

**Electronic Supplementary Information**

Interrogation of fractional crystallization behavior of newly exploited chiral  
resolution method for racemic 1-(pyridin-2-yl)ethylamine via DFT-D3  
calculation of cohesive energy

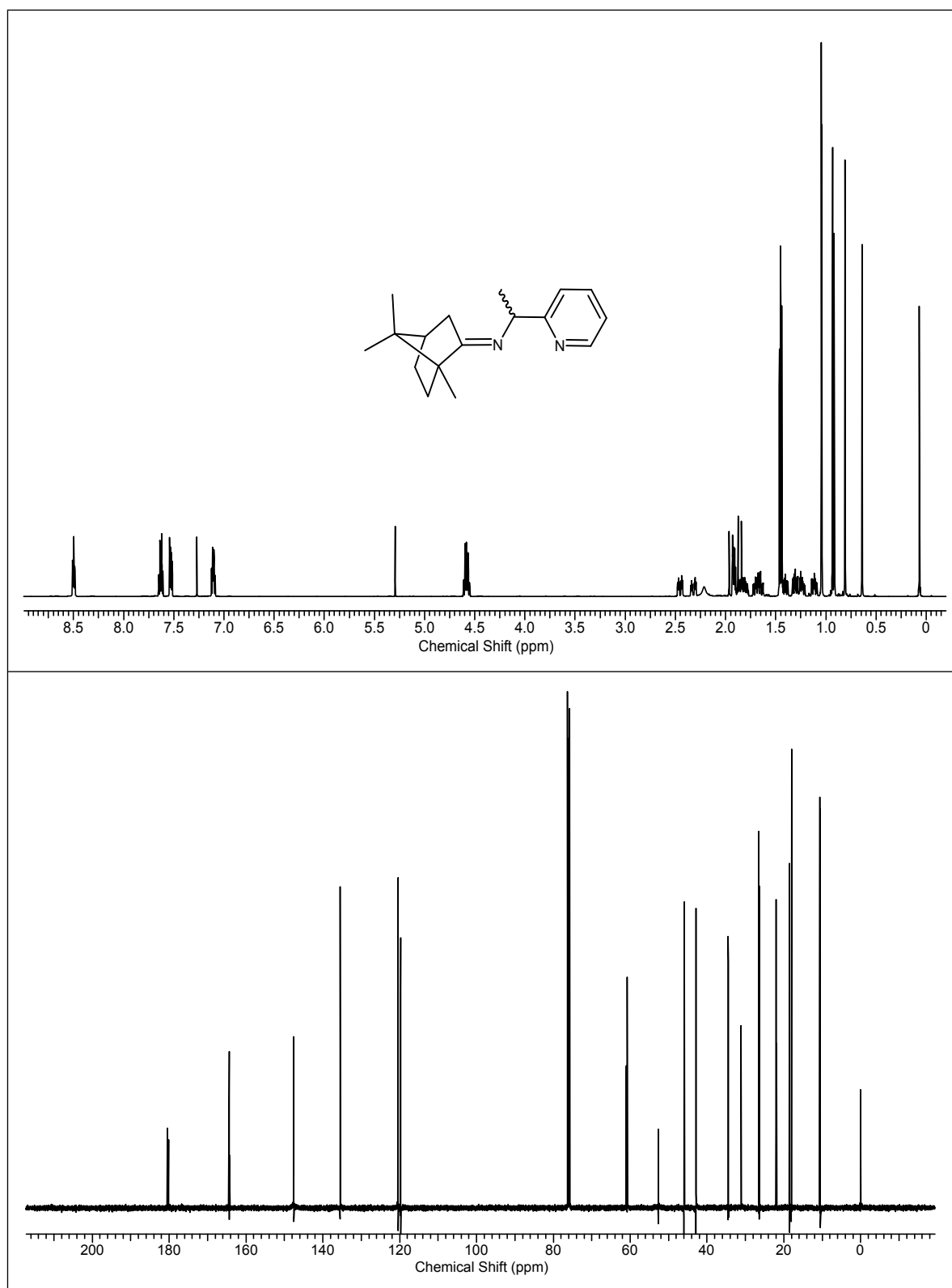
<sup>1</sup>Juhyun Cho, <sup>1</sup>Jong Hwa Jeong\*, <sup>2</sup>Myung Won Lee\* and <sup>3</sup>Youn K. Kang\*

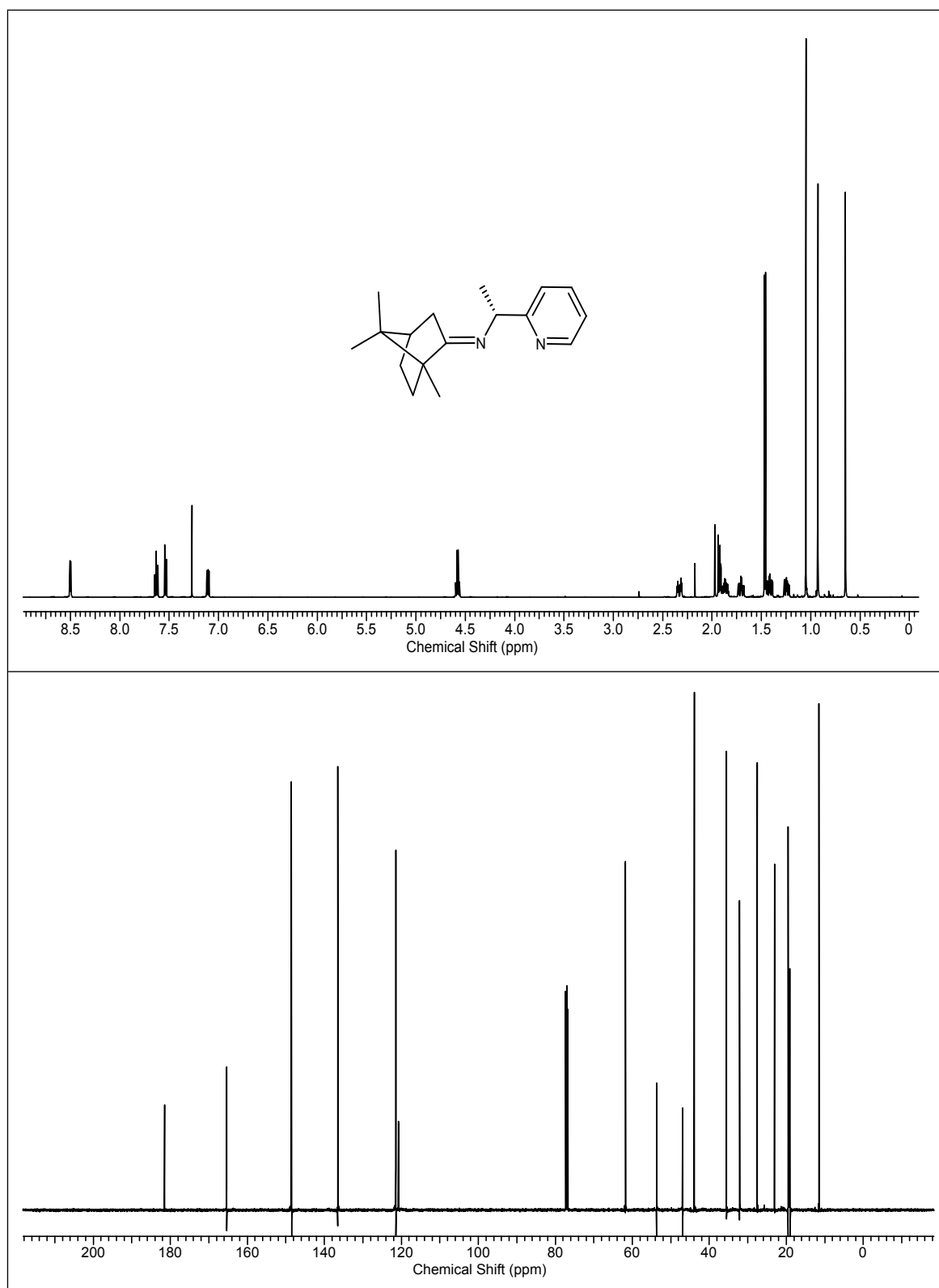
<sup>1</sup> Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Daegu 41566, Republic of Korea, <sup>2</sup>Pukyong National University, Busan 48513, Republic of Korea, <sup>3</sup>Department of Chemistry, Sangmyung University, Seoul 03016, Republic of Korea.

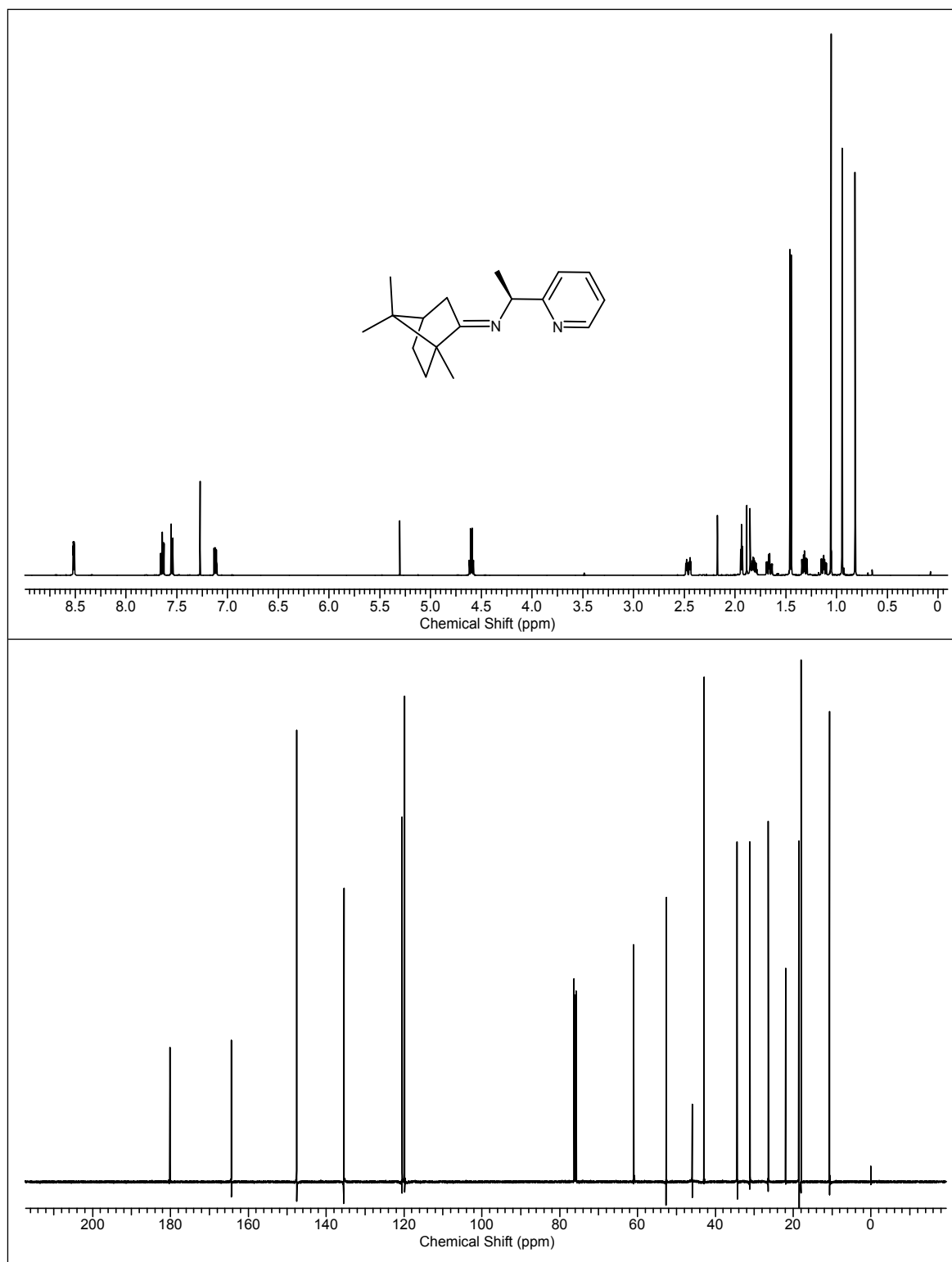
I. Full reference of Gaussian 16 program

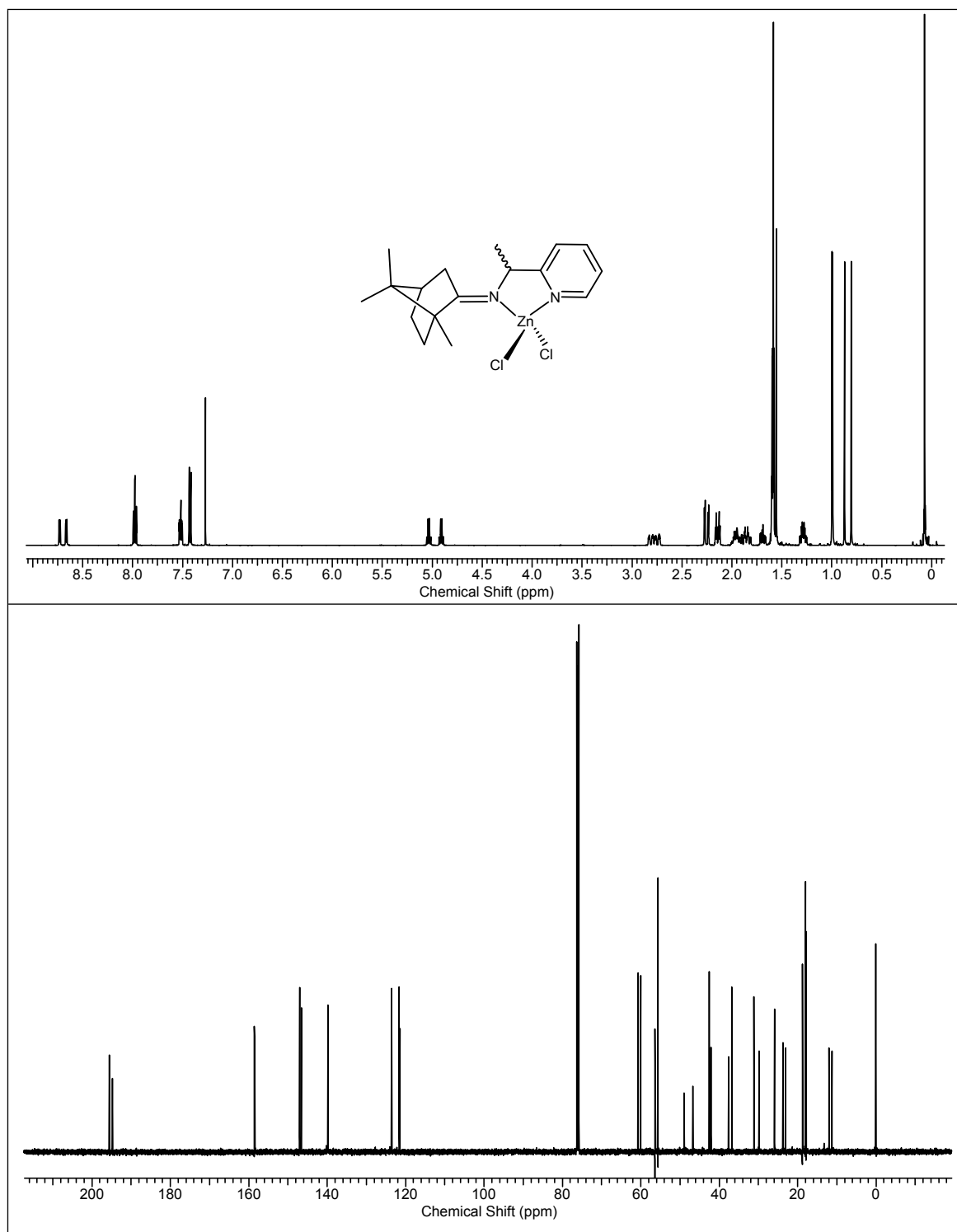
Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

