

Supplementary

A Selective Fluorescent Optode for Lead(II) Based on the Dansylamidopropyl Pendant Arm Derivative of 1,4-dioxo-7,13-dithia-10-Azacyclopentadecane ([15]aneNS₂O₂)

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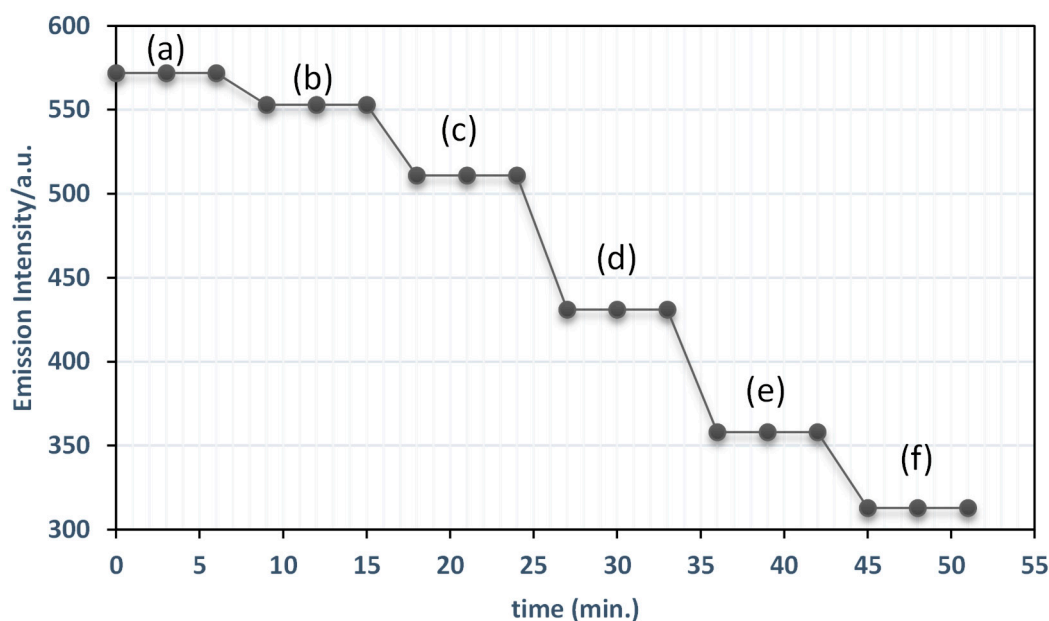


Figure S1. Plot of the fluorescence emission intensity *versus* time of the optode at the optimized composition for step changes in the concentration of Pb(II): (a) 0; (b) 1.0×10^{-8} ; (c) 1.0×10^{-7} ; (d) 1.0×10^{-6} ; (e) 1.0×10^{-5} ; (f) 1.0×10^{-4} M.

Table S1. DFT (mPW1PW/def2-SVP) gas-phase total electronic energy E, sum of total electronic energy and thermal free energy G, thermal enthalpy H calculated for L, the free Pb²⁺ ion and the complexes [Pb(L)]²⁺ and [Pb(L)₂]²⁺; reaction free energy ΔG_r and total electronic energy stabilization energy ΔE_r calculated for the formation of the 1:1 and 1:2 complexes [Pb(L)]²⁺ and [Pb(L)₂]²⁺. All energies are provided in Hartree.

| | G | H | E | ΔG _r | ΔE _r |
|-------------------------------------|------------|------------|------------|----------------------|----------------------|
| L | −2633.5017 | −2633.3875 | −2634.0558 | — | — |
| Pb ⁺⁺ | −192.1677 | −192.1478 | −192.1501 | — | — |
| [Pb(L)] ²⁺ | −2826.0541 | −2825.9431 | −2826.6164 | −0.3847 ^a | −0.4105 ^c |
| [Pb(L) ₂] ²⁺ | −5459.5832 | −5459.3821 | −5460.7257 | −0.0275 ^b | −0.0535 ^d |

^{a–d} Corresponding to −241.4 (a), −17.2 (b), −257.6 (c), and −33.5 (d) kcal/mol, respectively.

