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# Zinc Metallo-β-Lactamase from *Bacteroides fragilis*: A Quantum Chemical Study on Model Systems of the Active Site

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## SUPPLEMENTARY MATERIAL

**Table S1**. Cartesian Coordinates of the HF/6-31G* optimized structures **$3_H$ / 3**.

| $[Zn(Me\text{-}Im)_3(H_2O)]^{2+}$ $3_H$ | | | | $[Zn(Me\text{-}Im)_3(OH)]^{+}$ **3** | | | |
|---|---|---|---|---|---|---|---|
| Zn | 0.005631 | -0.262434 | 0.592087 | Zn | 0.01684 | -0.23215 | 0.72213 |
| N | -1.003512 | 1.449733 | 0.244460 | N | -1.56882 | 0.96912 | 0.13879 |
| C | -0.708908 | 2.663976 | 0.627667 | C | -2.20314 | 1.33719 | -1.03100 |
| N | -1.604803 | 3.528999 | 0.173162 | C | -3.17319 | 2.23250 | -0.76190 |
| C | -2.552539 | 2.847951 | -0.562274 | N | -3.11841 | 2.40853 | 0.60585 |
| C | -2.164782 | 1.559454 | -0.508974 | C | -2.14747 | 1.63586 | 1.09405 |
| H | 0.135706 | 2.948632 | 1.219215 | H | -1.91714 | 0.93157 | -1.97772 |
| H | -1.590148 | 4.513570 | 0.337514 | C | -4.15168 | 2.95078 | -1.63283 |
| C | -3.708177 | 3.528211 | -1.222702 | H | -5.17394 | 2.71724 | -1.35345 |
| H | -3.367244 | 4.263442 | -1.943049 | H | -4.01033 | 2.65687 | -2.66446 |
| H | -4.333945 | 4.028952 | -0.492332 | H | -4.02066 | 4.02607 | -1.56856 |
| H | -4.314291 | 2.800320 | -1.744254 | H | -3.70093 | 3.01051 | 1.14410 |
| H | -2.624400 | 0.708339 | -0.962237 | H | -1.87413 | 1.57012 | 2.12637 |
| N | -0.725565 | -1.917806 | -0.307499 | N | -0.07478 | -2.10273 | -0.17948 |
| C | -1.944419 | -2.569763 | -0.134778 | C | 0.96583 | -2.72231 | -0.66156 |
| C | -2.002448 | -3.585576 | -1.015300 | N | 0.64262 | -3.93627 | -1.08831 |
| N | -0.822387 | -3.556671 | -1.722116 | C | -0.70359 | -4.11498 | -0.85995 |
| C | -0.096453 | -2.552594 | -1.268488 | C | -1.14468 | -2.97493 | -0.29418 |
| C | -2.952595 | -2.161724 | 0.893431 | H | 1.95594 | -2.32194 | -0.71130 |
| H | -2.590309 | -2.344005 | 1.900046 | H | 1.26724 | -4.59863 | -1.49062 |
| H | -3.209442 | -1.111064 | 0.811477 | H | -1.20857 | -5.02046 | -1.11508 |
| H | -3.862582 | -2.733085 | 0.769068 | C | -2.52088 | -2.62102 | 0.17136 |
| H | -2.758156 | -4.317261 | -1.200474 | H | -2.52656 | -2.39827 | 1.23325 |
| H | -0.557820 | -4.183504 | -2.452113 | H | -3.19908 | -3.44684 | -0.00143 |
| H | 0.872069 | -2.305051 | -1.649131 | H | -2.90066 | -1.75310 | -0.35519 |
| N | 1.992043 | 0.017519 | 0.303901 | N | 1.87429 | 0.53956 | 0.14985 |
| C | 2.551145 | 0.707697 | -0.764065 | C | 2.59465 | 1.00232 | 1.12952 |
| C | 3.893820 | 0.704235 | -0.654642 | N | 3.71409 | 1.56064 | 0.66715 |
| N | 4.148289 | -0.000819 | 0.503262 | C | 3.71939 | 1.45949 | -0.70888 |
| C | 2.995907 | -0.385382 | 1.035855 | C | 2.56917 | 0.82522 | -1.00937 |
| H | 1.946884 | 1.156216 | -1.523358 | H | 2.31385 | 0.94720 | 2.16051 |
| C | 4.977890 | 1.285518 | -1.504205 | H | 4.41864 | 1.98682 | 1.22713 |
| H | 4.546253 | 1.790602 | -2.357380 | C | 4.82881 | 1.99147 | -1.55643 |
| H | 5.643291 | 0.511417 | -1.869942 | H | 5.77403 | 1.51729 | -1.31277 |
| H | 5.565982 | 2.005444 | -0.945966 | H | 4.94435 | 3.06242 | -1.42570 |
| H | 5.051026 | -0.189225 | 0.885733 | H | 4.61731 | 1.80253 | -2.60058 |
| H | 2.924543 | -0.946154 | 1.943494 | H | 2.18885 | 0.56183 | -1.97333 |
| O | -0.090710 | -0.734575 | 2.657662 | O | 0.05993 | 0.03856 | 2.56133 |
| H | -0.310241 | -0.130084 | 3.361967 | H | -0.01529 | -0.67658 | 3.17424 |
| H | -0.229524 | -1.616593 | 2.992485 | | | | |