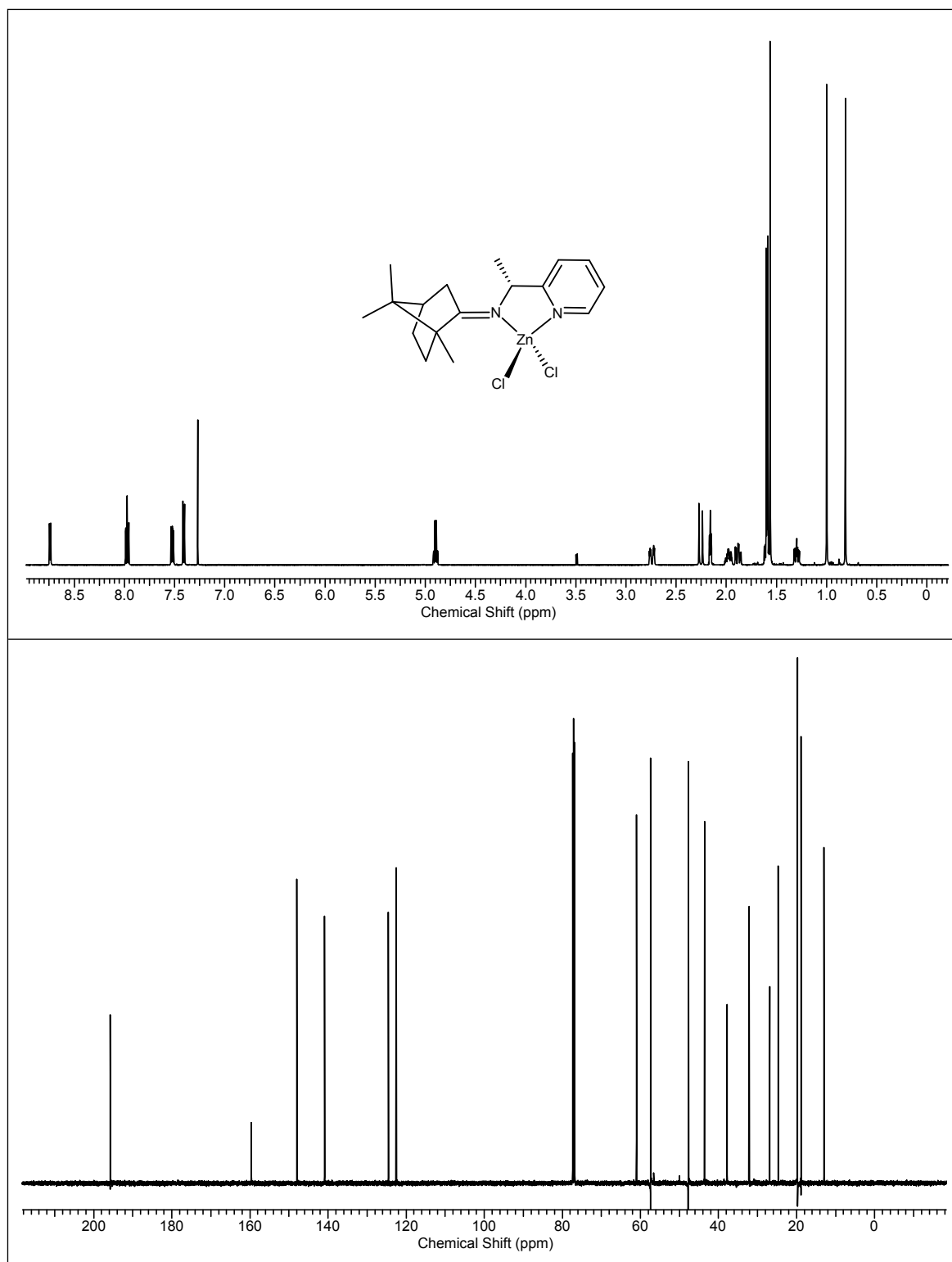
## II. NMR spectra for new compounds

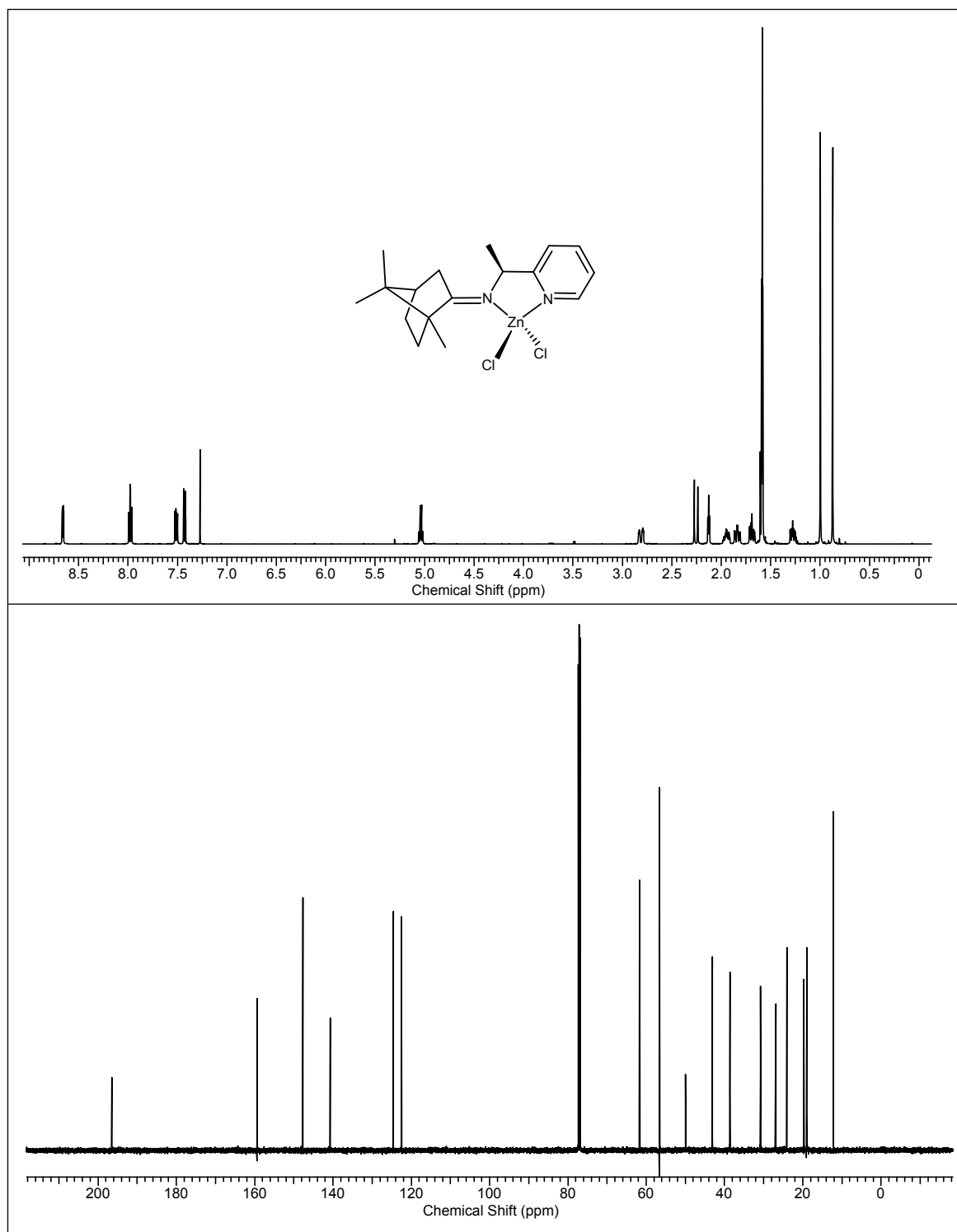




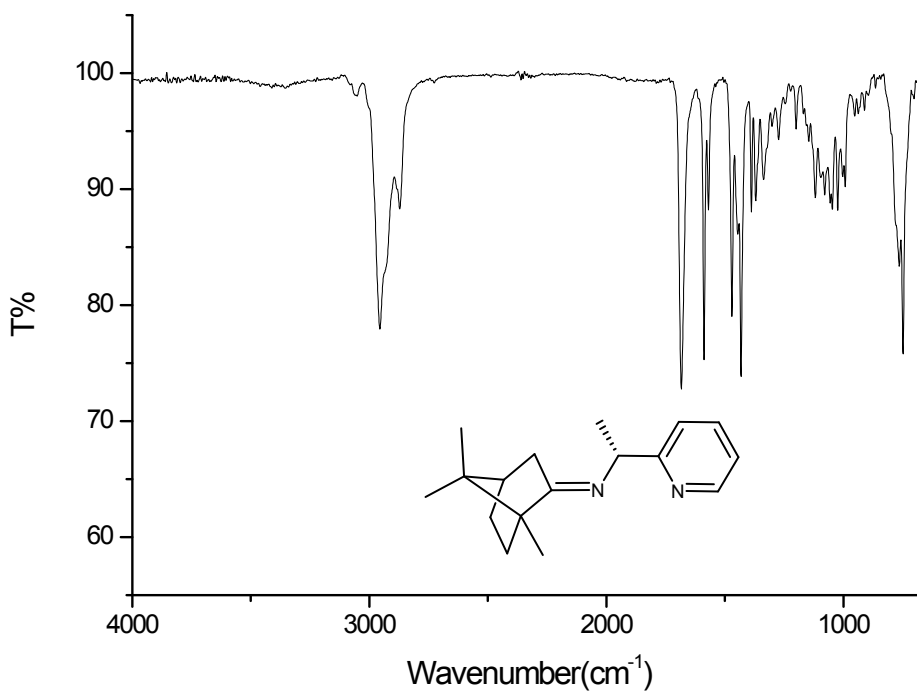
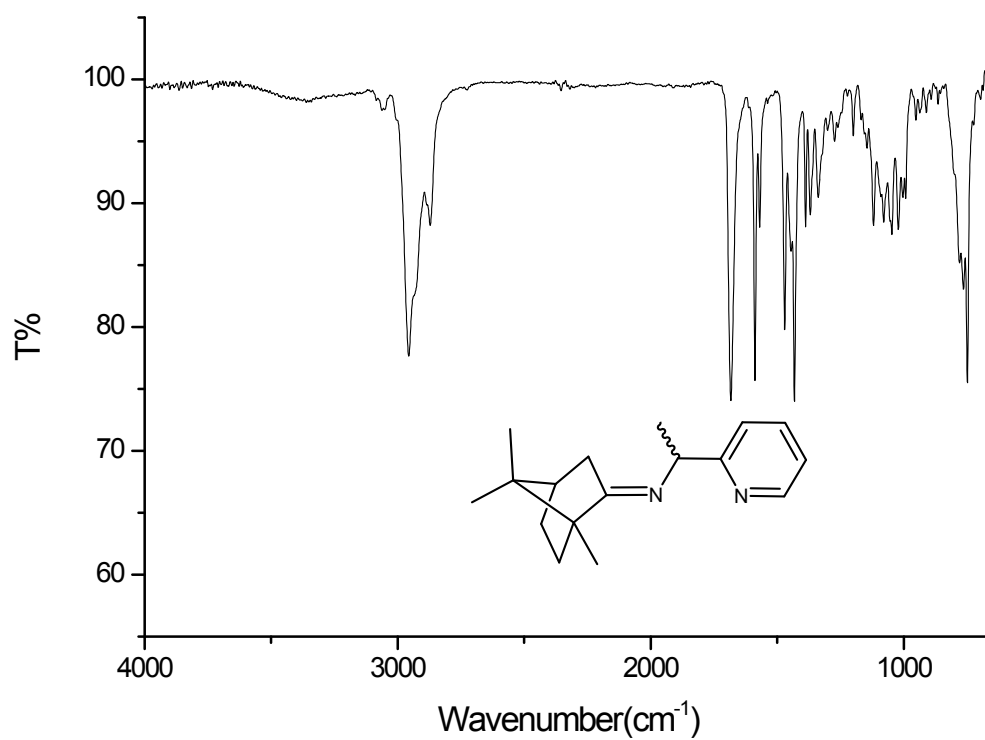


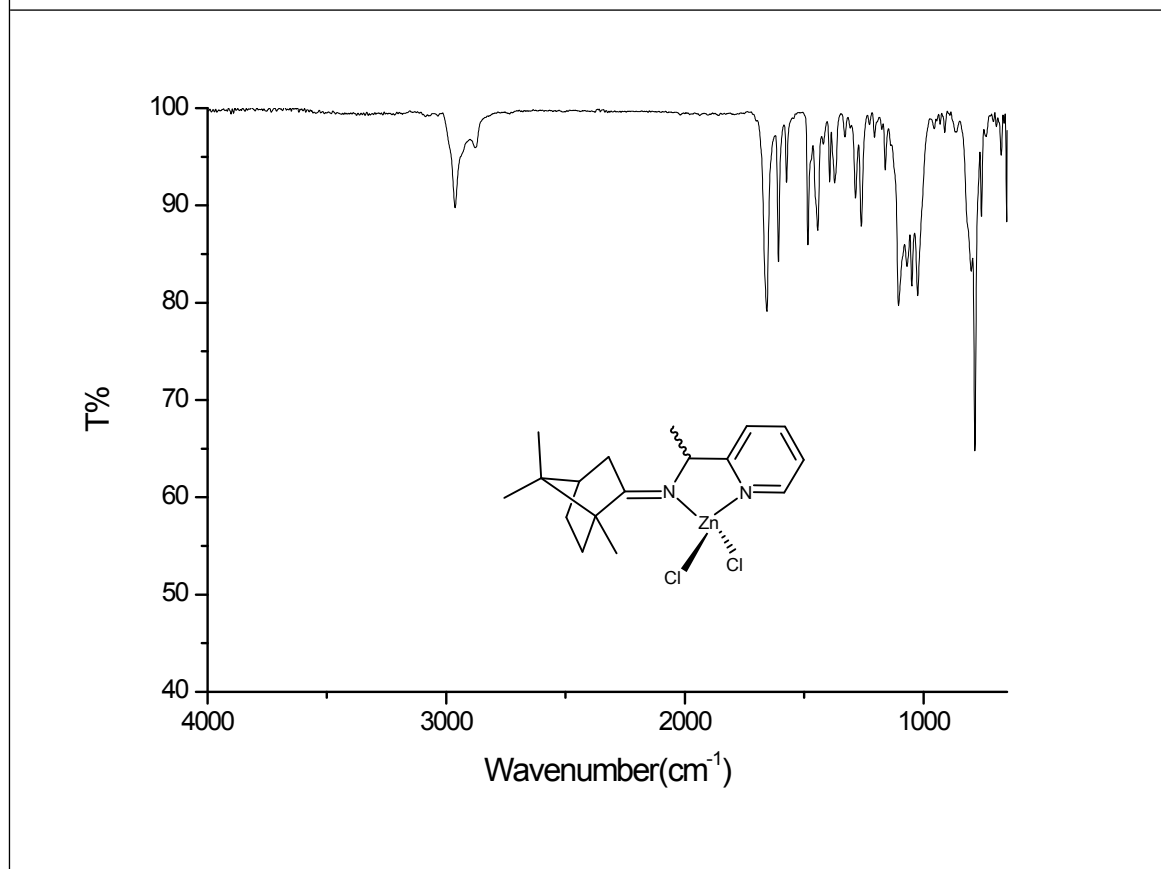
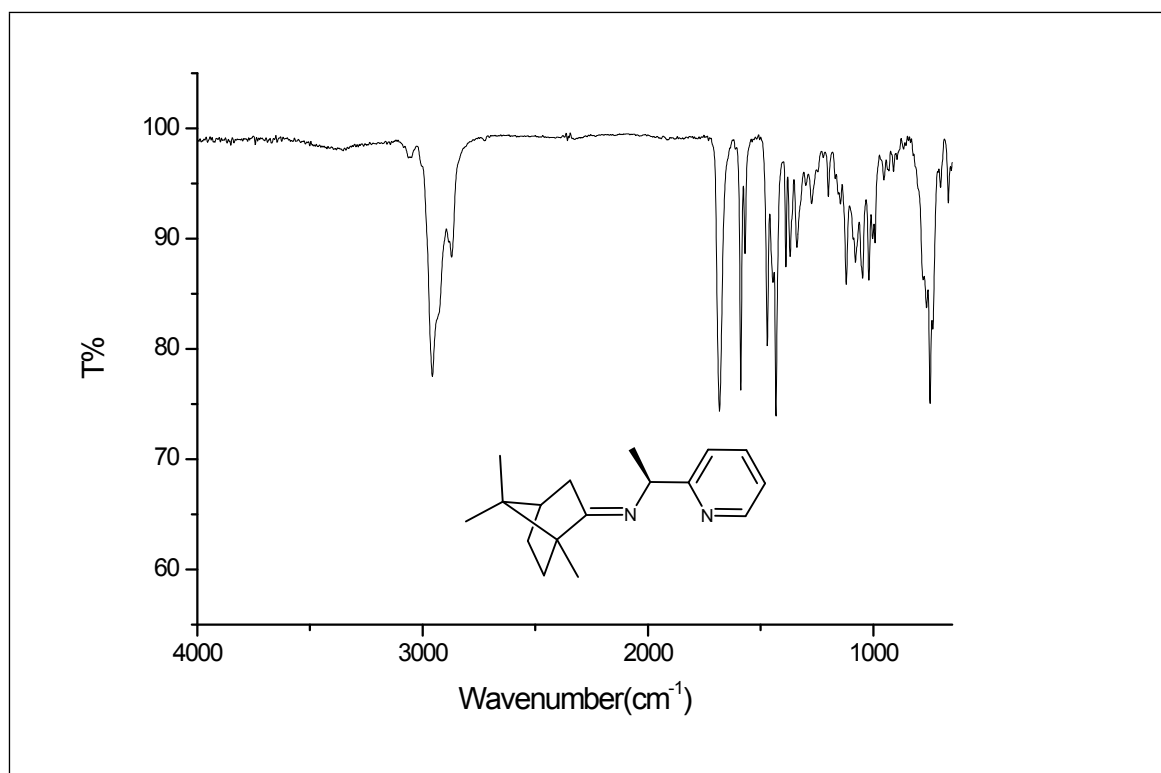


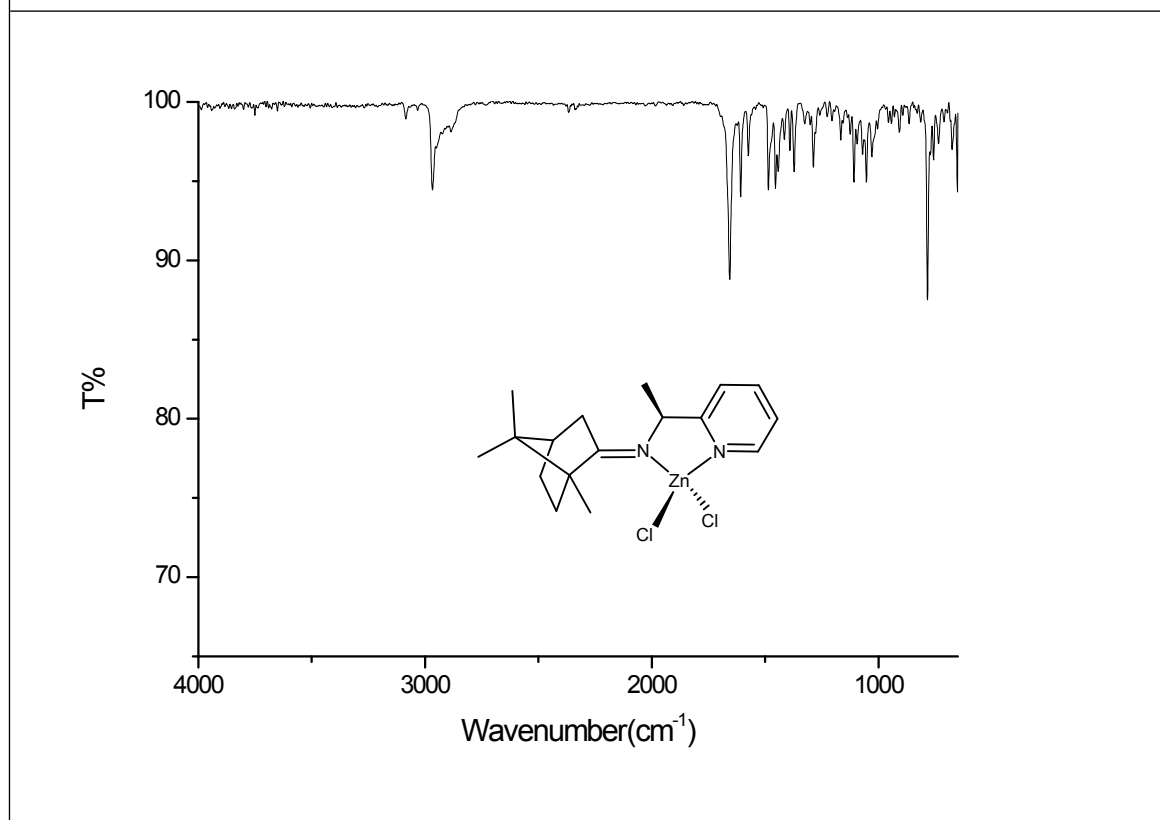
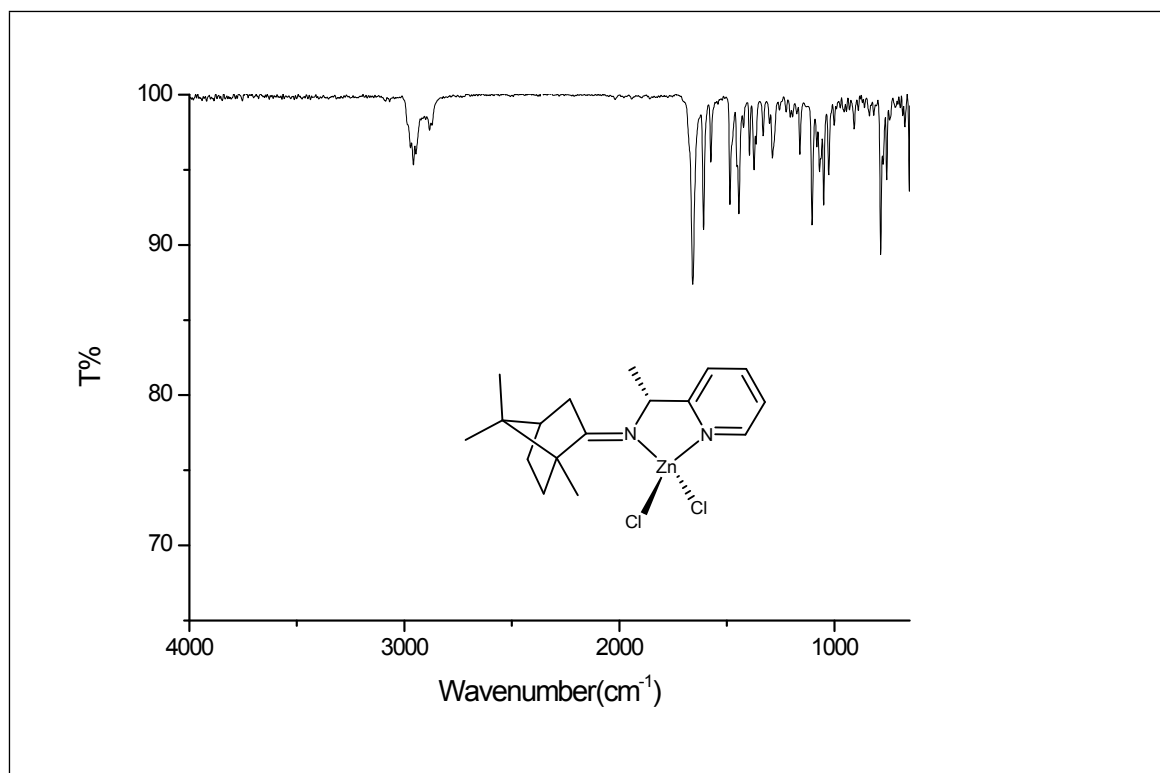