Table S2. DFT (mPW1PW/def2-SVP) gas-phase optimized geometry for L (C₂₅H₃₉N₃O₄S₃) in orthogonal Cartesian format.

| Center | Atomic | Coordinates (Angstroms) | | |
|--------|--------|-------------------------|-----------|-----------|
| Number | Number | X | Y | Z |
| 1 | 6 | −3.092183 | 1.271340 | 0.924713 |
| 2 | 1 | −3.451927 | 0.947579 | −0.064291 |
| 3 | 1 | −2.036828 | 1.565235 | 0.817574 |
| 4 | 6 | −3.253127 | 0.113629 | 1.927645 |
| 5 | 1 | −2.661308 | 0.328932 | 2.831290 |
| 6 | 1 | −4.306430 | 0.105734 | 2.258762 |
| 7 | 6 | −3.895808 | 3.846697 | 0.105774 |
| 8 | 1 | −2.828746 | 3.973945 | −0.133393 |
| 9 | 1 | −4.259943 | 4.808610 | 0.495091 |
| 10 | 6 | −4.674779 | 3.491327 | −1.147082 |
| 11 | 1 | −4.370730 | 2.491982 | −1.509074 |
| 12 | 1 | −4.399162 | 4.208794 | −1.945750 |
| 13 | 6 | −6.830897 | 2.583561 | −1.551829 |
| 14 | 1 | −6.480025 | 2.392364 | −2.582779 |
| 15 | 1 | −7.853569 | 2.980088 | −1.627130 |
| 16 | 6 | −6.834089 | 1.278698 | −0.770757 |
| 17 | 1 | −7.266355 | 1.456936 | 0.229550 |
| 18 | 1 | −5.786627 | 0.963560 | −0.607417 |
| 19 | 6 | −7.022727 | −0.997575 | −1.362845 |
| 20 | 1 | −7.519651 | −1.612966 | −2.126517 |
| 21 | 1 | −5.940725 | −1.007515 | −1.596812 |
| 22 | 6 | −7.246801 | −1.606720 | 0.019720 |
| 23 | 1 | −8.317099 | −1.802988 | 0.177779 |
| 24 | 1 | −6.934566 | −0.906258 | 0.808179 |
| 25 | 6 | −4.959031 | −2.593203 | 1.309796 |
| 26 | 1 | −4.535616 | −3.499005 | 1.768196 |
| 27 | 1 | −5.362036 | −1.984341 | 2.133496 |
| 28 | 6 | −3.871910 | −1.822405 | 0.555498 |
| 29 | 1 | −3.358908 | −2.512539 | −0.131327 |

| | | | | |
|----|----|-----------|-----------|-----------|
| 30 | 1 | -4.352384 | -1.072077 | -0.097001 |
| 31 | 7 | -2.920346 | -1.198422 | 1.442511 |
| 32 | 16 | -4.076601 | 2.691164 | 1.494589 |
| 33 | 8 | -6.050813 | 3.550845 | -0.901137 |
| 34 | 8 | -7.538940 | 0.299070 | -1.485593 |
| 35 | 16 | -6.347857 | -3.169665 | 0.285443 |
| 36 | 6 | -1.554496 | -1.648352 | 1.441294 |
| 37 | 1 | -1.079521 | -1.312904 | 2.378899 |
| 38 | 1 | -1.549393 | -2.751322 | 1.488522 |
| 39 | 6 | -0.681588 | -1.209311 | 0.257903 |
| 40 | 1 | -1.179350 | -1.495808 | -0.684642 |
| 41 | 1 | -0.587227 | -0.112879 | 0.240728 |
| 42 | 6 | 0.703351 | -1.832734 | 0.307751 |
| 43 | 1 | 0.629753 | -2.933724 | 0.323883 |
| 44 | 1 | 1.214408 | -1.546741 | 1.239162 |
| 45 | 7 | 1.514177 | -1.366689 | -0.809654 |
| 46 | 1 | 1.101209 | -1.480033 | -1.732538 |
| 47 | 8 | 3.382663 | -2.058576 | -2.322717 |
| 48 | 16 | 3.110211 | -1.845585 | -0.907054 |
| 49 | 8 | 3.337148 | -2.913864 | 0.061642 |
| 50 | 6 | 4.033471 | -0.411613 | -0.367388 |
| 51 | 6 | 5.456587 | -0.519635 | -0.267301 |
| 52 | 6 | 3.373117 | 0.762229 | -0.087211 |
| 53 | 6 | 6.166748 | -1.728214 | -0.488754 |
| 54 | 6 | 6.181018 | 0.658963 | 0.101071 |
| 55 | 6 | 4.096849 | 1.889590 | 0.350273 |
| 56 | 1 | 2.289793 | 0.801086 | -0.194474 |
| 57 | 6 | 7.531503 | -1.755408 | -0.339732 |
| 58 | 1 | 5.629161 | -2.636285 | -0.753088 |
| 59 | 6 | 7.616882 | 0.619258 | 0.168068 |
| 60 | 6 | 5.466386 | 1.834465 | 0.443638 |
| 61 | 1 | 3.561371 | 2.800123 | 0.622948 |
| 62 | 6 | 8.258774 | -0.591054 | -0.022039 |
| 63 | 1 | 8.070274 | -2.691763 | -0.494903 |
| 64 | 1 | 6.031694 | 2.689919 | 0.812185 |
| 65 | 1 | 9.345050 | -0.647147 | 0.043045 |
| 66 | 7 | 8.314737 | 1.809761 | 0.450439 |
| 67 | 6 | 8.330677 | 2.802614 | -0.608251 |
| 68 | 1 | 8.585507 | 3.790362 | -0.194883 |
| 69 | 1 | 9.072663 | 2.560525 | -1.395723 |
| 70 | 1 | 7.348445 | 2.877317 | -1.089165 |
| 71 | 6 | 9.592988 | 1.684573 | 1.105898 |