**Table S2**. Cartesian Coordinates of the HF/6-31G* optimized structures $\mathbf{4_H}$ / **4**.

| [Zn(Me-Im)($SCH_3$)($CH_3COO$)(**$H_2O$**)]($H_2O$) $\mathbf{4_H}$ | | | | [Zn(Me-Im)($SCH_3$)($CH_3COO$)(**OH**)]$^{-1}$($H_2O$) **4** | | | |
|---|---|---|---|---|---|---|---|
| Zn | 0.615322 | 0.373061 | 0.194138 | Zn | 0.784001 | 0.341367 | 0.030624 |
| S | 0.512323 | 2.644033 | -0.213072 | O | 1.558328 | -1.483869 | -0.249107 |
| C | 0.790888 | 2.824265 | -2.012362 | C | 2.549903 | -1.798176 | 0.478629 |
| H | 0.010723 | 2.339713 | -2.585351 | O | 3.039274 | -1.115739 | 1.354018 |
| H | 0.786349 | 3.879388 | -2.251069 | C | 3.138394 | -3.170448 | 0.173076 |
| H | 1.748533 | 2.411303 | -2.300657 | H | 3.499773 | -3.187313 | -0.850709 |
| N | -1.109806 | -0.755586 | -0.035698 | H | 3.951038 | -3.402786 | 0.849223 |
| C | -2.434518 | -0.411997 | 0.151974 | H | 2.364773 | -3.928394 | 0.254477 |
| C | -3.217024 | -1.470512 | -0.132884 | N | -1.235846 | -0.506010 | -0.240843 |
| N | -2.341396 | -2.475600 | -0.499860 | C | -1.450940 | -1.606797 | -0.874841 |
| C | -1.099737 | -1.992970 | -0.424993 | H | -0.691333 | -2.208107 | -1.326379 |
| H | -2.720878 | 0.571239 | 0.462155 | N | -2.759875 | -1.915983 | -0.878163 |
| C | -4.698448 | -1.656061 | -0.108076 | C | -3.423402 | -0.924485 | -0.178287 |
| H | -5.173336 | -0.732330 | 0.194956 | C | -2.458568 | -0.064652 | 0.206958 |
| H | -5.081621 | -1.925102 | -1.087934 | H | -3.166641 | -2.716155 | -1.302178 |
| H | -4.991032 | -2.431951 | 0.593266 | C | -4.900660 | -0.935681 | 0.036619 |
| H | -2.586231 | -3.398607 | -0.777487 | H | -5.446626 | -0.901074 | -0.903471 |
| H | -0.221533 | -2.552935 | -0.663441 | H | -5.223865 | -1.823207 | 0.575812 |
| O | 1.866116 | -0.926770 | -0.571230 | H | -5.187458 | -0.070030 | 0.620280 |
| C | 2.924884 | -1.362509 | -0.014706 | H | -2.539230 | 0.827291 | 0.793186 |
| O | 3.209848 | -1.210693 | 1.162972 | S | 1.300444 | 1.777734 | -1.795755 |
| C | 3.855932 | -2.136607 | -0.920555 | C | 0.972484 | 3.424497 | -1.069277 |
| H | 4.162902 | -1.503998 | -1.745963 | H | 1.205689 | 3.437147 | -0.011910 |
| H | 4.723382 | -2.479969 | -0.375533 | H | 1.583928 | 4.171586 | -1.565277 |
| H | 3.327439 | -2.984604 | -1.343331 | H | -0.067942 | 3.710965 | -1.192977 |
| O | 1.249813 | 0.249964 | 2.189769 | O | 0.560654 | 1.137173 | 1.737505 |
| H | 2.040679 | -0.306181 | 2.056180 | H | 1.258495 | 0.872412 | 2.319746 |
| H | 1.540414 | 1.079645 | 2.551445 | H | -0.878799 | 1.987668 | 2.220442 |
| O | -2.828153 | 2.883620 | 0.675683 | O | -1.674350 | 2.548315 | 2.263014 |
| H | -2.822083 | 3.466737 | 1.422825 | H | -1.453413 | 3.266592 | 1.685430 |
| H | -1.954976 | 2.958996 | 0.295914 | | | | |