### III. IR spectra







#### IV. Energies of Stationary States from Gaussian Calculations

|                        | SCRF              | $E_0^1$<br>a.u | $E^2$<br>a.u | $H_{298}^3$<br>a.u | $G_{298}^4$<br>a.u | ZPE<br>a.u |
|------------------------|-------------------|----------------|--------------|--------------------|--------------------|------------|
| RE_PIC <sup>5</sup>    |                   | -770.7248      | -770.7066    | -770.7057          | -770.7718          |            |
| RZ_PIC <sup>5</sup>    |                   | -770.7149      | -770.6969    | -770.6960          | -770.7616          |            |
| SE_PIC <sup>5</sup>    |                   | -770.7247      | -770.7065    | -770.7056          | -770.7716          |            |
| SZ_PIC <sup>5</sup>    |                   | -770.7147      | -770.6967    | -770.6958          | -770.7619          |            |
| RE_PIC <sup>5</sup>    | toluene           | -770.7301      | -770.7119    | -770.7110          | -770.7769          |            |
| RZ_PIC <sup>5</sup>    | toluene           | -770.7204      | -770.7024    | -770.7015          | -770.7666          |            |
| SE_PIC <sup>5</sup>    | toluene           | -770.7300      | -770.7118    | -770.7109          | -770.7769          |            |
| SZ_PIC <sup>5</sup>    | toluene           | -770.7202      | -770.7022    | -770.7013          | -770.7663          |            |
| RE_PIC_Zn <sup>6</sup> |                   | -1916.5993     | -1916.5762   | -1916.5753         | -1916.6519         | 0.3854     |
| SE_PIC_Zn <sup>6</sup> |                   | -1916.6000     | -1916.5768   | -1916.5759         | -1916.6531         | 0.3853     |
| RE_PIC_Zn <sup>6</sup> | MeOH              | -1916.6293     | -1916.6061   | -1916.6052         | -1916.6826         | 0.3853     |
| SE_PIC_Zn <sup>6</sup> | MeOH              | -1916.6298     | -1916.6066   | -1916.6066         | -1916.6827         | 0.3853     |
| RE_PIC_Zn <sup>6</sup> | CHCl <sub>3</sub> | -1916.6224     | -1916.5991   | -1916.5981         | -1916.6757         | 0.3852     |
| SE_PIC_Zn <sup>6</sup> | CHCl <sub>3</sub> | -1916.6230     | -1916.5998   | -1916.5988         | -1916.6755         | 0.3853     |

1.  $E_0 = E_{\text{elec}} + \text{ZPE}$  2.  $E = E_0 + E_{\text{vib}} + E_{\text{rot}} + E_{\text{trans}}$  3.  $H = E + RT$  4.  $G = H - TS$

5. PBE0/def2TZVP 6. PBE+D3/def2TZVP+SDD

## V. Energies and Lattice Parameters for Optimized Structures from PBC Calculations

|                                                           | $E_{\text{elec}}^1$<br>eV | $a, b, c$<br>Å            | $\alpha, \beta, \gamma$<br>° |
|-----------------------------------------------------------|---------------------------|---------------------------|------------------------------|
| 4RE-PIC-Zn <sup>2</sup>                                   | -1079.0801                | 10.9678, 12.4979, 13.1706 | 90, 90, 90                   |
| 4SE-PIC-Zn <sup>2</sup>                                   | -1079.3168                | 9.6497, 10.3948, 17.8049  | 90, 90, 90                   |
| 2RE-PIC-Zn / 2SE-PIC-Zn / 4CHCl <sub>3</sub> <sup>2</sup> | -1157.8709                | 12.5453, 13.4385, 13.4490 | 90, 93.8264, 90              |
| 2RE-PIC-Zn / 2SE-PIC-Zn <sup>2</sup>                      | -1077.8700                | 12.3268, 13.2261, 13.2917 | 90, 94.8175, 90              |
| RE-PIC-Zn <sup>3</sup>                                    | -267.8444                 | 25, 20, 20                | 90, 90, 90                   |
| SE-PIC-Zn <sup>3</sup>                                    | -267.8621                 | 25, 20, 20                | 90, 90, 90                   |
| CHCl <sub>3</sub> <sup>3</sup>                            | -19.1853                  | 19, 18, 19                | 90, 90, 90                   |

1. PBE-D3 calculations with cutoff energy of 600 eV and 2×2×2 k-point mesh
2. Molecular crystals
3. One molecule in a large unit cell

## VI. Atomic coordinates from DFT Calculations

| RE_PIC in gas phase |           |           |           |
|---------------------|-----------|-----------|-----------|
| Atomic Number       | x         | y         | z         |
| 7                   | -3.379664 | 0.580574  | 0.818765  |
| 7                   | -0.350755 | 0.768400  | 0.418541  |
| 6                   | -4.421125 | -0.205599 | 1.057236  |
| 1                   | -5.018661 | 0.045117  | 1.930293  |
| 6                   | -4.765396 | -1.289872 | 0.263886  |
| 1                   | -5.629488 | -1.896437 | 0.506769  |
| 6                   | -3.976823 | -1.562149 | -0.841360 |
| 1                   | -4.207627 | -2.395068 | -1.496406 |
| 6                   | -2.887034 | -0.747424 | -1.095578 |
| 1                   | -2.247038 | -0.927694 | -1.952246 |
| 6                   | -2.617524 | 0.315301  | -0.238011 |
| 6                   | -1.409940 | 1.200256  | -0.477330 |
| 1                   | -1.127073 | 1.081598  | -1.532955 |
| 6                   | -1.716812 | 2.666011  | -0.211687 |
| 1                   | -2.529244 | 3.012745  | -0.854441 |
| 1                   | -0.831590 | 3.275072  | -0.407462 |
| 1                   | -2.015605 | 2.796678  | 0.827743  |
| 6                   | 0.780527  | 0.461963  | -0.046875 |
| 6                   | 1.285082  | 0.425047  | -1.485378 |
| 1                   | 1.192986  | 1.394174  | -1.983189 |
| 1                   | 0.716480  | -0.295838 | -2.079017 |
| 6                   | 2.742817  | -0.002089 | -1.292789 |
| 1                   | 3.208230  | -0.406366 | -2.194393 |
| 6                   | 3.477541  | 1.200258  | -0.686359 |
| 1                   | 3.275485  | 2.115270  | -1.247666 |
| 1                   | 4.559456  | 1.056644  | -0.694769 |
| 6                   | 2.919745  | 1.250602  | 0.754428  |
| 1                   | 2.403006  | 2.185019  | 0.982324  |
| 1                   | 3.710057  | 1.134758  | 1.499940  |
| 6                   | 1.948227  | 0.047120  | 0.828914  |
| 6                   | 1.572892  | -0.374046 | 2.224981  |
| 1                   | 1.048762  | 0.435158  | 2.736768  |
| 1                   | 2.460472  | -0.634998 | 2.807375  |
| 1                   | 0.896605  | -1.231500 | 2.213295  |
| 6                   | 2.652926  | -0.986980 | -0.101745 |
| 6                   | 4.009804  | -1.461443 | 0.401772  |
| 1                   | 3.892293  | -2.079441 | 1.295736  |
| 1                   | 4.692127  | -0.648789 | 0.649952  |
| 1                   | 4.495933  | -2.080342 | -0.358366 |
| 6                   | 1.803415  | -2.222629 | -0.381907 |
| 1                   | 2.236980  | -2.808725 | -1.197621 |
| 1                   | 0.770963  | -1.988031 | -0.645627 |
| 1                   | 1.769499  | -2.867785 | 0.499629  |

| RZ_PIC in gas phase |           |           |           |
|---------------------|-----------|-----------|-----------|
| Atomic Number       | x         | y         | z         |
| 7                   | 3.486895  | 0.786277  | -0.660648 |
| 7                   | 0.423540  | 0.609746  | -0.712140 |
| 6                   | 4.629013  | 0.137632  | -0.847619 |
| 1                   | 5.321659  | 0.584806  | -1.556464 |
| 6                   | 4.961412  | -1.040336 | -0.195759 |
| 1                   | 5.910792  | -1.525712 | -0.387312 |
| 6                   | 4.048211  | -1.564706 | 0.703818  |
| 1                   | 4.263518  | -2.480627 | 1.243181  |
| 6                   | 2.853941  | -0.894140 | 0.902883  |
| 1                   | 2.113603  | -1.273023 | 1.599006  |
| 6                   | 2.606973  | 0.280146  | 0.197476  |
| 6                   | 1.288740  | 1.010842  | 0.379515  |
| 1                   | 0.903208  | 0.721132  | 1.360727  |
| 6                   | 1.469683  | 2.520388  | 0.341706  |
| 1                   | 2.168591  | 2.844617  | 1.116066  |
| 1                   | 0.510561  | 3.016857  | 0.504712  |
| 1                   | 1.864292  | 2.820478  | -0.628341 |
| 6                   | -0.752263 | 0.171308  | -0.583906 |
| 6                   | -1.530676 | -0.236989 | -1.827762 |
| 1                   | -0.982818 | -0.995458 | -2.391124 |
| 1                   | -1.652399 | 0.624345  | -2.487718 |
| 6                   | -2.852000 | -0.741183 | -1.258475 |
| 1                   | -3.670262 | -0.774895 | -1.980886 |
| 6                   | -2.558434 | -2.081263 | -0.574330 |
| 1                   | -1.999897 | -2.749077 | -1.233376 |
| 1                   | -3.474750 | -2.603700 | -0.293133 |
| 6                   | -1.743460 | -1.659284 | 0.668828  |
| 1                   | -0.738180 | -2.086193 | 0.682685  |
| 1                   | -2.231613 | -1.968273 | 1.596847  |
| 6                   | -1.693975 | -0.111457 | 0.598413  |
| 6                   | -1.454151 | 0.550328  | 1.938358  |
| 1                   | -0.627086 | 0.092036  | 2.483274  |
| 1                   | -2.342172 | 0.437175  | 2.566750  |
| 1                   | -1.245979 | 1.617943  | 1.843686  |
| 6                   | -3.074897 | 0.213601  | -0.065712 |
| 6                   | -4.282969 | -0.159417 | 0.785039  |
| 1                   | -4.394484 | 0.523310  | 1.631189  |
| 1                   | -4.243325 | -1.174229 | 1.181004  |
| 1                   | -5.193683 | -0.075809 | 0.184801  |
| 6                   | -3.218942 | 1.680822  | -0.457932 |
| 1                   | -4.106568 | 1.824625  | -1.080712 |
| 1                   | -2.358589 | 2.067700  | -1.005614 |
| 1                   | -3.344699 | 2.302050  | 0.433019  |

| SE_PIC in gas phase |           |           |           |
|---------------------|-----------|-----------|-----------|
| Atomic Number       | x         | y         | z         |
| 7                   | 3.352178  | 0.766607  | 0.724080  |
| 7                   | 0.341678  | 0.803584  | 0.262077  |
| 6                   | 4.413060  | 0.073927  | 1.116570  |
| 1                   | 4.979715  | 0.495828  | 1.943035  |
| 6                   | 4.813535  | -1.118683 | 0.532618  |
| 1                   | 5.691390  | -1.640393 | 0.894211  |
| 6                   | 4.062512  | -1.609366 | -0.522198 |
| 1                   | 4.337969  | -2.534371 | -1.016791 |
| 6                   | 2.952363  | -0.893425 | -0.936039 |
| 1                   | 2.341090  | -1.244389 | -1.759988 |
| 6                   | 2.626025  | 0.292367  | -0.284002 |
| 6                   | 1.397580  | 1.079042  | -0.697567 |
| 1                   | 1.128558  | 0.747673  | -1.710442 |
| 6                   | 1.664188  | 2.575932  | -0.721210 |
| 1                   | 1.956601  | 2.912371  | 0.272789  |
| 1                   | 0.763228  | 3.112018  | -1.027248 |
| 1                   | 2.467624  | 2.814091  | -1.422182 |
| 6                   | -0.727868 | 0.252611  | -0.115682 |
| 6                   | -1.174844 | -0.206713 | -1.499514 |
| 1                   | -1.215975 | 0.636398  | -2.194420 |
| 1                   | -0.495803 | -0.946281 | -1.932180 |
| 6                   | -2.559695 | -0.788962 | -1.202611 |
| 1                   | -3.199589 | -0.879800 | -2.083058 |
| 6                   | -2.330333 | -2.104895 | -0.448326 |
| 1                   | -3.250555 | -2.685642 | -0.363616 |
| 1                   | -1.603046 | -2.737605 | -0.962110 |
| 6                   | -1.829790 | -1.624062 | 0.932860  |
| 1                   | -0.825110 | -1.978098 | 1.172379  |
| 1                   | -2.485218 | -1.957549 | 1.740945  |
| 6                   | -1.864131 | -0.078940 | 0.833824  |
| 6                   | -1.812155 | 0.637523  | 2.157192  |
| 1                   | -0.875110 | 0.415658  | 2.671194  |
| 1                   | -2.641549 | 0.332258  | 2.800617  |
| 1                   | -1.851985 | 1.720913  | 2.024874  |
| 6                   | -3.094378 | 0.152333  | -0.096066 |
| 6                   | -4.422780 | -0.296555 | 0.498726  |
| 1                   | -5.213511 | -0.225369 | -0.254146 |
| 1                   | -4.708646 | 0.352161  | 1.330775  |
| 1                   | -4.411905 | -1.321611 | 0.868510  |
| 6                   | -3.251060 | 1.603134  | -0.540106 |
| 1                   | -2.320389 | 2.051250  | -0.891328 |
| 1                   | -3.610183 | 2.217653  | 0.289241  |
| 1                   | -3.987978 | 1.679888  | -1.344972 |

| SZ_PIC in gas phase |           |           |           |
|---------------------|-----------|-----------|-----------|
| Atomic Number       | x         | y         | z         |
| 7                   | 3.517043  | -0.932158 | -0.421064 |
| 7                   | 0.447891  | -0.562588 | -0.567484 |
| 6                   | 4.694065  | -0.422533 | -0.760988 |
| 1                   | 5.364389  | -1.086996 | -1.300773 |
| 6                   | 5.087236  | 0.873048  | -0.462147 |
| 1                   | 6.062474  | 1.235195  | -0.764455 |
| 6                   | 4.199783  | 1.676824  | 0.234156  |
| 1                   | 4.462149  | 2.696063  | 0.495893  |
| 6                   | 2.969968  | 1.152164  | 0.591167  |
| 1                   | 2.247031  | 1.750531  | 1.134640  |
| 6                   | 2.662110  | -0.159115 | 0.240937  |
| 6                   | 1.303906  | -0.738269 | 0.591252  |
| 1                   | 0.944191  | -0.188070 | 1.465141  |
| 6                   | 1.393619  | -2.216879 | 0.938932  |
| 1                   | 1.736897  | -2.781387 | 0.072606  |
| 1                   | 0.414242  | -2.592055 | 1.244131  |
| 1                   | 2.100436  | -2.378687 | 1.755797  |
| 6                   | -0.787824 | -0.311564 | -0.523279 |
| 6                   | -1.564201 | -0.173574 | -1.826714 |
| 1                   | -1.164891 | 0.663057  | -2.403816 |
| 1                   | -1.449281 | -1.068681 | -2.441658 |
| 6                   | -2.996099 | 0.059031  | -1.356279 |
| 1                   | -3.649322 | 0.509405  | -2.106681 |
| 6                   | -3.498766 | -1.277089 | -0.800577 |
| 1                   | -4.570849 | -1.256187 | -0.596021 |
| 1                   | -3.324346 | -2.091666 | -1.506416 |
| 6                   | -2.677506 | -1.433486 | 0.498209  |
| 1                   | -2.042019 | -2.321200 | 0.494808  |
| 1                   | -3.321676 | -1.509451 | 1.378073  |
| 6                   | -1.831636 | -0.134652 | 0.589911  |
| 6                   | -1.398893 | 0.191844  | 2.001217  |
| 1                   | -0.847482 | -0.629695 | 2.461926  |
| 1                   | -2.282576 | 0.367863  | 2.621413  |
| 1                   | -0.777379 | 1.088873  | 2.048213  |
| 6                   | -2.786836 | 0.906695  | -0.081694 |
| 6                   | -4.074689 | 1.163711  | 0.691106  |
| 1                   | -4.760247 | 1.756198  | 0.078148  |
| 1                   | -3.878231 | 1.738675  | 1.599684  |
| 1                   | -4.598652 | 0.253272  | 0.982152  |
| 6                   | -2.119148 | 2.254826  | -0.334544 |
| 1                   | -1.141157 | 2.168984  | -0.810341 |
| 1                   | -1.978820 | 2.793497  | 0.606606  |
| 1                   | -2.749943 | 2.879789  | -0.973232 |