| | | | | |
|----|---|-----------|----------|----------|
| 72 | 1 | 10.409147 | 1.344292 | 0.435545 |
| 73 | 1 | 9.890196 | 2.665347 | 1.505985 |
| 74 | 1 | 9.521471 | 0.982273 | 1.946686 |

Table S3. DFT (mPW1PW/def2-SVP) gas-phase optimized geometry for [Pb(L)]²⁺ (C₂₅H₃₉N₃O₄PbS₃²⁺) in orthogonal Cartesian format.

| Center Number | Atomic Number | Coordinates (Angstroms) | | |
|------------------|------------------|-------------------------|-----------|-----------|
| | | X | Y | Z |
| 1 | 82 | 1.724837 | -0.051136 | 0.353303 |
| 2 | 16 | 3.175814 | 2.508352 | 0.795483 |
| 3 | 7 | 1.162859 | 1.636240 | -1.660679 |
| 4 | 16 | 1.500602 | -1.701445 | -2.081039 |
| 5 | 8 | 3.162994 | -2.446689 | 0.320228 |
| 6 | 8 | 4.301099 | -0.241844 | 1.389551 |
| 7 | 6 | 3.721759 | -2.548771 | 1.615773 |
| 8 | 1 | 2.943213 | -2.397938 | 2.387235 |
| 9 | 1 | 4.157755 | -3.548845 | 1.777205 |
| 10 | 6 | 4.813848 | -1.517685 | 1.740769 |
| 11 | 1 | 5.184115 | -1.518993 | 2.779253 |
| 12 | 1 | 5.655207 | -1.770455 | 1.073156 |
| 13 | 6 | 1.969510 | -3.375479 | -1.520523 |
| 14 | 1 | 1.136853 | -4.039810 | -1.787080 |
| 15 | 1 | 2.842974 | -3.680494 | -2.112220 |
| 16 | 6 | 2.246625 | -3.462604 | -0.033922 |
| 17 | 1 | 2.668803 | -4.457821 | 0.188141 |
| 18 | 1 | 1.311283 | -3.365025 | 0.547474 |
| 19 | 6 | 5.156119 | 0.840461 | 1.712991 |
| 20 | 1 | 6.211738 | 0.535343 | 1.619628 |
| 21 | 1 | 4.992692 | 1.153472 | 2.758657 |
| 22 | 6 | 4.923213 | 1.986790 | 0.752726 |
| 23 | 1 | 5.181444 | 1.688650 | -0.273571 |
| 24 | 1 | 5.552422 | 2.841781 | 1.036587 |
| 25 | 6 | 2.902922 | 3.282168 | -0.833079 |
| 26 | 1 | 3.652342 | 2.911820 | -1.546061 |
| 27 | 1 | 3.055262 | 4.365384 | -0.731210 |
| 28 | 6 | 3.017517 | -1.082137 | -2.894915 |
| 29 | 1 | 3.881226 | -1.624395 | -2.489842 |
| 30 | 1 | 2.933574 | -1.319939 | -3.965113 |
| 31 | 6 | -1.195324 | 1.856065 | -0.709857 |
| 32 | 1 | -1.235900 | 2.947005 | -0.593680 |