**Table S3.** Cartesian Coordinates of the HF/6-31G* optimized structures $\mathbf{5_H}$ / **5**.

| $[Zn1(Me\text{-}Im)_3(H_2O)Zn2(Me\text{-}Im)(SCH_3)(CH_3COO)]^{2+}(H_2O)$ **$5A_H$** | | | | $[Zn1(Me\text{-}Im)_3(OH)Zn2(Me\text{-}Im)(SCH_3)(CH_3COO)]^{+}(H_2O)$ **5** | | | |
|---|---|---|---|---|---|---|---|
| C | -4.735568 | -0.946556 | 0.366271 | Zn | 1.359034 | 0.054334 | 0.431982 |
| N | -3.817060 | -0.023681 | 0.395818 | O | -0.545546 | -0.086105 | 0.660505 |
| C | -4.418314 | 1.098864 | 0.938904 | H | -0.790465 | -0.904591 | 1.095187 |
| C | -5.705049 | 0.829214 | 1.231353 | Zn | -1.946844 | -0.212245 | -0.816270 |
| N | -5.883029 | -0.486389 | 0.855967 | N | 2.368289 | -0.844666 | 2.028817 |
| Zn | -1.940113 | -0.141366 | -0.417055 | C | 2.388589 | -2.167397 | 2.447130 |
| O | -1.295969 | 2.729121 | 1.066076 | C | 3.102647 | -2.238238 | 3.587115 |
| C | -6.799404 | 1.656107 | 1.824215 | N | 3.518491 | -0.954777 | 3.864729 |
| O | -0.340825 | 0.033610 | 0.843130 | C | 3.050767 | -0.164787 | 2.908034 |
| Zn | 1.545100 | 0.148664 | 0.276793 | C | 1.690212 | -3.262480 | 1.704854 |
| N | 2.247848 | 2.036852 | -0.138174 | H | 2.029694 | -3.314731 | 0.675864 |
| C | 3.216760 | 2.636272 | 0.494770 | H | 1.897082 | -4.216593 | 2.173467 |
| N | 3.456967 | 3.833107 | -0.031104 | H | 0.616558 | -3.115974 | 1.699964 |
| C | 2.580592 | 4.038188 | -1.076341 | H | 3.347152 | -3.064349 | 4.217713 |
| C | 1.838729 | 2.915010 | -1.129827 | H | 4.059992 | -0.664329 | 4.647529 |
| C | 2.572800 | 5.289204 | -1.893945 | H | 3.220914 | 0.890019 | 2.877593 |
| N | 1.820929 | -1.177429 | -1.274275 | N | 2.179039 | -0.733478 | -1.286318 |
| C | 1.634278 | -0.942583 | -2.543304 | C | 1.674402 | -0.640367 | -2.484998 |
| N | 1.903089 | -2.024894 | -3.267255 | N | 2.441816 | -1.280046 | -3.364957 |
| C | 2.287242 | -3.042596 | -2.420183 | C | 3.517967 | -1.829633 | -2.700127 |
| C | 2.228617 | -2.501016 | -1.188434 | C | 3.338886 | -1.479183 | -1.412722 |
| C | 2.664044 | -4.403892 | -2.908869 | H | 0.774842 | -0.118290 | -2.745704 |
| N | 2.832538 | -0.492227 | 1.793047 | H | 2.247367 | -1.354694 | -4.339091 |
| C | 2.691125 | -0.365060 | 3.169017 | C | 4.578450 | -2.623657 | -3.390407 |
| C | 3.788272 | -0.880155 | 3.756841 | H | 5.319886 | -2.950257 | -2.673215 |
| N | 4.599722 | -1.325013 | 2.738999 | H | 5.080860 | -2.033439 | -4.149873 |
| C | 3.988272 | -1.070631 | 1.592172 | H | 4.161294 | -3.504131 | -3.868027 |
| C | 1.489812 | 0.256575 | 3.807987 | H | 3.953394 | -1.707935 | -0.568720 |
| S | -1.357976 | 1.210917 | -2.172313 | N | 1.977107 | 2.033162 | 0.487010 |
| C | -2.764183 | 1.341011 | -3.336897 | C | 1.333989 | 3.045333 | 0.998996 |
| O | -1.881900 | -2.232366 | -0.370497 | N | 1.987618 | 4.181390 | 0.757720 |
| C | -1.342496 | -3.000518 | 0.404228 | C | 3.127605 | 3.894485 | 0.034919 |
| O | -0.599263 | -2.593726 | 1.386049 | C | 3.102790 | 2.558227 | -0.123859 |
| C | -1.494861 | -4.485180 | 0.318409 | H | 0.406998 | 2.988671 | 1.535060 |
| H | -0.558372 | 0.815014 | 1.347878 | H | 1.681670 | 5.086707 | 1.038057 |
| H | -0.525302 | -1.623551 | 1.390936 | C | 4.087603 | 4.946394 | -0.416365 |
| H | 1.279211 | -0.026318 | -2.963037 | H | 3.605013 | 5.661838 | -1.074052 |
| H | 1.824458 | -2.084760 | -4.259488 | H | 4.904573 | 4.490181 | -0.959491 |
| H | 2.437919 | -2.964938 | -0.248705 | H | 4.504142 | 5.488778 | 0.426272 |
| H | 3.518994 | -4.357209 | -3.574651 | H | 3.801365 | 1.935390 | -0.639874 |
| H | 1.843575 | -4.869157 | -3.444547 | S | -1.543539 | 1.174096 | -2.631761 |
| H | 2.924204 | -5.038572 | -2.072296 | C | -1.481086 | 2.880623 | -1.978217 |
| H | 1.338947 | 1.273192 | 3.458114 | H | -2.410945 | 3.158101 | -1.496933 |
| H | 0.592538 | -0.311964 | 3.594227 | H | -1.319543 | 3.555445 | -2.808403 |
| H | 1.615767 | 0.291917 | 4.882043 | H | -0.674136 | 3.014529 | -1.268560 |
| H | 4.061714 | -0.974341 | 4.784855 | N | -3.776005 | 0.105410 | 0.146898 |
| H | 5.488143 | -1.765113 | 2.841974 | C | -4.775011 | 0.970227 | -0.252990 |
| H | 4.405477 | -1.312681 | 0.637484 | C | -5.865561 | 0.796825 | 0.518603 |
| H | 3.760855 | 2.239783 | 1.324889 | N | -5.512775 | -0.200283 | 1.405884 |
| H | 4.154067 | 4.472731 | 0.283284 | C | -4.262115 | -0.582213 | 1.136441 |
| H | 2.378164 | 6.160357 | -1.277533 | H | -4.635131 | 1.635439 | -1.077540 |
| H | 3.522872 | 5.434757 | -2.396713 | C | -7.210654 | 1.446616 | 0.521811 |
| H | 1.799112 | 5.229334 | -2.647328 | H | -7.258437 | 2.192343 | -0.260646 |
| H | 1.035931 | 2.676146 | -1.793084 | H | -7.412197 | 1.938060 | 1.468552 |
| H | -2.543315 | 2.129014 | -4.042213 | H | -7.998834 | 0.722296 | 0.342831 |
| H | -3.677871 | 1.589256 | -2.815151 | H | -6.095875 | -0.593823 | 2.109987 |
| H | -2.899870 | 0.415801 | -3.878735 | H | -3.743784 | -1.359384 | 1.657529 |
| H | -3.873108 | 2.005495 | 1.079909 | O | -1.864595 | -2.149749 | -1.164836 |
| H | -6.432906 | 2.651082 | 2.037762 | C | -1.847860 | -2.947345 | -0.184848 |
| H | -7.160696 | 1.223416 | 2.751009 | C | -1.933370 | -4.416360 | -0.532594 |
| H | -7.637180 | 1.745425 | 1.141007 | O | -1.766043 | -2.596306 | 0.992096 |
| H | -6.729972 | -1.006905 | 0.928740 | H | -2.829570 | -4.597715 | -1.114808 |
| H | -4.607167 | -1.940759 | -0.004104 | H | -1.088486 | -4.687550 | -1.156757 |
| H | -1.903513 | -4.858773 | 1.249961 | H | -1.941905 | -5.026723 | 0.359283 |
| H | -0.517955 | -4.935565 | 0.188739 | O | -1.286259 | 2.041282 | 2.357484 |
| H | -2.137767 | -4.748226 | -0.506992 | H | -1.158809 | 1.255446 | 1.822395 |
| H | -1.294419 | 2.893829 | 0.126937 | H | -2.218738 | 2.210650 | 2.366091 |
| H | -1.411902 | 3.569727 | 1.492296 | | | | |

**Table S4.** Cartesian Coordinates of the HF/6-31G* optimized structures **5B$_H$** and **5C$_H$**.

| [Zn1(Me-Im)$_3$(**H$_2$O**)Zn2(Me-Im)(SCH$_3$)(CH$_3$COO)(H$_2$O)]$^{2+}$ **5B$_H$** | | | |
|---|---|---|---|
| C | -3.235999 | 4.814040 | -1.539325 |
| C | -2.768047 | 3.397910 | -1.442005 |
| N | -2.503488 | 2.620096 | -2.550719 |
| C | -2.509541 | 2.594882 | -0.392732 |
| C | -2.104406 | 1.418737 | -2.145972 |
| N | -2.097012 | 1.349171 | -0.844253 |
| C | -1.350160 | -0.964177 | 3.823570 |
| C | -2.647704 | -0.445926 | 3.289669 |
| N | -2.839125 | -0.120669 | 1.953009 |
| C | -3.793606 | -0.203056 | 3.954502 |
| C | -4.072157 | 0.303987 | 1.850428 |
| N | -4.686605 | 0.272807 | 3.023067 |
| C | -1.987005 | -4.883906 | -2.942528 |
| C | -2.092827 | -3.871804 | -1.847658 |
| N | -2.837487 | -4.078419 | -0.706563 |
| C | -1.570046 | -2.637205 | -1.700244 |
| C | -2.743494 | -2.998130 | 0.063789 |
| N | -1.985443 | -2.095479 | -0.491798 |
| Zn | -1.538801 | -0.242968 | 0.313884 |
| O | 0.340570 | -0.095949 | 0.893272 |
| C | 1.958887 | 4.351183 | 0.683683 |
| C | 1.615853 | 2.895935 | 0.636299 |
| O | 0.757660 | 2.521592 | 1.541618 |
| O | 2.092167 | 2.119849 | -0.162849 |
| C | 1.787699 | 1.081185 | -3.618550 |
| S | 1.149955 | -0.312681 | -2.619939 |
| C | 6.694995 | -1.624708 | 2.196660 |
| C | 5.658563 | -0.947659 | 1.359616 |
| N | 5.941983 | 0.124263 | 0.541195 |
| C | 4.338694 | -1.163636 | 1.194699 |
| C | 4.818910 | 0.503348 | -0.065430 |
| N | 3.819721 | -0.247304 | 0.295831 |
| Zn | 1.897704 | -0.042793 | -0.453205 |
| O | 1.806664 | -2.427056 | -0.125307 |
| H | -4.185505 | 4.878011 | -2.059805 |
| H | -2.517290 | 5.428649 | -2.070635 |
| H | -3.366467 | 5.228479 | -0.548689 |
| H | -2.584576 | 2.907624 | -3.502019 |
| H | -2.574236 | 2.821679 | 0.649573 |
| H | -1.807592 | 0.639271 | -2.813193 |
| H | -0.563342 | -0.224441 | 3.724627 |
| H | -1.042573 | -1.868894 | 3.306954 |
| H | -1.447339 | -1.204827 | 4.873891 |
| H | -4.052045 | -0.317463 | 4.984393 |
| H | -4.541163 | 0.639112 | 0.949518 |
| H | -2.959454 | -5.094415 | -3.374267 |
| H | -1.569170 | -5.815844 | -2.577085 |
| H | -1.343974 | -4.508908 | -3.727106 |
| H | -3.364275 | -4.897354 | -0.491276 |
| H | -0.937874 | -2.094795 | -2.370728 |
| H | -3.232778 | -2.907394 | 1.009948 |
| H | 7.140804 | -0.933432 | 2.903756 |
| H | 7.486545 | -2.038527 | 1.581165 |
| H | 6.245511 | -2.434341 | 2.755697 |
| H | 6.837094 | 0.543853 | 0.413584 |
| H | 3.724609 | -1.904196 | 1.658969 |
| H | 4.766284 | 1.321398 | -0.751372 |
| H | 1.330594 | 1.035038 | -4.597300 |
| H | 2.858578 | 1.001523 | -3.744095 |
| H | 1.554641 | 2.034644 | -3.164012 |
| H | 2.603413 | -2.809768 | -0.478664 |
| H | -5.627409 | 0.552922 | 3.196750 |
| H | 2.424323 | 4.574869 | 1.636856 |
| H | 1.051787 | 4.939629 | 0.618980 |
| H | 2.627862 | 4.603757 | -0.124235 |
| H | 1.100033 | -2.798072 | -0.642886 |
| H | 0.564170 | -0.739864 | 1.554520 |
| H | 0.578500 | 1.573088 | 1.453757 |