| RE_PIC in toluene |           |           |           |
|-------------------|-----------|-----------|-----------|
| Atomic Number     | x         | y         | z         |
| 7                 | -3.321926 | 0.508994  | 0.896853  |
| 7                 | -0.351287 | 0.719231  | 0.438758  |
| 6                 | -4.384706 | -0.253533 | 1.124180  |
| 1                 | -4.923295 | -0.061579 | 2.048771  |
| 6                 | -4.819770 | -1.245903 | 0.258040  |
| 1                 | -5.696281 | -1.836228 | 0.495683  |
| 6                 | -4.103549 | -1.449214 | -0.909609 |
| 1                 | -4.405208 | -2.210425 | -1.620463 |
| 6                 | -2.991967 | -0.659490 | -1.153053 |
| 1                 | -2.405465 | -0.789640 | -2.055535 |
| 6                 | -2.630168 | 0.310603  | -0.223411 |
| 6                 | -1.405025 | 1.171799  | -0.455471 |
| 1                 | -1.123276 | 1.053523  | -1.510016 |
| 6                 | -1.689365 | 2.643115  | -0.188825 |
| 1                 | -2.494066 | 3.003265  | -0.834049 |
| 1                 | -0.794653 | 3.238565  | -0.383058 |
| 1                 | -1.987389 | 2.781666  | 0.850385  |
| 6                 | 0.788098  | 0.444771  | -0.031363 |
| 6                 | 1.295195  | 0.472555  | -1.467370 |
| 1                 | 1.193471  | 1.461112  | -1.923105 |
| 1                 | 0.732646  | -0.227652 | -2.090557 |
| 6                 | 2.756839  | 0.051811  | -1.291012 |
| 1                 | 3.225355  | -0.312816 | -2.207465 |
| 6                 | 3.479823  | 1.236021  | -0.637248 |
| 1                 | 3.270847  | 2.169962  | -1.163536 |
| 1                 | 4.562786  | 1.101090  | -0.646057 |
| 6                 | 2.917003  | 1.226371  | 0.802270  |
| 1                 | 2.390183  | 2.146785  | 1.062544  |
| 1                 | 3.705939  | 1.090082  | 1.545639  |
| 6                 | 1.958403  | 0.009608  | 0.829533  |
| 6                 | 1.594239  | -0.471669 | 2.209233  |
| 1                 | 1.077776  | 0.313947  | 2.764424  |
| 1                 | 2.487906  | -0.756482 | 2.770507  |
| 1                 | 0.921352  | -1.331102 | 2.166998  |
| 6                 | 2.675665  | -0.979948 | -0.140076 |
| 6                 | 4.036328  | -1.459151 | 0.348721  |
| 1                 | 3.922437  | -2.118235 | 1.213399  |
| 1                 | 4.707279  | -0.649933 | 0.636096  |
| 1                 | 4.532113  | -2.036920 | -0.437050 |
| 6                 | 1.840927  | -2.213203 | -0.470947 |
| 1                 | 2.291675  | -2.767171 | -1.299525 |
| 1                 | 0.810558  | -1.979608 | -0.743666 |
| 1                 | 1.801971  | -2.887036 | 0.388802  |

| RZ_PIC in toluene |           |           |           |  |
|-------------------|-----------|-----------|-----------|--|
| Atomic Number     | x         | y         | z         |  |
| 7                 | 3.424500  | 0.717967  | -0.764089 |  |
| 7                 | 0.417382  | 0.608114  | -0.722201 |  |
| 6                 | 4.576237  | 0.083838  | -0.948911 |  |
| 1                 | 5.217327  | 0.473958  | -1.735462 |  |
| 6                 | 4.979259  | -1.013727 | -0.202518 |  |
| 1                 | 5.932278  | -1.490173 | -0.397491 |  |
| 6                 | 4.130612  | -1.470278 | 0.792107  |  |
| 1                 | 4.401566  | -2.322764 | 1.405006  |  |
| 6                 | 2.926466  | -0.814995 | 0.989872  |  |
| 1                 | 2.235256  | -1.143803 | 1.757826  |  |
| 6                 | 2.606559  | 0.277093  | 0.189116  |  |
| 6                 | 1.283122  | 0.995734  | 0.375514  |  |
| 1                 | 0.897147  | 0.691472  | 1.350583  |  |
| 6                 | 1.460792  | 2.507325  | 0.364245  |  |
| 1                 | 2.153531  | 2.819655  | 1.149185  |  |
| 1                 | 0.500204  | 2.999386  | 0.531115  |  |
| 1                 | 1.858465  | 2.828261  | -0.598529 |  |
| 6                 | -0.760877 | 0.172037  | -0.590453 |  |
| 6                 | -1.547079 | -0.227809 | -1.831699 |  |
| 1                 | -1.003339 | -0.981819 | -2.405335 |  |
| 1                 | -1.678071 | 0.638698  | -2.483397 |  |
| 6                 | -2.863179 | -0.739259 | -1.256934 |  |
| 1                 | -3.685494 | -0.769556 | -1.974557 |  |
| 6                 | -2.560507 | -2.082810 | -0.583701 |  |
| 1                 | -2.004949 | -2.744631 | -1.251341 |  |
| 1                 | -3.473437 | -2.608688 | -0.298353 |  |
| 6                 | -1.737409 | -1.666345 | 0.655860  |  |
| 1                 | -0.730878 | -2.090299 | 0.661820  |  |
| 1                 | -2.219055 | -1.980124 | 1.585386  |  |
| 6                 | -1.693099 | -0.117267 | 0.595656  |  |
| 6                 | -1.447088 | 0.535856  | 1.938912  |  |
| 1                 | -0.618684 | 0.072945  | 2.477727  |  |
| 1                 | -2.333354 | 0.417739  | 2.568514  |  |
| 1                 | -1.241121 | 1.604509  | 1.850872  |  |
| 6                 | -3.079736 | 0.207683  | -0.057137 |  |
| 6                 | -4.280181 | -0.174421 | 0.800406  |  |
| 1                 | -4.387624 | 0.504130  | 1.650383  |  |
| 1                 | -4.233420 | -1.190947 | 1.191038  |  |
| 1                 | -5.194506 | -0.091169 | 0.205636  |  |
| 6                 | -3.232101 | 1.676968  | -0.438647 |  |
| 1                 | -4.126950 | 1.820795  | -1.050933 |  |
| 1                 | -2.379459 | 2.070575  | -0.993807 |  |
| 1                 | -3.349350 | 2.291539  | 0.458004  |  |

| SE_PIC in toluene |           |           |           |  |
|-------------------|-----------|-----------|-----------|--|
| Atomic Number     | x         | y         | z         |  |
| 7                 | 3.297582  | 0.721292  | 0.794017  |  |
| 7                 | 0.338134  | 0.801002  | 0.274749  |  |
| 6                 | 4.368813  | 0.040294  | 1.183027  |  |
| 1                 | 4.888016  | 0.423038  | 2.058073  |  |
| 6                 | 4.835438  | -1.095442 | 0.537585  |  |
| 1                 | 5.717673  | -1.609145 | 0.899505  |  |
| 6                 | 4.143020  | -1.540494 | -0.576073 |  |
| 1                 | 4.470143  | -2.420861 | -1.118001 |  |
| 6                 | 3.022587  | -0.837373 | -0.986773 |  |
| 1                 | 2.455799  | -1.155066 | -1.854540 |  |
| 6                 | 2.628385  | 0.290829  | -0.273665 |  |
| 6                 | 1.394667  | 1.066807  | -0.689466 |  |
| 1                 | 1.124555  | 0.724800  | -1.696968 |  |
| 6                 | 1.658921  | 2.564469  | -0.735937 |  |
| 1                 | 1.954145  | 2.920610  | 0.250952  |  |
| 1                 | 0.756193  | 3.094254  | -1.047600 |  |
| 1                 | 2.458382  | 2.793208  | -1.444636 |  |
| 6                 | -0.731342 | 0.247826  | -0.105897 |  |
| 6                 | -1.165063 | -0.216794 | -1.490593 |  |
| 1                 | -1.197211 | 0.624176  | -2.188344 |  |
| 1                 | -0.481561 | -0.958291 | -1.912360 |  |
| 6                 | -2.553844 | -0.795722 | -1.206442 |  |
| 1                 | -3.184614 | -0.886407 | -2.093144 |  |
| 6                 | -2.334371 | -2.110182 | -0.447153 |  |
| 1                 | -3.257094 | -2.687380 | -0.366398 |  |
| 1                 | -1.604238 | -2.745602 | -0.953190 |  |
| 6                 | -1.843173 | -1.626218 | 0.936065  |  |
| 1                 | -0.840787 | -1.981971 | 1.183257  |  |
| 1                 | -2.505162 | -1.955741 | 1.740278  |  |
| 6                 | -1.875662 | -0.080520 | 0.834089  |  |
| 6                 | -1.843854 | 0.635196  | 2.158636  |  |
| 1                 | -0.924283 | 0.399881  | 2.698194  |  |
| 1                 | -2.691571 | 0.338155  | 2.781455  |  |
| 1                 | -1.871745 | 1.719298  | 2.027485  |  |
| 6                 | -3.097527 | 0.149315  | -0.107980 |  |
| 6                 | -4.431275 | -0.296565 | 0.477201  |  |
| 1                 | -5.212701 | -0.233166 | -0.285955 |  |
| 1                 | -4.727223 | 0.359490  | 1.300002  |  |
| 1                 | -4.422541 | -1.318350 | 0.856005  |  |
| 6                 | -3.249485 | 1.598908  | -0.557945 |  |
| 1                 | -2.318294 | 2.042458  | -0.913886 |  |
| 1                 | -3.606623 | 2.217895  | 0.269096  |  |
| 1                 | -3.986679 | 1.672660  | -1.362718 |  |

| SZ_PIC in toluene |           |           |           |  |
|-------------------|-----------|-----------|-----------|--|
| Atomic Number     | x         | y         | z         |  |
| 7                 | 3.415664  | -0.886722 | -0.566812 |  |
| 7                 | 0.432808  | -0.652116 | -0.531857 |  |
| 6                 | 4.595019  | -0.400247 | -0.933597 |  |
| 1                 | 5.190864  | -1.030461 | -1.589134 |  |
| 6                 | 5.079754  | 0.833802  | -0.524924 |  |
| 1                 | 6.051715  | 1.178734  | -0.855991 |  |
| 6                 | 4.286741  | 1.597736  | 0.314568  |  |
| 1                 | 4.621783  | 2.568117  | 0.663746  |  |
| 6                 | 3.053745  | 1.097548  | 0.700226  |  |
| 1                 | 2.403551  | 1.667421  | 1.354461  |  |
| 6                 | 2.650542  | -0.150343 | 0.236350  |  |
| 6                 | 1.298255  | -0.711720 | 0.631450  |  |
| 1                 | 0.934367  | -0.099923 | 1.459418  |  |
| 6                 | 1.416433  | -2.155841 | 1.102386  |  |
| 1                 | 1.775263  | -2.784315 | 0.286996  |  |
| 1                 | 0.443538  | -2.526235 | 1.432572  |  |
| 1                 | 2.118696  | -2.232740 | 1.935773  |  |
| 6                 | -0.800268 | -0.378560 | -0.498865 |  |
| 6                 | -1.594470 | -0.373784 | -1.798619 |  |
| 1                 | -1.193351 | 0.387929  | -2.470720 |  |
| 1                 | -1.504863 | -1.333933 | -2.311613 |  |
| 6                 | -3.015345 | -0.066304 | -1.337857 |  |
| 1                 | -3.671766 | 0.309452  | -2.125302 |  |
| 6                 | -3.529339 | -1.323985 | -0.630372 |  |
| 1                 | -4.597091 | -1.260848 | -0.412898 |  |
| 1                 | -3.379177 | -2.214476 | -1.244202 |  |
| 6                 | -2.689255 | -1.349659 | 0.665314  |  |
| 1                 | -2.067904 | -2.243241 | 0.751960  |  |
| 1                 | -3.319667 | -1.315231 | 1.557365  |  |
| 6                 | -1.822323 | -0.062350 | 0.601514  |  |
| 6                 | -1.366249 | 0.411874  | 1.962903  |  |
| 1                 | -0.835350 | -0.367409 | 2.512818  |  |
| 1                 | -2.239821 | 0.682745  | 2.562552  |  |
| 1                 | -0.720132 | 1.290429  | 1.902348  |  |
| 6                 | -2.772436 | 0.913910  | -0.169079 |  |
| 6                 | -4.043447 | 1.276622  | 0.589184  |  |
| 1                 | -4.731509 | 1.802537  | -0.079180 |  |
| 1                 | -3.823457 | 1.951065  | 1.420601  |  |
| 1                 | -4.572812 | 0.413715  | 0.993363  |  |
| 6                 | -2.089546 | 2.214838  | -0.579860 |  |
| 1                 | -1.124360 | 2.061763  | -1.064932 |  |
| 1                 | -1.918668 | 2.847911  | 0.295025  |  |
| 1                 | -2.726012 | 2.777643  | -1.268676 |  |

| RE_PIC_Zn in gas phase |           |           |           |
|------------------------|-----------|-----------|-----------|
| Atomic Number          | x         | y         | z         |
| 30                     | -1.097379 | -1.232781 | 0.205662  |
| 17                     | -1.450351 | -2.422999 | -1.654591 |
| 17                     | -0.877230 | -1.932155 | 2.318976  |
| 7                      | -2.610545 | 0.251985  | -0.092510 |
| 7                      | 0.082664  | 0.568585  | 0.177599  |
| 6                      | -3.853421 | -0.005019 | -0.527779 |
| 1                      | -4.125367 | -1.060587 | -0.586380 |
| 6                      | -4.726245 | 1.009585  | -0.908619 |
| 1                      | -5.731405 | 0.765869  | -1.251971 |
| 6                      | -4.275203 | 2.329994  | -0.856217 |
| 1                      | -4.926498 | 3.150593  | -1.161892 |
| 6                      | -2.975931 | 2.588183  | -0.423148 |
| 1                      | -2.587047 | 3.607165  | -0.383916 |
| 6                      | -2.166266 | 1.516539  | -0.039311 |
| 6                      | -0.768995 | 1.719698  | 0.516100  |
| 1                      | -0.361501 | 2.649870  | 0.084555  |
| 6                      | -0.848256 | 1.852329  | 2.050552  |
| 1                      | -1.520308 | 2.674903  | 2.331819  |
| 1                      | 0.148080  | 2.051178  | 2.468461  |
| 1                      | -1.217721 | 0.911424  | 2.483145  |
| 6                      | 1.348254  | 0.743021  | 0.069414  |
| 6                      | 2.111174  | 2.060897  | 0.127159  |
| 1                      | 1.920204  | 2.619449  | 1.055683  |
| 1                      | 1.801919  | 2.710566  | -0.706970 |
| 6                      | 3.571332  | 1.592694  | -0.003537 |
| 1                      | 4.264190  | 2.384548  | -0.320065 |
| 6                      | 3.927893  | 0.920296  | 1.339308  |
| 1                      | 3.678086  | 1.567391  | 2.192474  |
| 1                      | 5.001997  | 0.702281  | 1.408950  |
| 6                      | 3.077015  | -0.378245 | 1.302594  |
| 1                      | 2.333617  | -0.450893 | 2.108637  |
| 1                      | 3.698056  | -1.282974 | 1.364533  |
| 6                      | 2.376316  | -0.356039 | -0.101359 |
| 6                      | 1.884157  | -1.711264 | -0.557499 |
| 1                      | 1.302777  | -2.210127 | 0.233484  |
| 1                      | 2.738390  | -2.369260 | -0.774114 |
| 1                      | 1.252994  | -1.656485 | -1.454425 |
| 6                      | 3.448518  | 0.386625  | -0.983312 |
| 6                      | 4.754264  | -0.392962 | -1.162590 |
| 1                      | 4.596489  | -1.267600 | -1.809973 |
| 1                      | 5.187407  | -0.751585 | -0.220995 |
| 1                      | 5.505223  | 0.245238  | -1.653049 |
| 6                      | 2.922628  | 0.752738  | -2.378005 |
| 1                      | 3.629569  | 1.418844  | -2.895560 |
| 1                      | 1.941093  | 1.246089  | -2.363839 |
| 1                      | 2.811769  | -0.153256 | -2.991117 |

| SE_PIC_Zn in gas phase |           |           |           |
|------------------------|-----------|-----------|-----------|
| Atomic Number          | x         | y         | z         |
| 30                     | 1.083760  | -1.266807 | 0.080455  |
| 17                     | 1.205859  | -2.216526 | 2.093254  |
| 17                     | 1.090949  | -2.122747 | -1.989195 |
| 7                      | 2.602127  | 0.229245  | -0.117619 |
| 7                      | -0.077630 | 0.530332  | 0.262406  |
| 6                      | 3.838444  | 0.018097  | -0.593594 |
| 1                      | 4.100405  | -1.023362 | -0.789651 |
| 6                      | 4.723569  | 1.062458  | -0.842211 |
| 1                      | 5.722050  | 0.853895  | -1.225850 |
| 6                      | 4.293821  | 2.369144  | -0.602188 |
| 1                      | 4.955504  | 3.214830  | -0.796996 |
| 6                      | 3.003239  | 2.582795  | -0.122146 |
| 1                      | 2.632135  | 3.591935  | 0.065135  |
| 6                      | 2.178507  | 1.480403  | 0.116185  |
| 6                      | 0.787176  | 1.633687  | 0.704288  |
| 1                      | 0.389658  | 2.608439  | 0.376724  |
| 6                      | 0.867959  | 1.602434  | 2.243604  |
| 1                      | 1.223427  | 0.616078  | 2.575914  |
| 1                      | -0.126897 | 1.775583  | 2.677354  |
| 1                      | 1.552392  | 2.380230  | 2.609707  |
| 6                      | -1.316894 | 0.755092  | 0.024202  |
| 6                      | -2.037272 | 2.098016  | 0.051251  |
| 1                      | -1.998123 | 2.544221  | 1.056474  |
| 1                      | -1.576076 | 2.821366  | -0.639958 |
| 6                      | -3.464842 | 1.699260  | -0.360754 |
| 1                      | -4.225940 | 2.447073  | -0.098373 |
| 6                      | -3.406478 | 1.338808  | -1.861796 |
| 1                      | -4.412385 | 1.222212  | -2.286871 |
| 1                      | -2.904687 | 2.125165  | -2.444017 |
| 6                      | -2.619925 | -0.002216 | -1.865471 |
| 1                      | -1.682242 | 0.029793  | -2.436706 |
| 1                      | -3.212756 | -0.829173 | -2.280985 |
| 6                      | -2.342857 | -0.296415 | -0.353913 |
| 6                      | -2.003217 | -1.738852 | -0.039355 |
| 1                      | -1.267198 | -2.141639 | -0.750653 |
| 1                      | -2.902631 | -2.365486 | -0.128746 |
| 1                      | -1.598997 | -1.858842 | 0.976430  |
| 6                      | -3.628438 | 0.313996  | 0.330093  |
| 6                      | -4.929610 | -0.403623 | -0.039324 |
| 1                      | -5.788654 | 0.159550  | 0.356531  |
| 1                      | -4.961981 | -1.406020 | 0.411367  |
| 1                      | -5.078660 | -0.520235 | -1.119465 |
| 6                      | -3.530179 | 0.348920  | 1.861649  |
| 1                      | -2.584608 | 0.765112  | 2.235109  |
| 1                      | -3.608075 | -0.669139 | 2.269511  |
| 1                      | -4.353693 | 0.941188  | 2.288739  |