| | | | | |
|----|----|-----------|-----------|-----------|
| 33 | 1 | -2.222750 | 1.550834 | -0.965738 |
| 34 | 7 | -0.774124 | 1.308682 | 0.585920 |
| 35 | 1 | -0.888204 | 1.968213 | 1.356577 |
| 36 | 16 | -1.330511 | -0.220216 | 1.127145 |
| 37 | 8 | -0.658508 | -0.331859 | 2.418947 |
| 38 | 8 | -0.853972 | -1.106534 | 0.046484 |
| 39 | 6 | -3.068226 | -0.214106 | 1.321978 |
| 40 | 6 | -3.989849 | -0.363504 | 0.226590 |
| 41 | 6 | -3.478578 | -0.013910 | 2.634423 |
| 42 | 6 | -3.640519 | -0.771148 | -1.079963 |
| 43 | 6 | -5.377898 | -0.145939 | 0.544645 |
| 44 | 6 | -4.843625 | 0.048767 | 2.926469 |
| 45 | 1 | -2.738507 | 0.055965 | 3.431640 |
| 46 | 6 | -4.633390 | -0.941380 | -2.025775 |
| 47 | 1 | -2.611210 | -1.019778 | -1.323192 |
| 48 | 6 | -6.375503 | -0.196173 | -0.504225 |
| 49 | 6 | -5.761612 | -0.005268 | 1.896516 |
| 50 | 1 | -5.174010 | 0.130908 | 3.961643 |
| 51 | 6 | -5.975671 | -0.653450 | -1.759832 |
| 52 | 1 | -4.362953 | -1.290342 | -3.024165 |
| 53 | 1 | -6.824195 | 0.019807 | 2.133272 |
| 54 | 1 | -6.704739 | -0.751318 | -2.561825 |
| 55 | 7 | -7.683456 | 0.138658 | -0.237588 |
| 56 | 6 | -8.026517 | 1.399289 | 0.402083 |
| 57 | 1 | -8.460778 | 2.094055 | -0.337734 |
| 58 | 1 | -8.768304 | 1.256931 | 1.203094 |
| 59 | 1 | -7.140724 | 1.883423 | 0.826006 |
| 60 | 6 | -8.730531 | -0.370622 | -1.096707 |
| 61 | 1 | -9.688897 | -0.303167 | -0.564590 |
| 62 | 1 | -8.830969 | 0.198008 | -2.039737 |
| 63 | 1 | -8.554165 | -1.426871 | -1.334679 |
| 64 | 6 | 3.174409 | 0.418495 | -2.680576 |
| 65 | 1 | 3.957313 | 0.766744 | -3.371292 |
| 66 | 1 | 3.576078 | 0.607000 | -1.669451 |
| 67 | 6 | 1.899259 | 1.250079 | -2.897511 |
| 68 | 1 | 2.141647 | 2.166741 | -3.458444 |
| 69 | 1 | 1.210504 | 0.689858 | -3.546014 |
| 70 | 6 | 1.475332 | 3.027099 | -1.287892 |
| 71 | 1 | 0.802085 | 3.336823 | -0.477684 |
| 72 | 1 | 1.260885 | 3.696372 | -2.142041 |
| 73 | 6 | -0.293965 | 1.459826 | -1.874689 |
| 74 | 1 | -0.456238 | 0.400480 | -2.116140 |

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|----|---|-----------|----------|-----------|
| 75 | 1 | -0.623684 | 2.044846 | -2.752566 |
|----|---|-----------|----------|-----------|

Table S4. DFT (mPW1PW/def2-SVP) gas-phase optimized geometry for $[\text{Pb}(\text{L})_2]^{2+}$ ($\text{C}_{50}\text{H}_{78}\text{N}_6\text{O}_8\text{PbS}_6^{2+}$) in orthogonal Cartesian format.