| [Zn1(Me-Im)$_3$(**H$_2$O**)Zn2(Me-Im)(SCH$_3$)(CH$_3$COO)(H$_2$O)]$^{2+}$ **5C$_H$** | | | |
|---|---|---|---|
| Zn | 1.343925 | 0.236437 | -0.116205 |
| N | 1.945042 | 1.231589 | 1.606065 |
| C | 1.532506 | 1.039031 | 2.828523 |
| N | 2.148622 | 1.864713 | 3.670395 |
| C | 2.767498 | 2.494848 | -2.096046 |
| C | 2.884867 | 2.249092 | 1.679651 |
| C | 2.700122 | -2.460647 | 0.566075 |
| N | 2.853705 | -3.538613 | -1.298151 |
| H | 0.794119 | 0.326557 | 3.125561 |
| N | 2.204108 | -1.653768 | -0.441428 |
| C | 2.315341 | -2.342265 | -1.538068 |
| H | 2.029551 | -2.014073 | -2.515040 |
| N | 2.778643 | 1.252964 | -1.471953 |
| C | 3.975607 | 0.767655 | -1.658073 |
| H | 4.329736 | -0.170098 | -1.288266 |
| O | -0.345235 | 0.842419 | -1.002936 |
| H | -0.242440 | 1.093019 | -1.911624 |
| Zn | -2.084721 | -0.211685 | -0.384670 |
| O | -3.044238 | 1.611562 | 0.047437 |
| C | -2.636315 | 2.744500 | 0.246481 |
| O | -1.412321 | 3.085668 | 0.021454 |
| C | -3.528416 | 3.827574 | 0.764948 |
| H | -0.911621 | 2.326938 | -0.334583 |
| N | -3.973661 | -1.162063 | -0.380751 |
| C | -5.088999 | -0.640732 | 0.037340 |
| N | -6.056528 | -1.556983 | 0.081742 |
| C | -4.244517 | -2.500786 | -0.609902 |
| H | -5.227483 | 0.381914 | 0.310697 |
| S | -0.767331 | -1.049912 | 1.376364 |
| C | -0.934228 | -2.866270 | 1.462901 |
| H | -0.574183 | -3.342490 | 0.560329 |
| H | -0.354931 | -3.228520 | 2.300250 |
| H | -1.968678 | -3.135469 | 1.622330 |
| O | -2.176794 | -0.873263 | -2.513462 |
| H | -3.034479 | -1.138583 | -2.828473 |
| H | -1.609795 | -0.775962 | -3.268969 |
| C | -5.536976 | -2.764068 | -0.330841 |
| C | -6.347784 | -4.018540 | -0.394439 |
| H | -6.995296 | -1.392097 | 0.372919 |
| H | -3.489627 | -3.176929 | -0.950039 |
| H | -5.734724 | -4.839025 | -0.743093 |
| H | -7.184810 | -3.910158 | -1.075362 |
| H | -6.738266 | -4.281787 | 0.582632 |
| H | -3.930865 | 3.519096 | 1.722550 |
| H | -4.359578 | 3.952710 | 0.081146 |
| H | -2.994494 | 4.759179 | 0.870608 |
| C | 3.023682 | 2.655277 | 2.955414 |
| C | 3.880445 | 3.700026 | 3.593631 |
| H | 1.992998 | 1.902306 | 4.654072 |
| H | 3.386008 | 2.615646 | 0.812174 |
| H | 4.478933 | 4.195554 | 2.840953 |
| H | 4.552308 | 3.263737 | 4.325147 |
| H | 3.277411 | 4.451215 | 4.092541 |
| C | 3.978350 | 2.712437 | -2.646845 |
| N | 4.734068 | 1.601635 | -2.360036 |
| C | 1.582172 | 3.407738 | -2.112961 |
| H | 4.364121 | 3.538354 | -3.203396 |
| H | 5.682848 | 1.448965 | -2.621940 |
| H | 0.782672 | 3.015743 | -2.733486 |
| H | 1.862214 | 4.370475 | -2.520622 |
| H | 1.190300 | 3.570291 | -1.116287 |
| C | 3.111526 | -3.637386 | 0.052739 |
| C | 3.722270 | -4.850633 | 0.675979 |
| H | 2.715844 | -2.137103 | 1.583750 |
| H | 3.036847 | -4.240124 | -1.982140 |
| H | 3.122992 | -5.734037 | 0.483409 |
| H | 3.789853 | -4.717586 | 1.747238 |
| H | 4.722163 | -5.028319 | 0.294500 |

