 0.296742 33 70 -0.621877 -2.287604 0.018608 34 70 -1.755558 -1.566536 -0.074159 35 60 -2.868872 -2.225559 0.007644 36 60 -6.623612 -2.2003049 0.071038 37 60 -7.730237 -2.864927 0.250385 38 60 -9.020942 -2.373615 0.253757 39 60 -9.231970 -0.994192 0.084873 40 60 -8.168217 -0.122128 -0.097112 41 60 -6.847325 -0.611879 -0.120040 42 10 -7.540351 -3.925895 0.389703 43 10 -9.864268 -3.042709 0.393048 44 10 -10.242225 -0.595814 0.100927 45 10 -5.287220 -2.483071 0.090213 47 10 -5.287220 -2.483071 0.090213 47 10 -5.287220 -2.483071 0.090213 47 10 -5.287220 -2.48306 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -5.921304 1.667026 -0.581207 51 <td>31</td> <td>8</td> <td>0</td> <td>0.456759</td> <td>-0.236729</td> <td>-0.231941</td>	31	8	0	0.456759	-0.236729	-0.231941
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	32	8	0	7.109555	-2.652806	0.296742
3470 -1.75558 1.566536 -0.074159 35 60 -2.868872 -2.225559 0.007644 36 60 -6.623612 -2.003049 0.071038 37 60 -7.730237 -2.864927 0.250385 38 60 -9.020942 -2.373615 0.253757 39 60 -9.231970 -0.994192 0.084873 40 60 -8.168217 -0.122128 -0.097112 41 60 -7.540351 -3.925895 0.389703 43 10 -9.864268 -3.042709 0.393048 44 10 -10.242225 -0.595814 0.100927 45 10 -8.370011 0.935622 -0.204151 46 60 -5.287220 -2.483071 0.990213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -5.921304 1.667026 -0.581207 51 80 -5.921304 1.667026 -0.581207 52 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -6.28454 4.002260 0.4009511 59 <	33	7	0	-0.621877	-2.287604	0.018608
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	34	7	0	-1.755558	-1.566536	-0.074159
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	35	6	0	-2.868872	-2.225559	0.007644
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	36	6	0	-6.623612	-2.003049	0.071038
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	37	6	0	-7.730237	-2.864927	0.250385
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38	6	0	-9.020942	-2.373615	0.253757
4060 -8.168217 -0.122128 -0.097112 41 60 -6.847325 -0.611879 -0.120040 42 10 -7.540351 -3.925895 0.389703 43 10 -9.864268 -3.042709 0.393048 44 10 -10.242225 -0.595814 0.100927 45 10 -8.370011 0.935622 -0.204151 46 60 -5.287220 -2.483071 0.090213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 <	39	6	0	-9.231970	-0.994192	0.084873
4160 -6.847325 -0.611879 -0.120040 42 10 -7.540351 -3.925895 0.389703 43 10 -9.864268 -3.042709 0.393048 44 10 -10.242225 -0.595814 0.100927 45 10 -8.370011 0.935622 -0.204151 46 60 -5.287220 -2.483071 0.090213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.20592 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70	40	6	0	-8.168217	-0.122128	-0.097112
4210 -7.540351 -3.925895 0.389703 43 10 -9.864268 -3.042709 0.393048 44 10 -10.242225 -0.595814 0.100927 45 10 -8.370011 0.935622 -0.204151 46 60 -5.287220 -2.483071 0.090213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 <	41	6	0	-6.847325	-0.611879	-0.120040