| Center Number | Atomic Number | Coordinates (Angstroms) | | |
|------------------|------------------|-------------------------|---|---|
| | | X | Y | Z |

| | | | | |
|----|----|-----------|-----------|-----------|
| 1 | 82 | -0.829455 | -2.784792 | 1.032077 |
| 2 | 7 | -1.205774 | -0.047638 | -2.123159 |
| 3 | 7 | 2.022992 | -3.627152 | 0.463011 |
| 4 | 6 | -1.110060 | 1.193656 | -2.896420 |
| 5 | 1 | -2.057556 | 1.311669 | -3.443252 |
| 6 | 1 | -0.345526 | 1.001547 | -3.664853 |
| 7 | 6 | -0.781084 | 2.464594 | -2.123672 |
| 8 | 1 | -0.823382 | 3.292107 | -2.848366 |
| 9 | 1 | -1.570248 | 2.664215 | -1.383310 |
| 10 | 6 | 2.984123 | -4.079825 | 1.481371 |
| 11 | 1 | 2.888966 | -5.175107 | 1.510204 |
| 12 | 1 | 4.018005 | -3.873643 | 1.166543 |
| 13 | 6 | 2.754429 | -3.513567 | 2.875747 |
| 14 | 1 | 2.898651 | -2.427283 | 2.872780 |
| 15 | 1 | 3.586737 | -3.899649 | 3.482716 |
| 16 | 6 | 1.468996 | -3.934025 | 3.594828 |
| 17 | 1 | 1.727653 | -4.111517 | 4.655053 |
| 18 | 1 | 1.141695 | -4.910561 | 3.205263 |
| 19 | 7 | 0.983700 | 3.688708 | -0.787910 |
| 20 | 7 | 0.273890 | -3.044177 | 3.589789 |
| 21 | 6 | 0.245246 | 4.003680 | 0.427994 |
| 22 | 1 | -0.366942 | 4.915675 | 0.295159 |
| 23 | 1 | -0.467921 | 3.189876 | 0.635208 |
| 24 | 6 | 1.113872 | 4.210059 | 1.663677 |
| 25 | 1 | 1.854239 | 5.006216 | 1.522564 |
| 26 | 1 | 0.477586 | 4.513989 | 2.509165 |
| 27 | 6 | -0.709758 | -3.739234 | 4.456840 |
| 28 | 1 | -0.313416 | -3.778094 | 5.489633 |
| 29 | 1 | -0.769959 | -4.783890 | 4.117803 |
| 30 | 6 | -2.116506 | -3.178685 | 4.536622 |
| 31 | 1 | -2.168886 | -2.126372 | 4.841627 |
| 32 | 1 | -2.659287 | -3.759249 | 5.296501 |
| 33 | 6 | 0.943703 | -0.620464 | 3.143678 |