**Table S5**. Cartesian Coordinates of the HF/6-31G* optimized structures $\mathbf{6_H}$ / **6**.

| $[Zn1(Me\text{-}Im)_3(H_2O)]^{2+}\cdots[(CH_3COO)Zn2(Me\text{-}Im)(SCH_3)(H_2O)]$ $\mathbf{6_H}$ | | | | $[Zn1(Me\text{-}Im)_3(OH)]^{+}\cdots[(CH_3COO)Zn2(Me\text{-}Im)(SCH_3)(H_2O)]$ **6** | | | |
|---|---|---|---|---|---|---|---|
| Zn | 2.55832 | 0.10197 | -0.13738 | Zn | -2.074069 | 0.069952 | -0.188318 |
| N | 2.21232 | -0.08962 | 1.85397 | N | -1.685113 | 2.071905 | -0.126158 |
| C | 1.16107 | -0.60236 | 2.43257 | C | -0.572863 | 2.624154 | -0.530441 |
| N | 1.30201 | -0.58215 | 3.75409 | N | -0.578191 | 3.925471 | -0.257026 |
| C | 3.17632 | 3.14843 | -0.22888 | C | -2.318887 | -1.836877 | 2.283759 |
| C | 3.07339 | 0.28145 | 2.87564 | C | -2.438097 | 3.086223 | 0.443360 |
| C | 4.72331 | -2.12110 | -0.31633 | C | -5.181893 | -0.152703 | -0.770274 |
| N | 4.30635 | -3.04278 | -2.22347 | N | -5.139814 | -1.141759 | -2.689053 |
| H | 0.29295 | -0.98573 | 1.93566 | H | 0.236487 | 2.110073 | -1.015755 |
| N | 3.66378 | -1.44972 | -0.90394 | N | -3.862862 | -0.373631 | -1.117361 |
| C | 3.44875 | -2.04252 | -2.04435 | C | -3.885645 | -0.968471 | -2.273543 |
| H | 2.69031 | -1.77603 | -2.74957 | H | -3.021602 | -1.281962 | -2.819444 |
| N | 3.52245 | 1.84608 | -0.56788 | N | -1.959322 | -0.616129 | 1.729015 |
| C | 4.62586 | 1.92158 | -1.26750 | C | -1.315011 | 0.043624 | 2.656131 |
| H | 5.15666 | 1.09130 | -1.68222 | H | -0.856541 | 1.000333 | 2.534806 |
| O | 0.85694 | -0.13290 | -1.18310 | O | -0.850729 | -0.827892 | -1.450240 |
| H | 0.26933 | -0.86390 | -0.96282 | Zn | 2.404716 | -0.136514 | -0.318384 |
| Zn | -3.33612 | -0.19427 | -0.72655 | O | 2.347878 | -2.122877 | -0.132347 |
| O | -3.04802 | 1.70355 | -0.92402 | C | 1.456407 | -2.999671 | 0.038013 |
| C | -1.98452 | 2.36984 | -1.11031 | O | 0.257217 | -2.856826 | -0.181430 |
| O | -0.86288 | 1.88637 | -1.18875 | C | 1.952382 | -4.337538 | 0.546752 |
| C | -2.17318 | 3.86407 | -1.22211 | H | -0.455765 | -1.629909 | -1.048479 |
| H | 0.25240 | 0.62694 | -1.28088 | N | 4.446842 | -0.121623 | -0.802421 |
| N | -5.24691 | -0.14666 | 0.00388 | C | 5.146384 | -1.187684 | -1.036112 |
| C | -5.86830 | 0.96424 | 0.27702 | N | 6.423750 | -0.874740 | -1.273595 |
| N | -7.08568 | 0.71657 | 0.75441 | C | 5.320646 | 0.941484 | -0.886334 |
| C | -6.12161 | -1.16779 | 0.32776 | H | 4.761448 | -2.184205 | -1.030980 |
| H | -5.46499 | 1.94419 | 0.13765 | S | 1.947829 | 1.239941 | 1.534812 |
| S | -1.69671 | -1.64086 | 0.04759 | C | 3.133742 | 0.712352 | 2.822956 |
| C | -2.39046 | -3.33334 | 0.01300 | H | 4.151067 | 0.754273 | 2.455262 |
| H | -2.79332 | -3.57427 | -0.96111 | H | 3.054110 | 1.380758 | 3.670922 |
| H | -1.60073 | -4.03470 | 0.24232 | H | 2.930691 | -0.297317 | 3.158502 |
| H | -3.16775 | -3.43720 | 0.75719 | O | 1.293534 | 0.506783 | -1.783904 |
| O | -3.82536 | -0.92617 | -2.68640 | H | 1.696027 | 0.504422 | -2.641431 |
| H | -4.55242 | -0.59732 | -3.20484 | H | -0.052397 | -0.290899 | -1.721482 |
| H | -3.18378 | -1.29449 | -3.28362 | C | 6.557922 | 0.495744 | -1.179673 |
| C | -7.27305 | -0.65013 | 0.79672 | C | 7.861114 | 1.197658 | -1.380181 |
| C | -8.53767 | -1.27975 | 1.28356 | H | 7.151103 | -1.524372 | -1.471084 |
| H | -7.74783 | 1.40724 | 1.03273 | H | 4.992398 | 1.944413 | -0.717376 |
| H | -5.85806 | -2.19536 | 0.19978 | H | 7.726116 | 2.263771 | -1.253483 |
| H | -8.45783 | -2.35690 | 1.22518 | H | 8.255093 | 1.025002 | -2.376863 |
| H | -9.38651 | -0.97167 | 0.68240 | H | 8.603935 | 0.866029 | -0.661488 |
| H | -8.73724 | -1.01198 | 2.31569 | H | 2.510390 | -4.194389 | 1.465296 |
| H | -2.50637 | 4.25215 | -0.26500 | H | 2.632956 | -4.766993 | -0.181324 |
| H | -2.94745 | 4.08329 | -1.94715 | H | 1.130330 | -5.018344 | 0.714948 |
| H | -1.25231 | 4.35112 | -1.50737 | C | -1.761604 | 4.246493 | 0.375600 |
| C | 2.52207 | -0.01907 | 4.06633 | C | -2.088143 | 5.631684 | 0.828872 |
| C | 2.99780 | 0.15801 | 5.47182 | H | 0.187660 | 4.539933 | -0.422347 |
| H | 0.62770 | -0.91907 | 4.40644 | H | -3.408312 | 2.906033 | 0.854691 |
| H | 4.01691 | 0.74303 | 2.67719 | H | -3.063900 | 5.646751 | 1.296386 |
| H | 3.97507 | 0.62143 | 5.47432 | H | -2.103725 | 6.325188 | -0.005618 |
| H | 3.07526 | -0.79618 | 5.98173 | H | -1.362258 | 5.988902 | 1.552080 |
| H | 2.32251 | 0.79173 | 6.03652 | C | -1.890035 | -1.862874 | 3.557508 |
| C | 4.10438 | 3.97558 | -0.74491 | N | -1.257270 | -0.656289 | 3.777230 |
| N | 5.01581 | 3.17761 | -1.40015 | C | -3.019811 | -2.900515 | 1.502418 |
| C | 1.95539 | 3.47673 | 0.56973 | H | -1.964897 | -2.612851 | 4.313526 |
| H | 4.20120 | 5.03836 | -0.71094 | H | -0.783318 | -0.374691 | 4.605461 |
| H | 5.82577 | 3.48755 | -1.89106 | H | -3.945699 | -2.532212 | 1.074194 |
| H | 1.05682 | 3.14115 | 0.06450 | H | -3.257420 | -3.739336 | 2.144746 |
| H | 1.88363 | 4.54755 | 0.71091 | H | -2.381675 | -3.259817 | 0.702411 |
| H | 1.99408 | 3.01371 | 1.55003 | C | -5.993166 | -0.624456 | -1.736368 |
| C | 5.13712 | -3.11623 | -1.12458 | C | -7.479927 | -0.651470 | -1.879680 |
| C | 6.21894 | -4.13900 | -0.99323 | H | -5.449389 | 0.323942 | 0.148201 |
| H | 5.10020 | -1.84514 | 0.64495 | H | -5.408256 | -1.576482 | -3.543869 |
| H | 4.33437 | -3.64363 | -3.01873 | H | -7.800148 | -0.103562 | -2.759795 |
| H | 5.81098 | -5.14374 | -1.01213 | H | -7.940665 | -0.194898 | -1.013852 |
| H | 6.73945 | -4.00490 | -0.05474 | H | -7.848958 | -1.668653 | -1.960308 |
| H | 6.94226 | -4.04994 | -1.79653 | | | | |