| RE_PIC_Zn in MeOH |           |           |           |
|-------------------|-----------|-----------|-----------|
| Atomic Number     | x         | y         | z         |
| 30                | -1.115769 | -1.162180 | 0.172091  |
| 17                | -1.438680 | -2.563275 | -1.608154 |
| 17                | -1.113361 | -2.168129 | 2.225709  |
| 7                 | -2.568928 | 0.320094  | -0.174455 |
| 7                 | 0.112265  | 0.561434  | 0.280648  |
| 6                 | -3.813882 | 0.108555  | -0.637848 |
| 1                 | -4.111768 | -0.935403 | -0.746661 |
| 6                 | -4.662920 | 1.156146  | -0.973405 |
| 1                 | -5.666700 | 0.948810  | -1.342421 |
| 6                 | -4.192143 | 2.464774  | -0.836413 |
| 1                 | -4.825893 | 3.311700  | -1.102453 |
| 6                 | -2.899048 | 2.677692  | -0.363983 |
| 1                 | -2.499519 | 3.686282  | -0.251851 |
| 6                 | -2.109197 | 1.574472  | -0.032127 |
| 6                 | -0.726902 | 1.739404  | 0.569255  |
| 1                 | -0.279179 | 2.647428  | 0.137475  |
| 6                 | -0.847043 | 1.910754  | 2.096047  |
| 1                 | -1.472641 | 2.781396  | 2.333104  |
| 1                 | 0.146443  | 2.058844  | 2.540076  |
| 1                 | -1.300165 | 1.014235  | 2.542254  |
| 6                 | 1.378873  | 0.734085  | 0.142144  |
| 6                 | 2.128634  | 2.055979  | 0.118039  |
| 1                 | 1.978027  | 2.644556  | 1.035018  |
| 1                 | 1.767046  | 2.673560  | -0.718728 |
| 6                 | 3.586060  | 1.600141  | -0.073755 |
| 1                 | 4.245665  | 2.385208  | -0.465851 |
| 6                 | 4.027659  | 0.996159  | 1.274587  |
| 1                 | 3.821157  | 1.681216  | 2.108522  |
| 1                 | 5.104418  | 0.782274  | 1.289728  |
| 6                 | 3.184317  | -0.305089 | 1.348589  |
| 1                 | 2.487275  | -0.327605 | 2.198090  |
| 1                 | 3.812593  | -1.203573 | 1.425368  |
| 6                 | 2.410650  | -0.359882 | -0.016898 |
| 6                 | 1.916971  | -1.741111 | -0.380935 |
| 1                 | 1.340733  | -2.186541 | 0.444657  |
| 1                 | 2.769879  | -2.410385 | -0.563739 |
| 1                 | 1.287014  | -1.739209 | -1.280878 |
| 6                 | 3.428248  | 0.348851  | -0.989225 |
| 6                 | 4.729124  | -0.431289 | -1.199537 |
| 1                 | 4.546233  | -1.332247 | -1.803156 |
| 1                 | 5.211183  | -0.747448 | -0.266594 |
| 1                 | 5.447592  | 0.193480  | -1.751529 |
| 6                 | 2.827161  | 0.646585  | -2.369921 |
| 1                 | 3.505767  | 1.289049  | -2.950492 |
| 1                 | 1.848223  | 1.143420  | -2.327910 |
| 1                 | 2.691635  | -0.287822 | -2.934240 |

| SE_PIC_Zn in MeOH |           |           |           |
|-------------------|-----------|-----------|-----------|
| Atomic Number     | x         | y         | z         |
| 30                | 1.124807  | -1.216030 | 0.078386  |
| 17                | 1.247412  | -2.270776 | 2.099761  |
| 17                | 1.126778  | -2.248751 | -1.960035 |
| 7                 | 2.617694  | 0.252187  | -0.113661 |
| 7                 | -0.088246 | 0.517066  | 0.225157  |
| 6                 | 3.878492  | 0.053484  | -0.537969 |
| 1                 | 4.176952  | -0.985598 | -0.685078 |
| 6                 | 4.748164  | 1.108602  | -0.787143 |
| 1                 | 5.763731  | 0.910394  | -1.127826 |
| 6                 | 4.282958  | 2.413040  | -0.601518 |
| 1                 | 4.932921  | 3.266302  | -0.799533 |
| 6                 | 2.974601  | 2.613776  | -0.167198 |
| 1                 | 2.578971  | 3.618922  | -0.016782 |
| 6                 | 2.163431  | 1.503104  | 0.075776  |
| 6                 | 0.761541  | 1.652398  | 0.634505  |
| 1                 | 0.351765  | 2.601257  | 0.258861  |
| 6                 | 0.825245  | 1.700724  | 2.173274  |
| 1                 | 1.230737  | 0.756231  | 2.562773  |
| 1                 | -0.179436 | 1.849994  | 2.591115  |
| 1                 | 1.467642  | 2.528666  | 2.501253  |
| 6                 | -1.335621 | 0.736701  | 0.000964  |
| 6                 | -2.050842 | 2.078406  | 0.042602  |
| 1                 | -1.979965 | 2.529060  | 1.043474  |
| 1                 | -1.603922 | 2.797689  | -0.661422 |
| 6                 | -3.492516 | 1.689105  | -0.327157 |
| 1                 | -4.239934 | 2.437233  | -0.032293 |
| 6                 | -3.483017 | 1.343375  | -1.831213 |
| 1                 | -4.500875 | 1.216216  | -2.222783 |
| 1                 | -3.005770 | 2.137455  | -2.422129 |
| 6                 | -2.684698 | 0.011081  | -1.868741 |
| 1                 | -1.760148 | 0.071264  | -2.459494 |
| 1                 | -3.277324 | -0.816339 | -2.283691 |
| 6                 | -2.372590 | -0.304855 | -0.366062 |
| 6                 | -2.040335 | -1.753977 | -0.085704 |
| 1                 | -1.291904 | -2.136888 | -0.794132 |
| 1                 | -2.939522 | -2.375719 | -0.201583 |
| 1                 | -1.652399 | -1.896425 | 0.933618  |
| 6                 | -3.641516 | 0.298544  | 0.355163  |
| 6                 | -4.949102 | -0.420551 | 0.011224  |
| 1                 | -5.798246 | 0.148675  | 0.418855  |
| 1                 | -4.975079 | -1.419945 | 0.469558  |
| 1                 | -5.116864 | -0.542781 | -1.065557 |
| 6                 | -3.507053 | 0.322839  | 1.884136  |
| 1                 | -2.560653 | 0.752651  | 2.239305  |
| 1                 | -3.567209 | -0.699088 | 2.286478  |
| 1                 | -4.327881 | 0.904071  | 2.329954  |

| RE_PIC_Zn in CHCl <sub>3</sub> |           |           |           |
|--------------------------------|-----------|-----------|-----------|
| Atomic Number                  | x         | y         | z         |
| 30                             | -1.113253 | -1.184672 | 0.181822  |
| 17                             | -1.452312 | -2.502218 | -1.639977 |
| 17                             | -1.000071 | -2.082828 | 2.263564  |
| 7                              | -2.594212 | 0.289135  | -0.123075 |
| 7                              | 0.100450  | 0.562747  | 0.227219  |
| 6                              | -3.846479 | 0.056401  | -0.552838 |
| 1                              | -4.141701 | -0.992036 | -0.616737 |
| 6                              | -4.705666 | 1.088150  | -0.913302 |
| 1                              | -5.715963 | 0.863629  | -1.253629 |
| 6                              | -4.235811 | 2.401890  | -0.840978 |
| 1                              | -4.876835 | 3.235847  | -1.130178 |
| 6                              | -2.933587 | 2.636348  | -0.404221 |
| 1                              | -2.533734 | 3.649341  | -0.342818 |
| 6                              | -2.135278 | 1.548819  | -0.042759 |
| 6                              | -0.742644 | 1.734114  | 0.527667  |
| 1                              | -0.312337 | 2.645747  | 0.084321  |
| 6                              | -0.840383 | 1.904646  | 2.056479  |
| 1                              | -1.479739 | 2.762189  | 2.305164  |
| 1                              | 0.156698  | 2.070621  | 2.485858  |
| 1                              | -1.265936 | 0.996539  | 2.506253  |
| 6                              | 1.367689  | 0.736433  | 0.104925  |
| 6                              | 2.121262  | 2.057432  | 0.114092  |
| 1                              | 1.946443  | 2.637651  | 1.032109  |
| 1                              | 1.785737  | 2.683787  | -0.727219 |
| 6                              | 3.582029  | 1.598384  | -0.040497 |
| 1                              | 4.257223  | 2.386600  | -0.399011 |
| 6                              | 3.979928  | 0.969836  | 1.311038  |
| 1                              | 3.747761  | 1.640664  | 2.150066  |
| 1                              | 5.055893  | 0.755953  | 1.356949  |
| 6                              | 3.134745  | -0.332280 | 1.336179  |
| 1                              | 2.413935  | -0.373319 | 2.164762  |
| 1                              | 3.760551  | -1.232530 | 1.412439  |
| 6                              | 2.399586  | -0.358734 | -0.050877 |
| 6                              | 1.909078  | -1.729854 | -0.456057 |
| 1                              | 1.325801  | -2.197624 | 0.351792  |
| 1                              | 2.763336  | -2.394676 | -0.648708 |
| 1                              | 1.284668  | -1.703436 | -1.359279 |
| 6                              | 3.446622  | 0.362996  | -0.980620 |
| 6                              | 4.751686  | -0.416609 | -1.165808 |
| 1                              | 4.584190  | -1.308998 | -1.786219 |
| 1                              | 5.207059  | -0.746700 | -0.224326 |
| 1                              | 5.486803  | 0.213484  | -1.689203 |
| 6                              | 2.886999  | 0.684477  | -2.373261 |
| 1                              | 3.581745  | 1.336489  | -2.923544 |
| 1                              | 1.906276  | 1.179156  | -2.351851 |
| 1                              | 2.767907  | -0.240285 | -2.956607 |

| SE_PIC_Zn in CHCl <sub>3</sub> |           |           |           |
|--------------------------------|-----------|-----------|-----------|
| Atomic Number                  | x         | y         | z         |
| 30                             | 1.120898  | -1.230633 | 0.079238  |
| 17                             | 1.216524  | -2.245671 | 2.107318  |
| 17                             | 1.124220  | -2.219181 | -1.970473 |
| 7                              | 2.619057  | 0.243485  | -0.108439 |
| 7                              | -0.084440 | 0.518796  | 0.221586  |
| 6                              | 3.876923  | 0.040644  | -0.536901 |
| 1                              | 4.169530  | -0.999681 | -0.687458 |
| 6                              | 4.750319  | 1.092864  | -0.787660 |
| 1                              | 5.764048  | 0.891008  | -1.131902 |
| 6                              | 4.290696  | 2.398630  | -0.599550 |
| 1                              | 4.943398  | 3.249732  | -0.798638 |
| 6                              | 2.983835  | 2.603536  | -0.162251 |
| 1                              | 2.591875  | 3.610175  | -0.010868 |
| 6                              | 2.169522  | 1.495302  | 0.081961  |
| 6                              | 0.767751  | 1.646929  | 0.641134  |
| 1                              | 0.362663  | 2.601765  | 0.273886  |
| 6                              | 0.830447  | 1.678512  | 2.180649  |
| 1                              | 1.223454  | 0.724249  | 2.559010  |
| 1                              | -0.173470 | 1.833151  | 2.598753  |
| 1                              | 1.481403  | 2.495658  | 2.519309  |
| 6                              | -1.330829 | 0.739962  | -0.001109 |
| 6                              | -2.047385 | 2.081809  | 0.049156  |
| 1                              | -1.976657 | 2.525636  | 1.053211  |
| 1                              | -1.602040 | 2.805891  | -0.651122 |
| 6                              | -3.488644 | 1.692818  | -0.322593 |
| 1                              | -4.237410 | 2.438572  | -0.024176 |
| 6                              | -3.478679 | 1.354758  | -1.828617 |
| 1                              | -4.496661 | 1.231170  | -2.221212 |
| 1                              | -3.001340 | 2.151970  | -2.415595 |
| 6                              | -2.681262 | 0.021962  | -1.873370 |
| 1                              | -1.757395 | 0.081945  | -2.464993 |
| 1                              | -3.275021 | -0.803014 | -2.291438 |
| 6                              | -2.367432 | -0.300972 | -0.372967 |
| 6                              | -2.032580 | -1.751136 | -0.099557 |
| 1                              | -1.291472 | -2.132522 | -0.816420 |
| 1                              | -2.932890 | -2.372601 | -0.208594 |
| 1                              | -1.634128 | -1.897409 | 0.915141  |
| 6                              | -3.635726 | 0.298430  | 0.352616  |
| 6                              | -4.943756 | -0.418656 | 0.006371  |
| 1                              | -5.792970 | 0.146431  | 0.419800  |
| 1                              | -4.968002 | -1.421398 | 0.457219  |
| 1                              | -5.113550 | -0.533457 | -1.070918 |
| 6                              | -3.499269 | 0.313965  | 1.881519  |
| 1                              | -2.551621 | 0.740234  | 2.237693  |
| 1                              | -3.557917 | -0.710301 | 2.277734  |
| 1                              | -4.319309 | 0.892139  | 2.333030  |

| 4RE-PIC-Zn (molecular crystal) (1/4) |           |           |           |
|--------------------------------------|-----------|-----------|-----------|
| Atomic Number                        | x         | y         | z         |
| 30                                   | 8.688491  | 5.077251  | 0.117480  |
| 30                                   | 7.763252  | 7.420649  | 6.702781  |
| 30                                   | 2.279338  | 11.326200 | 6.467821  |
| 30                                   | 3.204576  | 1.171699  | 13.053123 |
| 17                                   | 10.074957 | 6.814044  | 0.181045  |
| 17                                   | 6.376786  | 5.683856  | 6.766346  |
| 17                                   | 0.892872  | 0.565094  | 6.404255  |
| 17                                   | 4.591043  | 11.932805 | 12.989557 |
| 17                                   | 6.529121  | 5.564804  | 12.924833 |
| 17                                   | 9.922622  | 6.933095  | 6.339533  |
| 17                                   | 4.438707  | 11.813754 | 6.831069  |
| 17                                   | 1.045206  | 0.684145  | 0.245768  |
| 7                                    | 9.138787  | 4.056236  | 1.852596  |
| 7                                    | 7.312956  | 8.441663  | 8.437898  |
| 7                                    | 1.829041  | 10.305185 | 4.732705  |
| 7                                    | 3.654873  | 2.192714  | 11.318006 |
| 7                                    | 9.030954  | 3.210007  | 12.453667 |
| 7                                    | 7.420788  | 9.287892  | 5.868366  |
| 7                                    | 1.936874  | 9.458956  | 7.302236  |
| 7                                    | 3.547040  | 3.038943  | 0.716935  |
| 6                                    | 9.452257  | 4.606247  | 3.040786  |
| 6                                    | 6.999486  | 7.891652  | 9.626086  |
| 6                                    | 1.515572  | 10.855196 | 3.544516  |
| 6                                    | 3.968342  | 1.642702  | 10.129816 |
| 6                                    | 9.820720  | 3.833790  | 4.132959  |
| 6                                    | 6.631024  | 8.664109  | 10.718261 |
| 6                                    | 1.147109  | 10.082740 | 2.452342  |
| 6                                    | 4.336805  | 2.415159  | 9.037642  |
| 6                                    | 9.891576  | 2.446332  | 3.974427  |
| 6                                    | 6.560168  | 10.051567 | 10.559728 |
| 6                                    | 1.076254  | 8.695282  | 2.610874  |
| 6                                    | 4.407660  | 3.802617  | 9.196175  |
| 6                                    | 9.598579  | 1.887515  | 2.731373  |
| 6                                    | 6.853164  | 10.610384 | 9.316674  |
| 6                                    | 1.369249  | 8.136464  | 3.853928  |
| 6                                    | 4.114665  | 4.361434  | 10.439228 |
| 6                                    | 9.214404  | 2.723990  | 1.681675  |
| 6                                    | 7.237339  | 9.773910  | 8.266975  |
| 6                                    | 1.753425  | 8.972939  | 4.903626  |
| 6                                    | 3.730490  | 3.524959  | 11.488928 |
| 6                                    | 8.812479  | 2.183017  | 0.322932  |
| 6                                    | 7.639264  | 10.314882 | 6.908234  |
| 6                                    | 2.155350  | 8.431966  | 6.262369  |
| 6                                    | 3.328565  | 4.065932  | 12.847670 |
| 6                                    | 7.324607  | 1.791233  | 0.339829  |
| 6                                    | 9.127136  | 10.706666 | 6.925130  |