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|----|----|-----------|-----------|-----------|
| 34 | 1 | 1.193424 | 0.314176 | 3.666545 |
| 35 | 1 | 1.820362 | -0.857502 | 2.527593 |
| 36 | 6 | 0.574898 | -1.706398 | 4.140083 |
| 37 | 1 | -0.299611 | -1.364648 | 4.708616 |
| 38 | 1 | 1.394750 | -1.780582 | 4.878642 |
| 39 | 6 | 1.223330 | 4.783617 | -1.713440 |
| 40 | 1 | 1.800930 | 4.361828 | -2.551600 |
| 41 | 1 | 0.285533 | 5.184201 | -2.156161 |
| 42 | 6 | 2.026284 | 5.963610 | -1.170090 |
| 43 | 1 | 2.817774 | 5.637250 | -0.482139 |
| 44 | 1 | 2.506403 | 6.470918 | -2.019622 |
| 45 | 16 | -3.002966 | -3.404072 | 2.962710 |
| 46 | 16 | -0.309281 | -0.194672 | 1.899267 |
| 47 | 6 | -4.697816 | -2.838389 | 3.329984 |
| 48 | 1 | -5.311597 | -3.297339 | 2.542485 |
| 49 | 1 | -4.968399 | -3.318518 | 4.281795 |
| 50 | 6 | -4.952143 | -1.349334 | 3.380883 |
| 51 | 1 | -6.028458 | -1.220356 | 3.600293 |
| 52 | 1 | -4.762870 | -0.886073 | 2.393919 |
| 53 | 6 | -1.775822 | 0.311357 | 2.838513 |
| 54 | 1 | -2.465120 | 0.616464 | 2.038960 |
| 55 | 1 | -2.223124 | -0.540610 | 3.360743 |
| 56 | 6 | -1.560575 | 1.489765 | 3.785318 |
| 57 | 1 | -0.943318 | 1.197203 | 4.655803 |
| 58 | 1 | -1.025701 | 2.295960 | 3.263285 |
| 59 | 8 | -4.160890 | -0.754033 | 4.372053 |
| 60 | 8 | -2.786846 | 2.008189 | 4.195290 |
| 61 | 6 | -4.616535 | 0.512807 | 4.816138 |
| 62 | 1 | -5.318198 | 0.375197 | 5.657855 |
| 63 | 1 | -5.154876 | 1.037605 | 4.009274 |
| 64 | 6 | -3.467643 | 1.392917 | 5.261901 |
| 65 | 1 | -2.775394 | 0.818558 | 5.904510 |
| 66 | 1 | -3.887881 | 2.201155 | 5.879863 |
| 67 | 16 | 1.995389 | 2.727341 | 2.256904 |
| 68 | 16 | 0.955228 | 7.203327 | -0.362376 |
| 69 | 6 | 2.079248 | 8.622949 | -0.225265 |
| 70 | 1 | 2.658638 | 8.708751 | -1.157209 |
| 71 | 1 | 1.429168 | 9.507393 | -0.162722 |
| 72 | 6 | 2.999382 | 8.588610 | 0.975110 |
| 73 | 1 | 2.395986 | 8.518030 | 1.900175 |
| 74 | 1 | 3.571157 | 9.537446 | 1.026324 |
| 75 | 6 | 3.465056 | 2.665181 | 1.182702 |

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|-----|----|-----------|-----------|-----------|
| 76 | 1 | 3.782392 | 1.612789 | 1.159819 |
| 77 | 1 | 3.135361 | 2.946452 | 0.173459 |
| 78 | 6 | 4.613281 | 3.539628 | 1.639648 |
| 79 | 1 | 4.959538 | 3.232228 | 2.646618 |
| 80 | 1 | 5.464885 | 3.395461 | 0.943044 |
| 81 | 8 | 4.194758 | 4.869839 | 1.646377 |
| 82 | 8 | 3.859177 | 7.490897 | 0.867650 |
| 83 | 6 | 4.557527 | 7.172222 | 2.033907 |
| 84 | 1 | 5.341296 | 7.921350 | 2.259865 |
| 85 | 1 | 3.870484 | 7.139604 | 2.901250 |
| 86 | 6 | 5.201240 | 5.819033 | 1.866269 |
| 87 | 1 | 5.909583 | 5.838614 | 1.016090 |
| 88 | 1 | 5.779847 | 5.583913 | 2.779921 |
| 89 | 16 | -2.517586 | -0.396250 | -1.209227 |
| 90 | 8 | -2.801579 | 0.582111 | -0.159814 |
| 91 | 8 | -2.213132 | -1.772212 | -0.689246 |
| 92 | 6 | -3.855454 | -0.537063 | -2.359146 |
| 93 | 6 | -4.769577 | 0.533095 | -2.643907 |
| 94 | 6 | -3.927391 | -1.768135 | -2.988738 |
| 95 | 6 | -4.819962 | 1.772947 | -1.959361 |
| 96 | 6 | -5.726175 | 0.281003 | -3.690140 |
| 97 | 6 | -4.943271 | -2.019881 | -3.918952 |
| 98 | 1 | -3.211880 | -2.548631 | -2.732751 |
| 99 | 6 | -5.777463 | 2.701707 | -2.300876 |
| 100 | 1 | -4.131932 | 1.979390 | -1.145724 |
| 101 | 6 | -6.641443 | 1.320568 | -4.099409 |
| 102 | 6 | -5.818483 | -1.010053 | -4.255963 |
| 103 | 1 | -5.041808 | -3.010944 | -4.362069 |
| 104 | 6 | -6.677225 | 2.492711 | -3.358410 |
| 105 | 1 | -5.820659 | 3.645307 | -1.753916 |
| 106 | 1 | -6.630395 | -1.204531 | -4.955963 |
| 107 | 1 | -7.378650 | 3.283191 | -3.620254 |
| 108 | 16 | 2.283840 | -2.162875 | -0.355677 |
| 109 | 8 | 0.896202 | -1.801058 | -0.744210 |
| 110 | 8 | 2.978620 | -1.293326 | 0.580705 |
| 111 | 6 | 3.182634 | -2.483559 | -1.836248 |
| 112 | 6 | 4.615562 | -2.580023 | -1.857243 |
| 113 | 6 | 2.394944 | -2.742059 | -2.949145 |
| 114 | 6 | 5.460631 | -2.401381 | -0.737153 |
| 115 | 6 | 5.205786 | -2.914132 | -3.127207 |
| 116 | 6 | 2.995902 | -3.154242 | -4.143906 |
| 117 | 1 | 1.312029 | -2.639214 | -2.886623 |