**Table S6.** Bond-Critical-Point (BCP) Properties[a] of $\rho(r)$ for the Mononuclear $\mathbf{1_H/1}$ Zn Complexes.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | $\varepsilon$ | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| | | | **$1_H$ HF/6-31G*** | | | |
| **Zn-N** [b] | 0.074 | 0.253 | 0.012 | 1.871 | 2.061 | -0.029 |
| **Zn-O** | 0.060 | 0.289 | 0.094 | 1.915 | 1.996 | -0.016 |
| | | | **$1_H$ B3LYP/6-31G*** | | | |
| **Zn-N** [b] | 0.082 | 0.253 | 0.020 | 1.854 | 2.009 | -0.033 |
| **Zn-O** | 0.064 | 0.280 | 0.087 | 1.918 | 1.970 | -0.017 |
| | | | **$1_H$ MP2/6-31G*** | | | |
| **Zn-N** [b] | 0.082 | 0.280 | 0.014 | 1.835 | 2.017 | -0.034 |
| **Zn-O** | 0.065 | 0.312 | 0.094 | 1.888 | 1.966 | -0.018 |
| | | | **1 HF/6-31G*** | | | |
| **Zn-N** [b] | 0.065 | 0.243 | 0.007 | 1.921 | 2.104 | -0.021 |
| **Zn-O** | 0.122 | 0.619 | 0.071 | 1.662 | 1.768 | -0.051 |
| | | | **1 B3LYP/6-31G*** | | | |
| **Zn-N** [b] | 0.073 | 0.247 | 0.010 | 1.896 | 2.043 | -0.027 |
| **Zn-O** | 0.118 | 0.535 | 0.075 | 1.687 | 1.779 | -0.050 |
| | | | **1 MP2/6-31G*** | | | |
| **Zn-N** [b] | 0.073 | 0.270 | 0.008 | 1.876 | 2.051 | -0.028 |
| **Zn-O** | 0.121 | 0.610 | 0.080 | 1.665 | 1.775 | -0.051 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and $\varepsilon$ stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.

[b] Average values corresponding to the three Zn-N bonds.

**Table S7.** Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the Mononuclear **$2_H$/2** Zn Complexes.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| | | | **$2_H$ HF/6-31G*** | | | |
| **Zn-O(HCOO)** | 0.088 | 0.403 | 0.047 | 1.777 | 1.890 | -0.034 |
| **Zn-O(Wat)** | 0.053 | 0.248 | 0.029 | 1.974 | 2.083 | -0.012 |
| **Zn-N** | 0.069 | 0.252 | 0.018 | 1.894 | 2.081 | -0.025 |
| **Zn-S** | 0.074 | 0.151 | 0.078 | 1.960 | 2.361 | -0.029 |
| **O···HO** | 0.046 | 0.156 | 0.012 | 2.146 | 1.056 | -0.003 |
| | | | **$2_H$ B3LYP/6-31G*** | | | |
| **Zn-O(HCOO)** | 0.089 | 0.365 | 0.049 | 1.794 | 1.883 | -0.034 |
| **Zn-O(Wat)** | 0.062 | 0.251 | 0.023 | 1.953 | 2.034 | -0.016 |
| **Zn-N** | 0.080 | 0.260 | 0.025 | 1.859 | 2.013 | -0.032 |
| **Zn-S** | 0.080 | 0.146 | 0.064 | 1.949 | 2.304 | -0.033 |
| **O···HO** | 0.073 | 0.183 | 0.008 | 1.967 | 0.894 | -0.011 |
| | | | **$2_H$ MP2/6-31G*** | | | |
| **Zn-O(HCOO)** | 0.088 | 0.402 | 0.051 | 1.781 | 1.894 | -0.033 |
| **Zn-O(Wat)** | 0.060 | 0.275 | 0.023 | 1.931 | 2.042 | -0.016 |
| **Zn-N** | 0.079 | 0.284 | 0.019 | 1.844 | 2.024 | -0.033 |
| **Zn-S** | 0.083 | 0.160 | 0.082 | 1.916 | 2.294 | -0.037 |
| **O···HO** | 0.061 | 0.182 | 0.014 | 2.049 | 0.920 | -0.007 |
| | | | **2 HF/6-31G*** | | | |
| **Zn-O(HCOO)** | 0.078 | 0.348 | 0.058 | 1.827 | 1.942 | -0.028 |
| **Zn-O(Wat)** | 0.100 | 0.457 | 0.074 | 1.733 | 1.864 | -0.042 |
| **Zn-N** | 0.055 | 0.223 | 0.014 | 1.975 | 2.165 | -0.085 |
| **Zn-S** | 0.058 | 0.152 | 0.063 | 2.031 | 2.488 | -0.072 |
| **O···HO** | - | - | - | - | - | - |
| | | | **2 B3LYP/6-31G*** | | | |
| **Zn-O(HCOO)** | 0.082 | 0.328 | 0.035 | 1.835 | 1.919 | -0.029 |
| **Zn-O(Wat)** | 0.103 | 0.418 | 0.059 | 1.743 | 1.857 | -0.043 |
| **Zn-N** | 0.068 | 0.237 | 0.018 | 1.922 | 2.072 | -0.022 |
| **Zn-S** | 0.065 | 0.149 | 0.055 | 2.015 | 2.412 | -0.021 |
| **O···HO** | 0.019 | 0.059 | 0.079 | 2.517 | 1.532 | 0.000 |
| | | | **2 MP2/6-31G*** | | | |
| **Zn-O(HCOO)** | 0.078 | 0.350 | 0.057 | 1.827 | 1.943 | -0.028 |
| **Zn-O(Wat)** | 0.101 | 0.458 | 0.072 | 1.733 | 1.867 | -0.042 |
| **Zn-N** | 0.066 | 0.255 | 0.017 | 1.909 | 2.088 | -0.022 |
| **Zn-S** | 0.069 | 0.165 | 0.069 | 1.972 | 2.387 | -0.025 |
| **O···HO** | 0.013 | 0.050 | 0.227 | 2.689 | 1.699 | 0.000 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.