| 4RE-PIC-Zn (molecular crystal) (2/4) |           |           |           |  |
|--------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                        | x         | y         | z         |  |
| 6                                    | 3.643222  | 8.040183  | 6.245472  |  |
| 6                                    | 1.840693  | 4.457716  | 12.830773 |  |
| 6                                    | 9.221020  | 2.831762  | 11.238194 |  |
| 6                                    | 7.230722  | 9.666138  | 4.652894  |  |
| 6                                    | 1.746808  | 9.080712  | 8.517708  |  |
| 6                                    | 3.737107  | 3.417187  | 1.932407  |  |
| 6                                    | 9.360722  | 1.406796  | 10.724175 |  |
| 6                                    | 7.091022  | 11.091103 | 4.138874  |  |
| 6                                    | 1.607107  | 7.655746  | 9.031728  |  |
| 6                                    | 3.876807  | 4.842153  | 2.446427  |  |
| 6                                    | 9.384720  | 1.617402  | 9.200089  |  |
| 6                                    | 7.067022  | 10.880497 | 2.614787  |  |
| 6                                    | 1.583108  | 7.866352  | 10.555815 |  |
| 6                                    | 3.900807  | 4.631547  | 3.970514  |  |
| 6                                    | 7.955284  | 2.037623  | 8.799021  |  |
| 6                                    | 8.496460  | 10.460276 | 2.213721  |  |
| 6                                    | 3.012546  | 8.286572  | 10.956882 |  |
| 6                                    | 2.471369  | 4.211326  | 4.371580  |  |
| 6                                    | 7.843390  | 3.464340  | 9.399989  |  |
| 6                                    | 8.608354  | 9.033560  | 2.814688  |  |
| 6                                    | 3.124439  | 9.713289  | 10.355914 |  |
| 6                                    | 2.359476  | 2.784610  | 3.770613  |  |
| 6                                    | 9.254210  | 3.739784  | 10.030682 |  |
| 6                                    | 7.197535  | 8.758115  | 3.445381  |  |
| 6                                    | 1.713620  | 9.988734  | 9.725222  |  |
| 6                                    | 3.770295  | 2.509165  | 3.139920  |  |
| 6                                    | 9.558674  | 5.205901  | 10.232334 |  |
| 6                                    | 6.893069  | 7.291998  | 3.647034  |  |
| 6                                    | 1.409155  | 11.454851 | 9.523569  |  |
| 6                                    | 4.074760  | 1.043048  | 2.938267  |  |
| 6                                    | 10.193732 | 2.940578  | 9.060840  |  |
| 6                                    | 6.258010  | 9.557321  | 2.475539  |  |
| 6                                    | 0.774096  | 9.189528  | 10.695063 |  |
| 6                                    | 4.709819  | 3.308372  | 4.109762  |  |
| 6                                    | 10.218824 | 3.512719  | 7.644227  |  |
| 6                                    | 6.232919  | 8.985180  | 1.058925  |  |
| 6                                    | 0.749005  | 9.761669  | 12.111676 |  |
| 6                                    | 4.734910  | 2.736230  | 5.526376  |  |
| 6                                    | 0.672757  | 2.834383  | 9.551796  |  |
| 6                                    | 4.811157  | 9.663515  | 2.966495  |  |
| 6                                    | 10.295072 | 9.083333  | 10.204106 |  |
| 6                                    | 6.156672  | 3.414566  | 3.618806  |  |
| 1                                    | 9.406658  | 5.693874  | 3.093798  |  |
| 1                                    | 7.045085  | 6.804026  | 9.679099  |  |
| 1                                    | 1.561171  | 11.942823 | 3.491503  |  |
| 1                                    | 3.922744  | 0.555076  | 10.076804 |  |

| 4RE-PIC-Zn (molecular crystal) (3/4) |           |           |           |  |
|--------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                        | x         | y         | z         |  |
| 1                                    | 10.049806 | 4.323818  | 5.077895  |  |
| 1                                    | 6.401938  | 8.174081  | 11.663197 |  |
| 1                                    | 0.918023  | 10.572767 | 1.507406  |  |
| 1                                    | 4.565891  | 1.925132  | 8.092707  |  |
| 1                                    | 10.210032 | 1.807944  | 4.801660  |  |
| 1                                    | 6.241711  | 10.689956 | 11.386960 |  |
| 1                                    | 0.757797  | 8.056893  | 1.783641  |  |
| 1                                    | 4.726119  | 4.441006  | 8.368942  |  |
| 1                                    | 9.686260  | 0.814627  | 2.561004  |  |
| 1                                    | 6.765482  | 11.683272 | 9.146305  |  |
| 1                                    | 1.281568  | 7.063576  | 4.024297  |  |
| 1                                    | 4.202347  | 5.434323  | 10.609597 |  |
| 1                                    | 9.438138  | 1.300139  | 0.121902  |  |
| 1                                    | 7.013605  | 11.197761 | 6.707202  |  |
| 1                                    | 1.529691  | 7.549088  | 6.463399  |  |
| 1                                    | 3.954224  | 4.948811  | 13.048701 |  |
| 1                                    | 7.125567  | 1.073311  | 1.144391  |  |
| 1                                    | 9.326176  | 11.424588 | 7.729693  |  |
| 1                                    | 3.842262  | 7.322260  | 5.440910  |  |
| 1                                    | 1.641653  | 5.175639  | 12.026211 |  |
| 1                                    | 7.023717  | 1.323475  | 12.565237 |  |
| 1                                    | 9.428027  | 11.174424 | 5.979937  |  |
| 1                                    | 3.944112  | 7.572424  | 7.190666  |  |
| 1                                    | 1.539802  | 4.925474  | 0.605365  |  |
| 1                                    | 6.698877  | 2.680232  | 0.494351  |  |
| 1                                    | 9.752867  | 9.817666  | 7.079652  |  |
| 1                                    | 4.268952  | 8.929181  | 6.090950  |  |
| 1                                    | 1.214962  | 3.568717  | 12.676251 |  |
| 1                                    | 8.544879  | 0.750539  | 11.060648 |  |
| 1                                    | 7.906865  | 11.747360 | 4.475347  |  |
| 1                                    | 2.422951  | 6.999489  | 8.695255  |  |
| 1                                    | 3.060964  | 5.498411  | 2.109954  |  |
| 1                                    | 10.294639 | 0.973363  | 11.117342 |  |
| 1                                    | 6.157104  | 11.524535 | 4.532040  |  |
| 1                                    | 0.673189  | 7.222312  | 8.638561  |  |
| 1                                    | 4.810726  | 5.275587  | 2.053261  |  |
| 1                                    | 9.803580  | 0.776266  | 8.635740  |  |
| 1                                    | 6.648163  | 11.721633 | 2.050439  |  |
| 1                                    | 1.164249  | 7.025216  | 11.120163 |  |
| 1                                    | 4.319665  | 5.472683  | 4.534862  |  |
| 1                                    | 7.198960  | 1.354025  | 9.210221  |  |
| 1                                    | 9.252783  | 11.143873 | 2.624920  |  |
| 1                                    | 3.768868  | 7.602975  | 10.545681 |  |
| 1                                    | 1.715045  | 4.894925  | 3.960381  |  |
| 1                                    | 7.820354  | 2.045607  | 7.708924  |  |
| 1                                    | 8.631389  | 10.452291 | 1.123623  |  |

| 4RE-PIC-Zn (molecular crystal) (4/4) |           |           |           |  |
|--------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                        | x         | y         | z         |  |
| 1                                    | 3.147475  | 8.294557  | 12.046979 |  |
| 1                                    | 2.336440  | 4.203343  | 5.461678  |  |
| 1                                    | 7.051203  | 3.565839  | 10.153137 |  |
| 1                                    | 9.400539  | 8.932060  | 3.567836  |  |
| 1                                    | 3.916625  | 9.814788  | 9.602766  |  |
| 1                                    | 1.567289  | 2.683111  | 3.017465  |  |
| 1                                    | 7.648909  | 4.220510  | 8.626948  |  |
| 1                                    | 8.802834  | 8.277389  | 2.041647  |  |
| 1                                    | 3.318919  | 10.469460 | 11.128955 |  |
| 1                                    | 2.164995  | 2.028440  | 4.543653  |  |
| 1                                    | 8.778670  | 5.712549  | 10.817930 |  |
| 1                                    | 7.673072  | 6.785350  | 4.232628  |  |
| 1                                    | 2.189158  | 11.961498 | 8.937972  |  |
| 1                                    | 3.294757  | 0.536401  | 2.352672  |  |
| 1                                    | 9.601843  | 5.714679  | 9.258217  |  |
| 1                                    | 6.849900  | 6.783220  | 2.672915  |  |
| 1                                    | 1.365986  | 11.963629 | 10.497686 |  |
| 1                                    | 4.117929  | 0.534271  | 3.912386  |  |
| 1                                    | 10.512383 | 5.364223  | 10.750675 |  |
| 1                                    | 5.939360  | 7.133677  | 4.165375  |  |
| 1                                    | 0.455446  | 11.613173 | 9.005227  |  |
| 1                                    | 5.028469  | 0.884726  | 2.419926  |  |
| 1                                    | 10.690947 | 4.504350  | 7.632350  |  |
| 1                                    | 5.760796  | 7.993549  | 1.047050  |  |
| 1                                    | 0.276882  | 10.753300 | 12.123552 |  |
| 1                                    | 5.207032  | 1.744599  | 5.538251  |  |
| 1                                    | 9.223734  | 3.630428  | 7.198555  |  |
| 1                                    | 7.228009  | 8.867472  | 0.613254  |  |
| 1                                    | 1.744094  | 9.879377  | 12.557347 |  |
| 1                                    | 3.739820  | 2.618522  | 5.972047  |  |
| 1                                    | 10.814113 | 2.851405  | 7.001686  |  |
| 1                                    | 5.637630  | 9.646494  | 0.416385  |  |
| 1                                    | 0.153717  | 9.100355  | 12.754217 |  |
| 1                                    | 5.330198  | 3.397544  | 6.168916  |  |
| 1                                    | 1.229086  | 2.139302  | 8.908464  |  |
| 1                                    | 4.254828  | 10.358597 | 2.323162  |  |
| 1                                    | 9.738743  | 8.388250  | 10.847439 |  |
| 1                                    | 6.713001  | 4.109648  | 4.262138  |  |
| 1                                    | 0.764589  | 2.484139  | 10.588341 |  |
| 1                                    | 4.719325  | 10.013759 | 4.003039  |  |
| 1                                    | 10.203240 | 8.733088  | 9.167562  |  |
| 1                                    | 6.248504  | 3.764810  | 2.582262  |  |
| 1                                    | 1.171300  | 3.812212  | 9.489895  |  |
| 1                                    | 4.312614  | 8.685686  | 2.904594  |  |
| 1                                    | 9.796529  | 10.061162 | 10.266007 |  |
| 1                                    | 6.655215  | 2.436737  | 3.680707  |  |

| 4SE-PIC-Zn (molecular crystal) (1/4) |          |          |           |
|--------------------------------------|----------|----------|-----------|
| Atomic Number                        | x        | y        | z         |
| 30                                   | 1.801980 | 2.566243 | 2.799814  |
| 30                                   | 3.022892 | 7.828524 | 11.702252 |
| 30                                   | 7.847764 | 7.763628 | 6.102624  |
| 30                                   | 6.626853 | 2.631141 | 15.005062 |
| 17                                   | 2.024400 | 4.738997 | 2.331877  |
| 17                                   | 2.800472 | 5.655769 | 11.234316 |
| 17                                   | 7.625344 | 9.936381 | 6.570560  |
| 17                                   | 6.849272 | 0.458386 | 15.472999 |
| 17                                   | 3.161165 | 1.091863 | 1.823829  |
| 17                                   | 1.663706 | 9.302905 | 10.726267 |
| 17                                   | 6.488578 | 6.289246 | 7.078609  |
| 17                                   | 7.986037 | 4.105521 | 15.981048 |
| 7                                    | 9.484334 | 2.048493 | 2.429337  |
| 7                                    | 4.990282 | 8.346274 | 11.331775 |
| 7                                    | 0.165410 | 7.245877 | 6.473102  |
| 7                                    | 4.659462 | 3.148891 | 15.375540 |
| 7                                    | 1.250289 | 2.173301 | 4.748638  |
| 7                                    | 3.574583 | 8.221466 | 13.651075 |
| 7                                    | 8.399455 | 7.370685 | 4.153800  |
| 7                                    | 6.075161 | 3.024083 | 13.056239 |
| 6                                    | 8.914706 | 1.844167 | 1.224408  |
| 6                                    | 5.559910 | 8.550601 | 10.126846 |
| 6                                    | 0.735038 | 7.041551 | 7.678030  |
| 6                                    | 4.089834 | 3.353217 | 16.580467 |
| 6                                    | 7.591787 | 1.443928 | 1.094420  |
| 6                                    | 6.882829 | 8.950839 | 9.996858  |
| 6                                    | 2.057956 | 6.641312 | 7.808018  |
| 6                                    | 2.766915 | 3.753455 | 16.710457 |
| 6                                    | 6.838958 | 1.241637 | 2.254652  |
| 6                                    | 7.635658 | 9.153131 | 11.157090 |
| 6                                    | 2.810786 | 6.439021 | 6.647786  |
| 6                                    | 2.014086 | 3.955746 | 15.550224 |
| 6                                    | 7.435048 | 1.441533 | 3.497256  |
| 6                                    | 7.039568 | 8.953236 | 12.399693 |
| 6                                    | 2.214696 | 6.638916 | 5.405182  |
| 6                                    | 2.610176 | 3.755851 | 14.307621 |
| 6                                    | 8.766281 | 1.859342 | 3.552536  |
| 6                                    | 5.708335 | 8.535426 | 12.454975 |
| 6                                    | 0.883463 | 7.056726 | 5.349901  |
| 6                                    | 3.941409 | 3.338042 | 14.252339 |
| 6                                    | 9.430852 | 2.167724 | 4.879146  |
| 6                                    | 5.043765 | 8.227044 | 13.781585 |
| 6                                    | 0.218893 | 7.365108 | 4.023292  |
| 6                                    | 4.605979 | 3.029660 | 12.925730 |
| 6                                    | 8.978588 | 3.551449 | 5.388196  |
| 6                                    | 5.496028 | 6.843320 | 14.290634 |

| 4SE-PIC-Zn (molecular crystal) (2/4) |          |           |           |  |
|--------------------------------------|----------|-----------|-----------|--|
| Atomic Number                        | x        | y         | z         |  |
| 6                                    | 0.671156 | 8.748833  | 3.514241  |  |
| 6                                    | 4.153717 | 1.645935  | 12.416680 |  |
| 6                                    | 1.959836 | 1.746891  | 5.735962  |  |
| 6                                    | 2.865036 | 8.647877  | 14.638401 |  |
| 6                                    | 7.689907 | 6.944275  | 3.166476  |  |
| 6                                    | 6.784709 | 3.450493  | 12.068913 |  |
| 6                                    | 1.457631 | 1.074919  | 7.000531  |  |
| 6                                    | 3.367242 | 9.319848  | 15.902969 |  |
| 6                                    | 8.192113 | 6.272303  | 1.901908  |  |
| 6                                    | 6.282503 | 4.122465  | 10.804346 |  |
| 6                                    | 2.774006 | 0.700548  | 7.697419  |  |
| 6                                    | 2.050866 | 9.694220  | 16.599857 |  |
| 6                                    | 6.875738 | 5.897932  | 1.205019  |  |
| 6                                    | 7.598878 | 4.496836  | 10.107456 |  |
| 6                                    | 3.409880 | 9.967157  | 6.855566  |  |
| 6                                    | 1.414992 | 0.427611  | 15.758004 |  |
| 6                                    | 6.239864 | 4.769773  | 2.046872  |  |
| 6                                    | 8.234752 | 5.624994  | 10.949310 |  |
| 6                                    | 3.888184 | 0.308309  | 5.575993  |  |
| 6                                    | 0.936688 | 10.086458 | 14.478431 |  |
| 6                                    | 5.761560 | 5.505693  | 3.326445  |  |
| 6                                    | 8.713057 | 4.889075  | 12.228884 |  |
| 6                                    | 3.472157 | 1.794653  | 5.814139  |  |
| 6                                    | 1.352715 | 8.600115  | 14.716578 |  |
| 6                                    | 6.177586 | 6.992037  | 3.088299  |  |
| 6                                    | 8.297029 | 3.402731  | 11.990736 |  |
| 6                                    | 4.181219 | 2.820834  | 4.954368  |  |
| 6                                    | 0.643653 | 7.573935  | 13.856806 |  |
| 6                                    | 5.468525 | 8.018217  | 3.948070  |  |
| 6                                    | 9.006091 | 2.376550  | 12.850509 |  |
| 6                                    | 3.667737 | 1.926827  | 7.374675  |  |
| 6                                    | 1.157135 | 8.467940  | 16.277113 |  |
| 6                                    | 5.982007 | 7.124211  | 1.527763  |  |
| 6                                    | 8.492609 | 3.270557  | 10.430202 |  |
| 6                                    | 5.109551 | 1.751998  | 7.841297  |  |
| 6                                    | 9.365066 | 8.642770  | 16.743736 |  |
| 6                                    | 4.540193 | 6.949382  | 1.061141  |  |
| 6                                    | 0.284679 | 3.445386  | 9.963579  |  |
| 6                                    | 3.168092 | 3.264860  | 7.927598  |  |
| 6                                    | 1.656780 | 7.129907  | 16.830036 |  |
| 6                                    | 6.481653 | 8.462244  | 0.974840  |  |
| 6                                    | 7.992963 | 1.932523  | 9.877278  |  |
| 1                                    | 9.549437 | 2.020190  | 0.355560  |  |
| 1                                    | 4.925180 | 8.374578  | 9.257998  |  |
| 1                                    | 0.100308 | 7.217573  | 8.546879  |  |
| 1                                    | 4.724564 | 3.177195  | 17.449316 |  |