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|-----|---|-----------|-----------|-----------|
| 118 | 6 | 6.818575 | -2.602533 | -0.870212 |
| 119 | 1 | 5.054884 | -2.081129 | 0.218253 |
| 120 | 6 | 6.643724 | -2.989467 | -3.260269 |
| 121 | 6 | 4.370166 | -3.249330 | -4.215332 |
| 122 | 1 | 2.376178 | -3.411445 | -5.002833 |
| 123 | 6 | 7.411813 | -2.899734 | -2.104505 |
| 124 | 1 | 7.462711 | -2.477855 | 0.002123 |
| 125 | 1 | 4.837103 | -3.617051 | -5.128180 |
| 126 | 1 | 8.494947 | -2.992173 | -2.160338 |
| 127 | 7 | 7.208319 | -3.199359 | -4.507092 |
| 128 | 7 | -7.486412 | 1.096164 | -5.182499 |
| 129 | 6 | -6.888538 | 0.897601 | -6.494284 |
| 130 | 1 | -7.540109 | 0.271193 | -7.121255 |
| 131 | 1 | -6.738586 | 1.861278 | -7.016402 |
| 132 | 1 | -5.911849 | 0.408158 | -6.415766 |
| 133 | 6 | -8.720885 | 1.846189 | -5.244935 |
| 134 | 1 | -8.582285 | 2.893886 | -5.574973 |
| 135 | 1 | -9.394974 | 1.362003 | -5.965031 |
| 136 | 1 | -9.217406 | 1.847944 | -4.266352 |
| 137 | 6 | 6.962005 | -2.242325 | -5.576425 |
| 138 | 1 | 7.781008 | -1.502734 | -5.634979 |
| 139 | 1 | 6.896901 | -2.751821 | -6.549494 |
| 140 | 1 | 6.032005 | -1.689188 | -5.409182 |
| 141 | 6 | 8.529407 | -3.784718 | -4.573978 |
| 142 | 1 | 8.697500 | -4.164261 | -5.591053 |
| 143 | 1 | 9.337883 | -3.062994 | -4.351122 |
| 144 | 1 | 8.609595 | -4.631973 | -3.881459 |
| 145 | 6 | 0.592442 | 2.456745 | -1.438339 |
| 146 | 1 | 1.362165 | 2.206234 | -2.190822 |
| 147 | 1 | 0.628522 | 1.653646 | -0.683879 |
| 148 | 1 | -0.354609 | -0.422236 | -1.698302 |
| 149 | 1 | 1.819823 | -4.348016 | -0.230166 |

Table S5. Imaginary and low-energy harmonic frequencies (cm^{-1}) calculated for **L**, $[\text{Pb}(\text{L})]^{2+}$, $[\text{Pb}(\text{L})_2]^{2+}$ at DFT (mPW1PW/def2-SVP) in the gas-phase.

| L | -1.415 | -0.001 | 0.002 | 0.002 | 0.547 |
|--------------------------------|---------------|---------------|--------------|--------------|--------------|
| | 1.389 | 5.780 | 9.601 | 11.173 | |
| $[\text{Pb}(\text{L})]^{2+}$ | -6.054 | -2.497 | -0.002 | -0.002 | -0.001 |
| | 1.873 | 11.588 | 20.378 | 24.796 | |
| $[\text{Pb}(\text{L})_2]^{2+}$ | -2.798 | -1.616 | -0.004 | -0.001 | -0.001 |
| | 1.021 | 6.498 | 8.773 | 10.258 | |