**Table S8.** Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the Mononuclear $\mathbf{3_H/3}$ and $\mathbf{4_H/4}$ Zn Complexes at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| | | | **$3_H$ HF/6-31G*** | | | |
| **Zn1-Nε(His$_{99}$)** | 0.085 | 0.295 | 0.041 | 1.817 | 1.995 | -0.037 |
| **Zn1-Nδ(His$_{101}$)** | 0.084 | 0.291 | 0.058 | 1.820 | 1.999 | -0.037 |
| **Zn1-Nε(His$_{162}$)** | 0.083 | 0.289 | 0.063 | 1.826 | 2.004 | -0.036 |
| **Zn1-O(Wat1)** | 0.053 | 0.261 | 0.086 | 1.967 | 2.042 | -0.011 |
| | | | **3 HF/6-31G*** | | | |
| **Zn1-Nε(His$_{99}$)** | 0.073 | 0.266 | 0.056 | 1.875 | 2.043 | -0.028 |
| **Zn1-Nδ(His$_{101}$)** | 0.072 | 0.264 | 0.061 | 1.879 | 2.049 | -0.027 |
| **Zn1-Nε(His$_{162}$)** | 0.070 | 0.257 | 0.060 | 1.893 | 2.059 | -0.025 |
| **Zn1-O(Wat1)** | 0.111 | 0.528 | 0.050 | 1.699 | 1.817 | -0.046 |
| | | | **$4_H$ HF/6-31G*** | | | |
| **Zn2-Oδ(Asp$_{103}$)** | 0.084 | 0.382 | 0.052 | 1.796 | 1.908 | -0.031 |
| **Zn2-Sγ(Cys$_{181}$)** | 0.071 | 0.150 | 0.118 | 1.973 | 2.392 | -0.027 |
| **Zn2-Nε(His$_{222}$)** | 0.073 | 0.267 | 0.048 | 1.872 | 2.048 | -0.028 |
| **Zn2-O(Wat1)** | 0.060 | 0.276 | 0.040 | 1.927 | 2.038 | -0.016 |
| **Oδ(Asp$_{86}$)-H(Wat1)** | 0.042 | 0.146 | 0.019 | 2.178 | 1.088 | -0.002 |
| | | | **4 HF/6-31G*** | | | |
| **Zn2-Oδ(Asp$_{103}$)** | 0.079 | 0.310 | 0.057 | 1.832 | 1.952 | -0.029 |
| **Zn2-Sγ(Cys$_{181}$)** | 0.046 | 0.134 | 0.099 | 2.155 | 2.349 | -0.008 |
| **Zn2-Nε(His$_{222}$)** | 0.054 | 0.202 | 0.060 | 1.984 | 2.187 | -0.013 |
| **Zn2-O(Wat1)** | 0.102 | 0.458 | 0.090 | 1.729 | 1.855 | -0.043 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.

**Table S9.** Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the Binuclear [Zn1(Me-Im)$_3$(OH)Zn2(Me-Im)(SCH$_3$)(CH$_3$COO)]$^+$(H$_2$O) Complex (**5**) at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| **Zn1-O(Wat1)** | 0.094 | 0.428 | 0.059 | 1.756 | 1.879 | -0.038 |
| **Zn1-Nε(His$_{99}$)** | 0.070 | 0.257 | 0.053 | 1.889 | 2.064 | -0.026 |
| **Zn1-Nδ(His$_{101}$)** | 0.076 | 0.272 | 0.049 | 1.859 | 2.035 | -0.030 |
| **Zn1-Nε(His$_{162}$)** | 0.073 | 0.266 | 0.043 | 1.872 | 2.047 | -0.028 |
| **Zn2-O(Wat1)** | 0.070 | 0.310 | 0.040 | 1.870 | 1.984 | -0.024 |
| **Zn2-Sγ(Cys$_{181}$)** | 0.070 | 0.151 | 0.103 | 1.980 | 2.404 | -0.026 |
| **Zn2-Nε(His$_{222}$)** | 0.070 | 0.260 | 0.025 | 1.889 | 2.063 | -0.025 |
| **Zn2-Oδ(Asp$_{103}$)** | 0.083 | 0.372 | 0.027 | 1.802 | 1.922 | -0.031 |
| **Oδ(Asp$_{103}$)-H(Wat1)** | 0.027 | 0.092 | 0.050 | 2.373 | 1.330 | -0.001 |
| **O(Wat1)-H(Wat2)** | 0.031 | 0.104 | 0.044 | 2.321 | 1.227 | -0.002 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.



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**Table S10.** Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the binuclear $[Zn1(Me\text{-}Im)_3(H_2O)Zn2(Me\text{-}Im)(SCH_3)(CH_3COO)]^{2+}$ $(H_2O)$ Complex ($\mathbf{5A_H}$) at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| **Zn1-O(Wat1)** | 0.083 | 0.369 | 0.051 | 1.802 | 1.925 | -0.032 |
| **Zn1-Nε($His_{99}$)** | 0.071 | 0.256 | 0.043 | 1.885 | 2.063 | -0.026 |
| **Zn1-Nδ($His_{101}$)** | 0.076 | 0.271 | 0.053 | 1.857 | 2.034 | -0.031 |
| **Zn1-Nε($His_{162}$)** | 0.077 | 0.273 | 0.060 | 1.856 | 2.033 | -0.031 |
| **Zn2-O(Wat1)** | 0.070 | 0.306 | 0.075 | 1.871 | 1.990 | -0.023 |
| **Zn2-Sγ($Cys_{181}$)** | 0.074 | 0.151 | 0.112 | 1.961 | 2.369 | -0.029 |
| **Zn2-Nε($His_{222}$)** | 0.078 | 0.278 | 0.072 | 1.847 | 2.024 | -0.032 |
| **Zn2-Oδ($Asp_{103}$)** | 0.058 | 0.277 | 0.030 | 1.935 | 2.021 | -0.014 |
| **OH($Asp_{103}$)-O(Wat1)** | 0.040 | 0.137 | 0.042 | 1.112 | 2.204 | -0.002 |
| **H(Wat1)-O(Wat2)** | 0.019 | 0.073 | 0.019 | 1.470 | 2.447 | 0.000 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.