| 4SE-PIC-Zn (molecular crystal) (3/4) |          |           |           |  |
|--------------------------------------|----------|-----------|-----------|--|
| Atomic Number                        | x        | y         | z         |  |
| 1                                    | 7.172998 | 1.281919  | 0.101161  |  |
| 1                                    | 7.301618 | 9.112848  | 9.003599  |  |
| 1                                    | 2.476747 | 6.479302  | 8.801277  |  |
| 1                                    | 2.348126 | 3.915465  | 17.703714 |  |
| 1                                    | 5.788768 | 0.950900  | 2.191350  |  |
| 1                                    | 8.685848 | 9.443869  | 11.093788 |  |
| 1                                    | 3.860977 | 6.148283  | 6.711089  |  |
| 1                                    | 0.963895 | 4.246484  | 15.613526 |  |
| 1                                    | 6.890739 | 1.269622  | 4.424805  |  |
| 1                                    | 7.583877 | 9.125146  | 13.327243 |  |
| 1                                    | 2.759004 | 6.467006  | 4.477633  |  |
| 1                                    | 2.065868 | 3.927762  | 13.380072 |  |
| 1                                    | 9.101175 | 1.396128  | 5.591576  |  |
| 1                                    | 5.373441 | 8.998640  | 14.494013 |  |
| 1                                    | 0.548568 | 6.593513  | 3.310863  |  |
| 1                                    | 4.276303 | 3.801255  | 12.213302 |  |
| 1                                    | 9.294374 | 4.333068  | 4.684520  |  |
| 1                                    | 5.180242 | 6.061700  | 13.586957 |  |
| 1                                    | 0.355370 | 9.530451  | 4.217919  |  |
| 1                                    | 4.469502 | 0.864316  | 13.120358 |  |
| 1                                    | 9.427508 | 3.765495  | 6.367025  |  |
| 1                                    | 5.047108 | 6.629273  | 15.269463 |  |
| 1                                    | 0.222236 | 8.962879  | 2.535414  |  |
| 1                                    | 4.602636 | 1.431889  | 11.437852 |  |
| 1                                    | 7.887602 | 3.594539  | 5.496530  |  |
| 1                                    | 6.587014 | 6.800229  | 14.398968 |  |
| 1                                    | 1.762143 | 8.791923  | 3.405908  |  |
| 1                                    | 3.062729 | 1.602845  | 12.308347 |  |
| 1                                    | 0.850168 | 1.766342  | 7.602560  |  |
| 1                                    | 3.974704 | 8.628426  | 16.504997 |  |
| 1                                    | 8.799576 | 6.963727  | 1.299879  |  |
| 1                                    | 5.675040 | 3.431042  | 10.202317 |  |
| 1                                    | 0.805822 | 0.215038  | 6.779992  |  |
| 1                                    | 4.019050 | 10.179729 | 15.682431 |  |
| 1                                    | 8.843923 | 5.412422  | 2.122446  |  |
| 1                                    | 5.630694 | 4.982346  | 11.024883 |  |
| 1                                    | 2.655114 | 0.460668  | 8.760343  |  |
| 1                                    | 2.169758 | 9.934098  | 17.662781 |  |
| 1                                    | 6.994629 | 5.658052  | 0.142096  |  |
| 1                                    | 7.479987 | 4.736715  | 9.044534  |  |
| 1                                    | 4.251972 | 9.488407  | 7.371727  |  |
| 1                                    | 0.572900 | 0.906361  | 16.274164 |  |
| 1                                    | 5.397772 | 4.291022  | 1.530712  |  |
| 1                                    | 9.076843 | 6.103745  | 10.433149 |  |
| 1                                    | 2.679708 | 9.179439  | 6.639004  |  |
| 1                                    | 2.145164 | 1.215329  | 15.541442 |  |

| 4SE-PIC-Zn (molecular crystal) (4/4) |          |           |           |
|--------------------------------------|----------|-----------|-----------|
| Atomic Number                        | x        | y         | z         |
| 1                                    | 6.970037 | 3.982055  | 2.263434  |
| 1                                    | 7.504580 | 6.412713  | 11.165873 |
| 1                                    | 3.455323 | 10.315536 | 4.644737  |
| 1                                    | 1.369549 | 0.079233  | 13.547173 |
| 1                                    | 6.194421 | 5.118151  | 4.257701  |
| 1                                    | 8.280195 | 5.276617  | 13.160141 |
| 1                                    | 4.980378 | 0.254310  | 5.469736  |
| 1                                    | 9.494238 | 10.140458 | 14.372173 |
| 1                                    | 4.669366 | 5.451694  | 3.432703  |
| 1                                    | 0.155506 | 4.943074  | 12.335141 |
| 1                                    | 4.216334 | 2.525377  | 3.896954  |
| 1                                    | 0.608537 | 7.869390  | 12.799391 |
| 1                                    | 5.433410 | 7.722761  | 5.005485  |
| 1                                    | 9.041206 | 2.672007  | 13.907924 |
| 1                                    | 5.221558 | 2.934950  | 5.289921  |
| 1                                    | 9.253057 | 7.459818  | 14.192358 |
| 1                                    | 4.428186 | 8.132333  | 3.612517  |
| 1                                    | 0.396686 | 2.262434  | 12.514956 |
| 1                                    | 3.698645 | 3.805093  | 5.017127  |
| 1                                    | 1.126227 | 6.589674  | 13.919565 |
| 1                                    | 5.951099 | 9.002477  | 3.885312  |
| 1                                    | 8.523516 | 1.392291  | 12.787749 |
| 1                                    | 5.116228 | 1.669227  | 8.937800  |
| 1                                    | 9.358389 | 8.725541  | 0.035361  |
| 1                                    | 4.533517 | 6.866611  | 17.769514 |
| 1                                    | 0.291355 | 3.528157  | 8.867076  |
| 1                                    | 5.720928 | 2.627583  | 7.577775  |
| 1                                    | 8.753687 | 7.767185  | 16.480215 |
| 1                                    | 3.928816 | 7.824967  | 1.324663  |
| 1                                    | 0.896056 | 2.569801  | 10.227099 |
| 1                                    | 5.611662 | 0.862282  | 7.449835  |
| 1                                    | 8.862955 | 9.532485  | 16.352274 |
| 1                                    | 4.038082 | 6.059666  | 1.452603  |
| 1                                    | 0.786790 | 4.335101  | 10.355042 |
| 1                                    | 2.190677 | 3.574586  | 7.537277  |
| 1                                    | 2.634195 | 6.820182  | 16.439716 |
| 1                                    | 7.459066 | 8.771970  | 1.365161  |
| 1                                    | 7.015550 | 1.622798  | 10.267598 |
| 1                                    | 3.881364 | 4.059324  | 7.672424  |
| 1                                    | 0.943508 | 6.335443  | 16.574862 |
| 1                                    | 5.768381 | 9.256707  | 1.230014  |
| 1                                    | 8.706235 | 1.138060  | 10.132452 |
| 1                                    | 3.094910 | 3.237261  | 9.023504  |
| 1                                    | 1.729962 | 7.157507  | 0.121066  |
| 1                                    | 6.554834 | 8.434645  | 17.683811 |
| 1                                    | 7.919782 | 1.960123  | 8.781373  |

| 2RE-PIC-Zn / 2SE-PIC-Zn (molecular crystal) (1/4) |           |           |           |  |
|---------------------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                                     | x         | y         | z         |  |
| 30                                                | 1.616065  | 11.890268 | 3.674266  |  |
| 30                                                | 9.594472  | 5.277227  | 9.570506  |  |
| 30                                                | 7.731150  | 6.314360  | 3.737077  |  |
| 30                                                | 3.479386  | 12.927402 | 9.507695  |  |
| 17                                                | 3.760561  | 11.264388 | 3.505903  |  |
| 17                                                | 7.449977  | 4.651346  | 9.738868  |  |
| 17                                                | 1.167317  | 0.838264  | 3.572996  |  |
| 17                                                | 10.043221 | 7.451305  | 9.671775  |  |
| 17                                                | 7.539300  | 4.104878  | 3.739938  |  |
| 17                                                | 3.671238  | 10.717920 | 9.504833  |  |
| 17                                                | 9.846885  | 7.071008  | 3.568785  |  |
| 17                                                | 1.363653  | 0.457966  | 9.675986  |  |
| 7                                                 | 0.703970  | 11.110545 | 5.361532  |  |
| 7                                                 | 10.506567 | 4.497502  | 7.883240  |  |
| 7                                                 | 0.458955  | 10.438900 | 2.736489  |  |
| 7                                                 | 10.751582 | 3.825859  | 10.508283 |  |
| 7                                                 | 6.715927  | 7.042243  | 5.390523  |  |
| 7                                                 | 4.494611  | 0.429201  | 7.854248  |  |
| 7                                                 | 6.587272  | 7.768443  | 2.764749  |  |
| 7                                                 | 4.623265  | 1.155400  | 10.480022 |  |
| 6                                                 | 0.691054  | 11.650372 | 6.595042  |  |
| 6                                                 | 10.519484 | 5.037331  | 6.649731  |  |
| 6                                                 | -0.059386 | 11.109493 | 7.630088  |  |
| 6                                                 | 11.269924 | 4.496450  | 5.614683  |  |
| 6                                                 | 11.485250 | 9.980650  | 7.371950  |  |
| 6                                                 | -0.274713 | 3.367608  | 5.872821  |  |
| 6                                                 | 11.493646 | 9.427238  | 6.093394  |  |
| 6                                                 | -0.283108 | 2.814197  | 7.151377  |  |
| 6                                                 | -0.037021 | 10.014621 | 5.107874  |  |
| 6                                                 | 11.247560 | 3.401579  | 8.136898  |  |
| 6                                                 | 0.066274  | 9.412503  | 3.723356  |  |
| 6                                                 | 11.144263 | 2.799462  | 9.521416  |  |
| 6                                                 | 1.098910  | 8.269879  | 3.723985  |  |
| 6                                                 | 10.111629 | 1.656837  | 9.520786  |  |
| 6                                                 | 0.030412  | 10.307485 | 1.530282  |  |
| 6                                                 | 11.180126 | 3.694443  | 11.714490 |  |
| 6                                                 | 11.413850 | 9.232713  | 1.018427  |  |
| 6                                                 | -0.203313 | 2.619671  | 12.226344 |  |
| 6                                                 | 10.127624 | 9.628923  | 12.790264 |  |
| 6                                                 | 1.082915  | 3.015881  | 0.454508  |  |
| 6                                                 | 9.271493  | 10.911804 | 12.784623 |  |
| 6                                                 | 1.939045  | 4.298762  | 0.460147  |  |
| 6                                                 | 11.357131 | 11.981844 | 0.108606  |  |
| 6                                                 | -0.146594 | 5.368803  | 13.136165 |  |
| 6                                                 | 0.363322  | 11.207703 | 0.358962  |  |
| 6                                                 | 10.847216 | 4.594661  | 12.885809 |  |

| 2RE-PIC-Zn / 2SE-PIC-Zn (molecular crystal) (2/4) |           |           |           |  |
|---------------------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                                     | x         | y         | z         |  |
| 6                                                 | 1.588536  | 12.085848 | 0.465032  |  |
| 6                                                 | 9.622003  | 5.472806  | 12.779740 |  |
| 6                                                 | -0.780483 | 10.153465 | 12.431827 |  |
| 6                                                 | 11.991020 | 3.540423  | 0.812945  |  |
| 6                                                 | 0.330593  | 9.101439  | 12.538713 |  |
| 6                                                 | 10.879944 | 2.488398  | 0.706058  |  |
| 6                                                 | -0.689032 | 10.765961 | 11.036046 |  |
| 6                                                 | 11.899570 | 4.152919  | 2.208725  |  |
| 6                                                 | 6.661818  | 6.482522  | 6.613730  |  |
| 6                                                 | 4.548720  | 13.095565 | 6.631041  |  |
| 6                                                 | 5.866071  | 7.000834  | 7.627287  |  |
| 6                                                 | 5.344466  | 0.387793  | 5.617484  |  |
| 6                                                 | 5.077835  | 8.122016  | 7.355111  |  |
| 6                                                 | 6.132702  | 1.508975  | 5.889660  |  |
| 6                                                 | 5.123056  | 8.690298  | 6.082702  |  |
| 6                                                 | 6.087481  | 2.077256  | 7.162069  |  |
| 6                                                 | 5.967916  | 8.129723  | 5.121666  |  |
| 6                                                 | 5.242622  | 1.516681  | 8.123104  |  |
| 6                                                 | 6.151813  | 8.768392  | 3.762325  |  |
| 6                                                 | 5.058724  | 2.155350  | 9.482447  |  |
| 6                                                 | 7.212743  | 9.881593  | 3.875664  |  |
| 6                                                 | 3.997795  | 3.268552  | 9.369108  |  |
| 6                                                 | 6.318369  | 8.004764  | 1.527407  |  |
| 6                                                 | 4.892169  | 1.391722  | 11.717364 |  |
| 6                                                 | 5.490707  | 9.152507  | 0.976138  |  |
| 6                                                 | 5.719831  | 2.539466  | 12.268634 |  |
| 6                                                 | 4.528470  | 8.965195  | 12.704031 |  |
| 6                                                 | 6.682068  | 2.352153  | 0.540740  |  |
| 6                                                 | 5.984140  | 9.348637  | 12.366711 |  |
| 6                                                 | 5.226397  | 2.735594  | 0.878060  |  |
| 6                                                 | 6.799413  | 8.187967  | 12.995375 |  |
| 6                                                 | 4.411126  | 1.574925  | 0.249396  |  |
| 6                                                 | 6.832628  | 7.221291  | 0.340790  |  |
| 6                                                 | 4.377910  | 0.608248  | 12.903981 |  |
| 6                                                 | 7.330337  | 5.820921  | 0.595097  |  |
| 6                                                 | 3.880201  | 12.433963 | 12.649673 |  |
| 6                                                 | 4.539498  | 7.418099  | 12.561084 |  |
| 6                                                 | 6.671039  | 0.805056  | 0.683687  |  |
| 6                                                 | 3.243838  | 6.731695  | 12.997195 |  |
| 6                                                 | 7.966700  | 0.118653  | 0.247575  |  |
| 6                                                 | 4.867020  | 6.943904  | 11.144318 |  |
| 6                                                 | 6.343518  | 0.330863  | 2.100453  |  |
| 1                                                 | 1.298767  | 12.544197 | 6.740940  |  |
| 1                                                 | 9.911771  | 5.931156  | 6.503832  |  |
| 1                                                 | -0.009198 | 11.576199 | 8.610899  |  |
| 1                                                 | 11.219735 | 4.963158  | 4.633871  |  |

| 2RE-PIC-Zn / 2SE-PIC-Zn (molecular crystal) (3/4) |           |           |           |  |
|---------------------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                                     | x         | y         | z         |  |
| 1                                                 | 10.877281 | 9.521708  | 8.153825  |  |
| 1                                                 | 0.333257  | 2.908666  | 5.090946  |  |
| 1                                                 | 10.891555 | 8.550546  | 5.845210  |  |
| 1                                                 | 0.318982  | 1.937505  | 7.399562  |  |
| 1                                                 | 11.409929 | 8.989861  | 3.474086  |  |
| 1                                                 | -0.199391 | 2.376821  | 9.770685  |  |
| 1                                                 | 1.145199  | 7.797764  | 2.733290  |  |
| 1                                                 | 10.065338 | 1.184721  | 10.511481 |  |
| 1                                                 | 0.806450  | 7.504056  | 4.453295  |  |
| 1                                                 | 10.404088 | 0.891013  | 8.791476  |  |
| 1                                                 | 2.095890  | 8.655688  | 3.978306  |  |
| 1                                                 | 9.114649  | 2.042645  | 9.266465  |  |
| 1                                                 | 10.473618 | 9.213045  | 1.589172  |  |
| 1                                                 | 0.736919  | 2.600003  | 11.655600 |  |
| 1                                                 | 11.849071 | 8.230711  | 1.141889  |  |
| 1                                                 | -0.638532 | 1.617667  | 12.102882 |  |
| 1                                                 | 9.757096  | 8.825929  | 12.144080 |  |
| 1                                                 | 1.453442  | 2.212887  | 1.100691  |  |
| 1                                                 | 9.495296  | 10.789371 | 0.164302  |  |
| 1                                                 | 1.715242  | 4.176330  | 13.080469 |  |
| 1                                                 | 8.921518  | 11.166323 | 11.775925 |  |
| 1                                                 | 2.289020  | 4.553282  | 1.468847  |  |
| 1                                                 | 10.996866 | 12.461143 | 1.027815  |  |
| 1                                                 | 0.213672  | 5.848101  | 12.216955 |  |
| 1                                                 | 10.436134 | 12.787217 | 12.632234 |  |
| 1                                                 | 0.774403  | 6.174174  | 0.612537  |  |
| 1                                                 | 1.446500  | 12.901879 | 1.186452  |  |
| 1                                                 | 9.764037  | 6.288837  | 12.058319 |  |
| 1                                                 | 0.681916  | 12.547376 | 12.734799 |  |
| 1                                                 | 10.528622 | 5.934334  | 0.509972  |  |
| 1                                                 | 2.471991  | 11.513814 | 0.774242  |  |
| 1                                                 | 8.738547  | 4.900772  | 12.470529 |  |
| 1                                                 | 1.301481  | 9.548801  | 12.283065 |  |
| 1                                                 | 9.909057  | 2.935759  | 0.961706  |  |
| 1                                                 | 0.140455  | 8.288902  | 11.823322 |  |
| 1                                                 | 11.070084 | 1.675860  | 1.421449  |  |
| 1                                                 | 1.545264  | 8.658234  | 0.294188  |  |
| 1                                                 | 9.665274  | 2.045193  | 12.950583 |  |
| 1                                                 | 0.305406  | 11.196321 | 10.858114 |  |
| 1                                                 | 10.905132 | 4.583279  | 2.386657  |  |
| 1                                                 | 10.896611 | 11.550721 | 10.841530 |  |
| 1                                                 | 0.313926  | 4.937679  | 2.403241  |  |
| 1                                                 | -0.846762 | 9.965778  | 10.300844 |  |
| 1                                                 | 12.057299 | 3.352737  | 2.943927  |  |
| 1                                                 | 7.276248  | 5.594769  | 6.770149  |  |
| 1                                                 | 3.934289  | 12.207810 | 6.474622  |  |

| 2RE-PIC-Zn / 2SE-PIC-Zn (molecular crystal) (4/4) |          |           |           |
|---------------------------------------------------|----------|-----------|-----------|
| Atomic Number                                     | x        | y         | z         |
| 1                                                 | 5.888800 | 6.526111  | 8.605832  |
| 1                                                 | 5.321738 | 13.139153 | 4.638940  |
| 1                                                 | 4.444619 | 8.566616  | 8.125070  |
| 1                                                 | 6.765918 | 1.953574  | 5.119702  |
| 1                                                 | 4.522964 | 9.565716  | 5.826581  |
| 1                                                 | 6.687574 | 2.952675  | 7.418190  |
| 1                                                 | 5.194834 | 9.221200  | 3.466359  |
| 1                                                 | 6.015703 | 2.608159  | 9.778412  |
| 1                                                 | 6.882749 | 10.641469 | 4.595441  |
| 1                                                 | 4.327788 | 4.028427  | 8.649330  |
| 1                                                 | 7.362551 | 10.370416 | 2.904076  |
| 1                                                 | 3.847987 | 3.757373  | 10.340694 |
| 1                                                 | 8.172204 | 9.458524  | 4.203723  |
| 1                                                 | 3.038334 | 2.845481  | 9.041048  |
| 1                                                 | 5.833769 | 10.132412 | 1.332790  |
| 1                                                 | 5.376770 | 3.519371  | 11.911981 |
| 1                                                 | 4.447892 | 9.064668  | 1.317817  |
| 1                                                 | 6.762646 | 2.451625  | 11.926953 |
| 1                                                 | 3.776067 | 9.484288  | 12.100044 |
| 1                                                 | 7.434470 | 2.871248  | 1.144727  |
| 1                                                 | 6.243935 | 10.324230 | 12.795809 |
| 1                                                 | 4.966603 | 3.711188  | 0.448962  |
| 1                                                 | 6.140353 | 9.428832  | 11.283695 |
| 1                                                 | 5.070185 | 2.815790  | 1.961075  |
| 1                                                 | 7.389102 | 7.641383  | 12.247042 |
| 1                                                 | 3.821435 | 1.028341  | 0.997730  |
| 1                                                 | 8.615015 | 8.509146  | 0.532590  |
| 1                                                 | 2.595522 | 1.896103  | 12.712181 |
| 1                                                 | 6.466803 | 5.337928  | 12.887042 |
| 1                                                 | 4.743735 | 11.950970 | 0.357729  |
| 1                                                 | 6.589171 | 5.208757  | 1.120701  |
| 1                                                 | 4.621366 | 11.821799 | 12.124070 |
| 1                                                 | 8.246984 | 5.820988  | 1.200354  |
| 1                                                 | 2.963554 | 12.434030 | 12.044417 |
| 1                                                 | 4.062464 | 6.949991  | 0.786772  |
| 1                                                 | 7.148073 | 0.336949  | 12.458000 |
| 1                                                 | 3.356533 | 5.642246  | 12.921421 |
| 1                                                 | 7.854005 | 12.255287 | 0.323350  |
| 1                                                 | 2.413839 | 7.024949  | 12.339877 |
| 1                                                 | 8.796700 | 0.411908  | 0.904894  |
| 1                                                 | 4.067124 | 7.259752  | 10.458479 |
| 1                                                 | 7.143413 | 0.646709  | 2.786293  |
| 1                                                 | 4.936328 | 5.848496  | 11.099509 |
| 1                                                 | 6.274209 | 12.461537 | 2.145262  |
| 1                                                 | 5.814201 | 7.335267  | 10.759016 |
| 1                                                 | 5.396336 | 0.722225  | 2.485755  |