4310 -9.864268 -3.042709 0.393048 4410 -10.242225 -0.595814 0.100927 4510 -8.370011 0.935622 -0.204151 4660 -5.287220 -2.483071 0.090213 4710 -5.124562 -3.548236 0.239291 4870 -5.744354 0.219078 -0.318282 4960 -4.434389 -0.226755 -0.256979 5060 -4.197823 -1.655559 -0.052907 5180 -3.523977 0.620665 -0.389097 5260 -5.921304 1.667026 -0.581207 5310 -5.086646 1.970632 -1.212573 5410 -6.838786 1.791034 -1.159970 5560 -5.940772 2.508540 0.699807 5610 -6.741296 2.156356 1.365033 5710 -4.992413 2.356530 1.228301 5860 -6.128454 4.002260 0.400951 5910 -7.070592 4.152925 -0.146222 6010 -2.805096 -3.307510 0.143458 6370 -1.291005 3.128996 -0.726021 6480 -1.336652 2.597911 0.418430 6580 -1.291084	42	1	0	-7.540351	-3.925895	0.389703
4410 -10.242225 -0.595814 0.100927 45 10 -8.370011 0.935622 -0.204151 46 60 -5.287220 -2.483071 0.090213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64	43	1	0	-9.864268	-3.042709	0.393048
4510 -8.370011 0.935622 -0.204151 46 60 -5.287220 -2.483071 0.090213 47 10 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.38786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 <td< td=""><td>44</td><td>1</td><td>0</td><td>-10.242225</td><td>-0.595814</td><td>0.100927</td></td<>	44	1	0	-10.242225	-0.595814	0.100927
46 6 0 -5.287220 -2.483071 0.090213 47 1 0 -5.124562 -3.548236 0.239291 48 7 0 -5.744354 0.219078 -0.318282 49 6 0 -4.434389 -0.226755 -0.256979 50 6 0 -4.197823 -1.655559 -0.052907 51 8 0 -3.523977 0.620665 -0.389097 52 6 0 -5.921304 1.667026 -0.581207 53 1 0 -5.086646 1.970632 -1.212573 54 1 0 -6.838786 1.791034 -1.159970 55 6 0 -5.940772 2.508540 0.699807 56 1 0 -6.741296 2.156356 1.365033 57 1 0 -4.992413 2.356530 1.228301 58 6 0 -6.128454 4.002260 0.400951 59 1 0 -7.070592 4.152925 -0.146222 60 1 0 -2.805096 -3.307510 0.143458 63 7 0 -1.291005 3.128996 -0.726021 64 8 0 -1.336652 2.597911 0.418430 65 8 0 -1.291084 2.294271 -1.671964 66 0 -6.129157 4.861469 1.669637 67 1 0 -6.262458 </td <td>45</td> <td>1</td> <td>0</td> <td>-8.370011</td> <td>0.935622</td> <td>-0.204151</td>	45	1	0	-8.370011	0.935622	-0.204151
4710 -5.124562 -3.548236 0.239291 48 70 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 0 -6.129157 4.861469 1.669637 67 1 <th< td=""><td>46</td><td>6</td><td>0</td><td>-5.287220</td><td>-2.483071</td><td>0.090213</td></th<>	46	6	0	-5.287220	-2.483071	0.090213
4870 -5.744354 0.219078 -0.318282 49 60 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.65559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 1	47	1	0	-5.124562	-3.548236	0.239291
4960 -4.434389 -0.226755 -0.256979 50 60 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -5.183122 4.759029 2.213715	48	7	0	-5.744354	0.219078	-0.318282
5060 -4.197823 -1.655559 -0.052907 51 80 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -6.939323 4.568294 2.348786 69 10 -5.183122 4.759029 2.213715	49	6	0	-4.434389	-0.226755	-0.256979
5180 -3.523977 0.620665 -0.389097 52 60 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -5.183122 4.759029 2.213715	50	6	0	-4.197823	-1.655559	-0.052907
5260 -5.921304 1.667026 -0.581207 53 10 -5.086646 1.970632 -1.212573 54 10 -6.838786 1.791034 -1.159970 55 60 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -6.939323 4.568294 2.348786 69 10 -5.183122 4.759029 2.213715	51	8	0	-3.523977	0.620665	-0.389097
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	52	6	0	-5.921304	1.667026	-0.581207