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**Table S11**. Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the Binuclear $[Zn1(Me\text{-}Im)_3(H_2O)Zn2(Me\text{-}Im)(SCH_3)(CH_3COO)]^{2+}$ $(H_2O)$ Complex ($\mathbf{5B_H}$) at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| **Zn1-O(Wat1)** | 0.083 | 0.370 | 0.055 | 1.803 | 1.924 | -0.031 |
| **Zn1-Nε($His_{99}$)** | 0.070 | 0.253 | 0.043 | 1.891 | 2.069 | -0.026 |
| **Zn1-Nδ($His_{101}$)** | 0.079 | 0.278 | 0.055 | 1.845 | 2.022 | -0.032 |
| **Zn1-Nε($His_{162}$)** | 0.075 | 0.267 | 0.061 | 1.865 | 2.044 | -0.029 |
| **Zn2-O(Wat1)** | 0.066 | 0.297 | 0.071 | 1.888 | 2.004 | -0.021 |
| **Zn2-Sγ($Cys_{181}$)** | 0.072 | 0.150 | 0.129 | 1.971 | 2.391 | -0.027 |
| **Zn2-Nε($His_{222}$)** | 0.074 | 0.264 | 0.075 | 1.868 | 2.049 | -0.028 |
| **Zn2-Oδ($Asp_{103}$)** | 0.045 | 0.224 | 0.029 | 2.035 | 2.106 | -0.006 |
| **Zn2-O(Wat2)** | 0.028 | 0.143 | 0.075 | 2.213 | 2.340 | 0.000 |
| **O(Wat1)-HO($Asp_{103}$)** | 0.038 | 0.130 | 0.052 | 2.230 | 1.128 | -0.002 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.



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**Table S12.** Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the Binuclear $[Zn1(Me\text{-}Im)_3(H_2O)Zn2(Me\text{-}Im)(SCH_3)(CH_3COO)]^{2+}$ $(H_2O)$ Complex ($\mathbf{5C_H}$) at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| **Zn1-O(Wat1)** | 0.077 | 0.341 | 0.088 | 1.831 | 1.952 | -0.027 |
| **Zn1-Nε($His_{99}$)** | 0.052 | 0.204 | 0.052 | 2.005 | 2.190 | -0.012 |
| **Zn1-Nδ($His_{101}$)** | 0.073 | 0.261 | 0.077 | 1.873 | 2.053 | -0.028 |
| **Zn1-Nε($His_{162}$)** | 0.068 | 0.251 | 0.042 | 1.895 | 2.077 | -0.024 |
| **Zn2-O(Wat1)** | 0.056 | 0.255 | 0.050 | 1.958 | 2.059 | -0.014 |
| **Zn2-Sγ($Cys_{181}$)** | 0.064 | 0.151 | 0.098 | 2.000 | 2.448 | -0.022 |
| **Zn2-Nε($His_{222}$)** | 0.067 | 0.244 | 0.066 | 1.910 | 2.086 | -0.023 |
| **Zn2-Oδ($Asp_{103}$)** | 0.055 | 0.268 | 0.047 | 1.948 | 2.032 | -0.012 |
| **Zn2-O(Wat2)** | 0.039 | 0.206 | 0.126 | 2.072 | 2.144 | -0.003 |
| **Zn1-Sγ($Cys_{181}$)** | 0.007 | 0.029 | - | 3.798 | 3.634 | 0.001 |
| **O(Wat1)-HO($Asp_{186}$)** | 0.044 | 0.144 | 0.051 | 2.186 | 1.071 | -0.003 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.



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**Table S13**. Bond-Critical-Point (BCP) Properties[a] of ρ(r) for the $[Zn1(Me\text{-}Im)_3(H_2O)]^{2+}\cdots[(CH_3COO)Zn2(Me\text{-}Im)(SCH_3)\ (H_2O)]$ Complex ($\mathbf{6_H}$) at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | ε | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| **Zn1-O(Wat1)** | 0.073 | 0.336 | 0.061 | 1.847 | 1.953 | -0.024 |
| **Zn1-Nε($His_{99}$)** | 0.080 | 0.282 | 0.055 | 1.837 | 2.015 | -0.034 |
| **Zn1-Nδ($His_{101}$)** | 0.082 | 0.288 | 0.049 | 1.830 | 2.007 | -0.035 |
| **Zn1-Nε($His_{162}$)** | 0.077 | 0.276 | 0.056 | 1.852 | 2.029 | -0.031 |
| **Zn2-Sγ($Cys_{181}$)** | 0.069 | 0.153 | 0.085 | 1.980 | 2.404 | -0.025 |
| **Zn2-Nε($His_{222}$)** | 0.078 | 0.280 | 0.047 | 1.845 | 2.022 | -0.032 |
| **Zn2-Oδ($Asp_{103}$)** | 0.090 | 0.420 | 0.022 | 1.770 | 1.878 | -0.034 |
| **Zn2-O(Wat2)** | 0.049 | 0.248 | 0.082 | 1.995 | 2.066 | -0.008 |
| **H(Wat1)-Oδ($Asp_{103}$)** | 0.001 | 0.007 | - | 2.994 | 3.930 | 0.000 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and ε stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.



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**Table S14.** Bond-Critical-Point (BCP) Properties[a] of $\rho(r)$ for the $[Zn1(Me\text{-}Im)_3(OH)]^+\cdots[(CH_3COO)Zn2(Me\text{-}Im)(SCH_3)\ (H_2O)]$ Complex (**6**) at the HF/6-31G* Level of Theory.

| | $\rho(r_c)$ | $\nabla^2\rho(r_c)$ | $\varepsilon$ | $r_1$ | $r_2$ | $H(r_c)$ |
|---|---|---|---|---|---|---|
| **Zn1-O(Wat1)** | 0.083 | 0.370 | 0.040 | 1.804 | 1.926 | -0.031 |
| **Zn1-Nε($His_{99}$)** | 0.075 | 0.272 | 0.057 | 1.863 | 2.038 | -0.029 |
| **Zn1-Nδ($His_{101}$)** | 0.080 | 0.282 | 0.053 | 1.839 | 2.015 | -0.034 |
| **Zn1-Nε($His_{162}$)** | 0.080 | 0.282 | 0.052 | 1.840 | 2.016 | -0.033 |
| **Zn2-Sγ($Cys_{181}$)** | 0.064 | 0.153 | 0.099 | 2.002 | 2.444 | -0.022 |
| **Zn2-Nε($His_{222}$)** | 0.068 | 0.257 | 0.060 | 1.896 | 2.070 | -0.024 |
| **Zn2-Oδ($Asp_{103}$)** | 0.074 | 0.346 | 0.040 | 1.842 | 1.932 | -0.025 |
| **Zn2-O(Wat2)** | 0.088 | 0.399 | 0.057 | 1.780 | 1.903 | -0.034 |

[a] $\rho(r_c)$, $\nabla^2\rho(r_c)$ and $\varepsilon$ stand for the electronic density, the Laplacian of the electronic density and ellipticity at BCP, respectively. $r_1$ and $r_2$ are the distances from the critical point to A and B in the bond A-B. $H(r_c)$ is the local energy density.



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