5410-6.8387861.791034-1.159970 55 60-5.9407722.5085400.699807 56 10-6.7412962.1563561.365033 57 10-4.9924132.3565301.228301 58 60-6.1284544.0022600.400951 59 10-7.0705924.152925-0.146222 60 10-5.3252624.339030-0.267914 61 300-1.4043000.602728-0.362664 62 10-2.805096-3.3075100.143458 63 70-1.2910053.128996-0.726021 64 80-1.3366522.5979110.418430 65 80-1.2910842.294271-1.671964 66 60-6.1291574.8614691.669637 67 10-6.2624585.9217171.428487 68 10-6.393234.5682942.348786 69 10-5.1831224.7590292.213715	53	1	0	-5.086646	1.970632	-1.212573
5560 -5.940772 2.508540 0.699807 56 10 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -6.939323 4.568294 2.348786 69 10 -5.183122 4.759029 2.213715	54	1	0	-6.838786	1.791034	-1.159970
5610 -6.741296 2.156356 1.365033 57 10 -4.992413 2.356530 1.228301 58 60 -6.128454 4.002260 0.400951 59 10 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 300 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -6.939323 4.568294 2.348786 69 10 -5.183122 4.759029 2.213715	55	6	0	-5.940772	2.508540	0.699807
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	56	1	0	-6.741296	2.156356	1.365033
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	57	1	0	-4.992413	2.356530	1.228301
5910 -7.070592 4.152925 -0.146222 60 10 -5.325262 4.339030 -0.267914 61 30 0 -1.404300 0.602728 -0.362664 62 10 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -6.939323 4.568294 2.348786 69 10 -5.183122 4.759029 2.213715	58	6	0	-6.128454	4.002260	0.400951
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	59	1	0	-7.070592	4.152925	-0.146222
61 30 0 -1.404300 0.602728 -0.362664 62 1 0 -2.805096 -3.307510 0.143458 63 7 0 -1.291005 3.128996 -0.726021 64 8 0 -1.336652 2.597911 0.418430 65 8 0 -1.291084 2.294271 -1.671964 66 6 0 -6.129157 4.861469 1.669637 67 1 0 -6.262458 5.921717 1.428487 68 1 0 -6.939323 4.568294 2.348786 69 1 0 -5.183122 4.759029 2.213715	60	1	0	-5.325262	4.339030	-0.267914
6210 -2.805096 -3.307510 0.143458 63 70 -1.291005 3.128996 -0.726021 64 80 -1.336652 2.597911 0.418430 65 80 -1.291084 2.294271 -1.671964 66 60 -6.129157 4.861469 1.669637 67 10 -6.262458 5.921717 1.428487 68 10 -6.939323 4.568294 2.348786 69 10 -5.183122 4.759029 2.213715	61	30	0	-1.404300	0.602728	-0.362664
6370-1.2910053.128996-0.7260216480-1.3366522.5979110.4184306580-1.2910842.294271-1.6719646660-6.1291574.8614691.6696376710-6.2624585.9217171.4284876810-6.9393234.5682942.3487866910-5.1831224.7590292.213715	62	1	0	-2.805096	-3.307510	0.143458
6480-1.3366522.5979110.4184306580-1.2910842.294271-1.6719646660-6.1291574.8614691.6696376710-6.2624585.9217171.4284876810-6.9393234.5682942.3487866910-5.1831224.7590292.213715	63	7	0	-1.291005	3.128996	-0.726021
6580-1.2910842.294271-1.6719646660-6.1291574.8614691.6696376710-6.2624585.9217171.4284876810-6.9393234.5682942.3487866910-5.1831224.7590292.213715	64	8	0	-1.336652	2.597911	0.418430
6660-6.1291574.8614691.6696376710-6.2624585.9217171.4284876810-6.9393234.5682942.3487866910-5.1831224.7590292.213715	65	8	0	-1.291084	2.294271	-1.671964
6710-6.2624585.9217171.4284876810-6.9393234.5682942.3487866910-5.1831224.7590292.213715	66	6	0	-6.129157	4.861469	1.669637
6810-6.9393234.5682942.3487866910-5.1831224.7590292.213715	67	1	0	-6.262458	5.921717	1.428487
69 1 0 -5.183122 4.759029 2.213715	68	1	0	-6.939323	4.568294	2.348786
	69	1	0	-5.183122	4.759029	2.213715