| 2RE-PIC-Zn / 2SE-PIC-Zn / 4CHCl <sub>3</sub> (molecular crystal) (1/5) |           |           |           |  |
|------------------------------------------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                                                          | x         | y         | z         |  |
| 30                                                                     | 1.708606  | 11.977855 | 3.700437  |  |
| 30                                                                     | 9.939208  | 5.258602  | 9.718537  |  |
| 30                                                                     | 7.913460  | 6.497365  | 3.774607  |  |
| 30                                                                     | 3.734354  | 13.216618 | 9.644367  |  |
| 17                                                                     | 3.865971  | 11.454786 | 3.559837  |  |
| 17                                                                     | 7.781844  | 4.735533  | 9.859138  |  |
| 17                                                                     | 1.135075  | 0.704070  | 3.569445  |  |
| 17                                                                     | 10.512739 | 7.423322  | 9.849529  |  |
| 17                                                                     | 7.530715  | 4.297018  | 3.753597  |  |
| 17                                                                     | 4.117098  | 11.016271 | 9.665377  |  |
| 17                                                                     | 10.057973 | 7.115225  | 3.595698  |  |
| 17                                                                     | 1.589841  | 0.395972  | 9.823276  |  |
| 17                                                                     | 3.188352  | 3.099664  | 3.927577  |  |
| 17                                                                     | 8.459462  | 9.818917  | 9.491397  |  |
| 17                                                                     | 3.506181  | 5.999599  | 3.613084  |  |
| 17                                                                     | 8.141634  | 12.718851 | 9.805891  |  |
| 17                                                                     | 4.123265  | 4.709278  | 6.159889  |  |
| 17                                                                     | 7.524549  | 11.428530 | 7.259084  |  |
| 17                                                                     | 9.581917  | 1.764773  | 3.941838  |  |
| 17                                                                     | 2.065898  | 8.484026  | 9.477137  |  |
| 17                                                                     | 10.224861 | 0.148753  | 6.273254  |  |
| 17                                                                     | 1.422953  | 6.868006  | 7.145720  |  |
| 17                                                                     | 9.801381  | 12.291997 | 3.685426  |  |
| 17                                                                     | 1.846433  | 5.572744  | 9.733548  |  |
| 7                                                                      | 0.817826  | 11.230515 | 5.414246  |  |
| 7                                                                      | 10.829988 | 4.511261  | 8.004729  |  |
| 7                                                                      | 0.474226  | 10.600327 | 2.779128  |  |
| 7                                                                      | 11.173589 | 3.881074  | 10.639847 |  |
| 7                                                                      | 6.957370  | 7.227550  | 5.456845  |  |
| 7                                                                      | 4.690444  | 0.508297  | 7.962129  |  |
| 7                                                                      | 6.715344  | 7.890892  | 2.809933  |  |
| 7                                                                      | 4.932469  | 1.171638  | 10.609040 |  |
| 6                                                                      | 0.873082  | 11.745442 | 6.657589  |  |
| 6                                                                      | 10.774733 | 5.026189  | 6.761386  |  |
| 6                                                                      | 0.122462  | 11.228750 | 7.704543  |  |
| 6                                                                      | 11.525352 | 4.509497  | 5.714431  |  |
| 6                                                                      | 11.805415 | 10.160728 | 7.445391  |  |
| 6                                                                      | -0.157602 | 3.441475  | 5.973583  |  |
| 6                                                                      | 11.742861 | 9.634006  | 6.157273  |  |
| 6                                                                      | -0.095046 | 2.914755  | 7.261702  |  |
| 6                                                                      | 0.005400  | 10.186090 | 5.161452  |  |
| 6                                                                      | 11.642413 | 3.466839  | 8.257524  |  |
| 6                                                                      | 0.054882  | 9.590623  | 3.771377  |  |
| 6                                                                      | 11.592932 | 2.871371  | 9.647597  |  |
| 6                                                                      | 1.048905  | 8.416111  | 3.746712  |  |
| 6                                                                      | 10.598908 | 1.696857  | 9.672262  |  |

| 2RE-PIC-Zn / 2SE-PIC-Zn / 4CHCl <sub>3</sub> (molecular crystal) (2/5) |           |           |           |
|------------------------------------------------------------------------|-----------|-----------|-----------|
| Atomic Number                                                          | x         | y         | z         |
| 6                                                                      | 0.023879  | 10.484256 | 1.578869  |
| 6                                                                      | 11.623935 | 3.765003  | 11.840106 |
| 6                                                                      | 11.588609 | 9.433367  | 1.088161  |
| 6                                                                      | 0.059204  | 2.714114  | 12.330812 |
| 6                                                                      | 10.508857 | 9.827521  | 13.035884 |
| 6                                                                      | 1.138958  | 3.108269  | 0.383090  |
| 6                                                                      | 9.685168  | 11.130497 | 13.040275 |
| 6                                                                      | 1.962646  | 4.411243  | 0.378699  |
| 6                                                                      | 11.588074 | 12.178791 | 0.165851  |
| 6                                                                      | 0.059741  | 5.459540  | 13.253123 |
| 6                                                                      | 0.360778  | 11.371406 | 0.397578  |
| 6                                                                      | 11.287037 | 4.652153  | 13.021397 |
| 6                                                                      | 1.614617  | 12.212476 | 0.477026  |
| 6                                                                      | 10.033197 | 5.493223  | 12.941950 |
| 6                                                                      | -0.609558 | 10.310493 | 12.651999 |
| 6                                                                      | 12.257372 | 3.591241  | 0.766975  |
| 6                                                                      | 0.475824  | 9.231353  | 12.766206 |
| 6                                                                      | 11.171988 | 2.512100  | 0.652768  |
| 6                                                                      | -0.525722 | 10.911287 | 11.249159 |
| 6                                                                      | 12.173535 | 4.192035  | 2.169814  |
| 6                                                                      | 6.970804  | 6.701747  | 6.696005  |
| 6                                                                      | 4.677009  | 13.421000 | 6.722969  |
| 6                                                                      | 6.172001  | 7.199761  | 7.717234  |
| 6                                                                      | 5.475812  | 0.480509  | 5.701740  |
| 6                                                                      | 5.303537  | 8.255565  | 7.432720  |
| 6                                                                      | 6.344276  | 1.536314  | 5.986254  |
| 6                                                                      | 5.279894  | 8.788172  | 6.144988  |
| 6                                                                      | 6.367920  | 2.068920  | 7.273986  |
| 6                                                                      | 6.135602  | 8.258464  | 5.178770  |
| 6                                                                      | 5.512212  | 1.539212  | 8.240204  |
| 6                                                                      | 6.259547  | 8.880960  | 3.805693  |
| 6                                                                      | 5.388267  | 2.161708  | 9.613281  |
| 6                                                                      | 7.287888  | 10.024993 | 3.874410  |
| 6                                                                      | 4.359926  | 3.305741  | 9.544564  |
| 6                                                                      | 6.436394  | 8.118272  | 1.572903  |
| 6                                                                      | 5.211421  | 1.399019  | 11.846071 |
| 6                                                                      | 5.585841  | 9.252467  | 1.024586  |
| 6                                                                      | 6.061973  | 2.533215  | 12.394388 |
| 6                                                                      | 4.852609  | 9.075403  | 12.925785 |
| 6                                                                      | 6.795206  | 2.356151  | 0.493189  |
| 6                                                                      | 6.300497  | 9.488119  | 12.596637 |
| 6                                                                      | 5.347317  | 2.768866  | 0.822337  |
| 6                                                                      | 7.137088  | 8.345806  | 13.228522 |
| 6                                                                      | 4.510727  | 1.626553  | 0.190451  |
| 6                                                                      | 6.967423  | 7.350296  | 0.384915  |
| 6                                                                      | 4.680391  | 0.631043  | 13.034059 |

| 2RE-PIC-Zn / 2SE-PIC-Zn / 4CHCl <sub>3</sub> (molecular crystal) (3/5) |           |           |           |  |
|------------------------------------------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                                                          | x         | y         | z         |  |
| 6                                                                      | 7.489971  | 5.954199  | 0.620165  |  |
| 6                                                                      | 4.157843  | 12.673451 | 12.798809 |  |
| 6                                                                      | 4.892977  | 7.529071  | 12.775025 |  |
| 6                                                                      | 6.754837  | 0.809818  | 0.643948  |  |
| 6                                                                      | 3.605929  | 6.821559  | 13.205683 |  |
| 6                                                                      | 8.041885  | 0.102306  | 0.213291  |  |
| 6                                                                      | 5.242027  | 7.058123  | 11.362247 |  |
| 6                                                                      | 6.405786  | 0.338871  | 2.056726  |  |
| 6                                                                      | 4.128100  | 4.519793  | 4.402692  |  |
| 6                                                                      | 7.519713  | 11.239047 | 9.016282  |  |
| 6                                                                      | 10.405859 | 0.312860  | 4.520604  |  |
| 6                                                                      | 1.241955  | 7.032114  | 8.898370  |  |
| 1                                                                      | 1.530623  | 12.603689 | 6.801112  |  |
| 1                                                                      | 10.117190 | 5.884437  | 6.617863  |  |
| 1                                                                      | 0.220133  | 11.673027 | 8.692698  |  |
| 1                                                                      | 11.427681 | 4.953774  | 4.726276  |  |
| 1                                                                      | 11.185039 | 9.737455  | 8.235711  |  |
| 1                                                                      | 0.462775  | 3.018203  | 5.183263  |  |
| 1                                                                      | 11.082524 | 8.802092  | 5.910507  |  |
| 1                                                                      | 0.565290  | 2.082840  | 7.508467  |  |
| 1                                                                      | 11.597936 | 9.205561  | 3.537467  |  |
| 1                                                                      | 0.049879  | 2.486310  | 9.881506  |  |
| 1                                                                      | 1.076845  | 7.960651  | 2.747910  |  |
| 1                                                                      | 10.570970 | 1.241398  | 10.671064 |  |
| 1                                                                      | 0.738792  | 7.645288  | 4.462008  |  |
| 1                                                                      | 10.909022 | 0.926035  | 8.956967  |  |
| 1                                                                      | 2.057979  | 8.763980  | 4.005762  |  |
| 1                                                                      | 9.589835  | 2.044726  | 9.413213  |  |
| 1                                                                      | 10.656027 | 9.443715  | 1.672543  |  |
| 1                                                                      | 0.991786  | 2.724463  | 11.746430 |  |
| 1                                                                      | 12.001258 | 8.421629  | 1.209854  |  |
| 1                                                                      | -0.353443 | 1.702375  | 12.209120 |  |
| 1                                                                      | 10.106523 | 9.029906  | 12.400931 |  |
| 1                                                                      | 1.541291  | 2.310654  | 1.018043  |  |
| 1                                                                      | 9.698527  | 11.035463 | 0.264362  |  |
| 1                                                                      | 1.949286  | 4.316212  | 13.154612 |  |
| 1                                                                      | 9.324761  | 11.389903 | 12.038881 |  |
| 1                                                                      | 2.323053  | 4.670652  | 1.380094  |  |
| 1                                                                      | 11.252714 | 12.668246 | 1.089063  |  |
| 1                                                                      | 0.395100  | 5.948993  | 12.329910 |  |
| 1                                                                      | 10.894222 | 12.974291 | 12.854191 |  |
| 1                                                                      | 0.753591  | 6.255037  | 0.564783  |  |
| 1                                                                      | 1.526304  | 13.009036 | 1.227788  |  |
| 1                                                                      | 10.121510 | 6.289783  | 12.191187 |  |
| 1                                                                      | 0.900170  | 12.700055 | 12.928041 |  |
| 1                                                                      | 10.747644 | 5.980803  | 0.490933  |  |

| 2RE-PIC-Zn / 2SE-PIC-Zn / 4CHCl <sub>3</sub> (molecular crystal) (4/5) |           |           |           |
|------------------------------------------------------------------------|-----------|-----------|-----------|
| Atomic Number                                                          | x         | y         | z         |
| 1                                                                      | 2.494228  | 11.605259 | 0.728291  |
| 1                                                                      | 9.153587  | 4.886006  | 12.690682 |
| 1                                                                      | 1.443973  | 9.626998  | 12.429599 |
| 1                                                                      | 10.203842 | 2.907745  | 0.989375  |
| 1                                                                      | 0.228584  | 8.377573  | 12.121341 |
| 1                                                                      | 11.419230 | 1.658320  | 1.297633  |
| 1                                                                      | 1.516417  | 8.854651  | 0.369557  |
| 1                                                                      | 10.131397 | 2.135400  | 13.049417 |
| 1                                                                      | 0.456584  | 11.370782 | 11.072493 |
| 1                                                                      | 11.191231 | 4.651528  | 2.346481  |
| 1                                                                      | 11.253704 | 11.669342 | 11.045362 |
| 1                                                                      | 0.394111  | 4.950090  | 2.373611  |
| 1                                                                      | -0.655146 | 10.104568 | 10.514592 |
| 1                                                                      | 12.302960 | 3.385316  | 2.904383  |
| 1                                                                      | 7.630811  | 5.849035  | 6.857168  |
| 1                                                                      | 4.017003  | 12.568287 | 6.561806  |
| 1                                                                      | 6.236652  | 6.748370  | 8.705015  |
| 1                                                                      | 5.411162  | 0.029117  | 4.713959  |
| 1                                                                      | 4.653275  | 8.668198  | 8.203418  |
| 1                                                                      | 6.994539  | 1.948945  | 5.215557  |
| 1                                                                      | 4.621147  | 9.616243  | 5.881723  |
| 1                                                                      | 7.026668  | 2.896992  | 7.537252  |
| 1                                                                      | 5.280640  | 9.295567  | 3.524760  |
| 1                                                                      | 6.367174  | 2.576314  | 9.894214  |
| 1                                                                      | 6.965323  | 10.783302 | 4.596700  |
| 1                                                                      | 4.682491  | 4.064049  | 8.822274  |
| 1                                                                      | 7.390143  | 10.511368 | 2.896200  |
| 1                                                                      | 4.257670  | 3.792115  | 10.522773 |
| 1                                                                      | 8.268882  | 9.633773  | 4.175586  |
| 1                                                                      | 3.378933  | 2.914520  | 9.243389  |
| 1                                                                      | 5.906381  | 10.238976 | 1.385361  |
| 1                                                                      | 5.741434  | 3.519725  | 12.033612 |
| 1                                                                      | 4.544140  | 9.139693  | 1.361919  |
| 1                                                                      | 7.103674  | 2.420440  | 12.057055 |
| 1                                                                      | 4.091361  | 9.585897  | 12.324436 |
| 1                                                                      | 7.556453  | 2.866646  | 1.094539  |
| 1                                                                      | 6.544947  | 10.471053 | 13.019280 |
| 1                                                                      | 5.102868  | 3.751801  | 0.399693  |
| 1                                                                      | 6.462825  | 9.558660  | 11.515642 |
| 1                                                                      | 5.184989  | 2.839407  | 1.903331  |
| 1                                                                      | 7.746855  | 7.816202  | 12.483621 |
| 1                                                                      | 3.900959  | 1.096949  | 0.935354  |
| 1                                                                      | 8.718997  | 8.681410  | 0.599536  |
| 1                                                                      | 2.928818  | 1.962157  | 12.819438 |
| 1                                                                      | 6.876075  | 5.499141  | 13.080487 |
| 1                                                                      | 4.771739  | 12.218394 | 0.338487  |

---

| 2RE-PIC-Zn / 2SE-PIC-Zn / 4CHCl <sub>3</sub> (molecular crystal) (5/5) |           |           |           |  |
|------------------------------------------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                                                          | x         | y         | z         |  |
| 1                                                                      | 6.748689  | 5.314007  | 1.112254  |  |
| 1                                                                      | 4.899125  | 12.033259 | 12.306721 |  |
| 1                                                                      | 8.392279  | 5.957826  | 1.247419  |  |
| 1                                                                      | 3.255536  | 12.677078 | 12.171555 |  |
| 1                                                                      | 4.165092  | 7.082644  | 0.797613  |  |
| 1                                                                      | 7.482721  | 0.363392  | 12.621362 |  |
| 1                                                                      | 3.755807  | 5.733744  | 13.196099 |  |
| 1                                                                      | 7.892006  | 12.452995 | 0.222875  |  |
| 1                                                                      | 2.791691  | 7.047004  | 12.504084 |  |
| 1                                                                      | 8.856122  | 0.327752  | 0.914891  |  |
| 1                                                                      | 4.463709  | 7.389723  | 10.661757 |  |
| 1                                                                      | 7.184105  | 0.670470  | 2.757216  |  |
| 1                                                                      | 5.284476  | 5.961339  | 11.314398 |  |
| 1                                                                      | 6.363338  | 12.680591 | 2.104576  |  |
| 1                                                                      | 6.207391  | 7.428753  | 11.000314 |  |
| 1                                                                      | 5.440423  | 0.709502  | 2.418660  |  |
| 1                                                                      | 5.170762  | 4.392731  | 4.079914  |  |
| 1                                                                      | 6.477053  | 11.111982 | 9.339059  |  |
| 1                                                                      | 11.475186 | 0.402829  | 4.285686  |  |
| 1                                                                      | 0.172628  | 7.122081  | 9.133289  |  |

---

| RE-PIC-Zn (in a unit cell) |           |           |           |
|----------------------------|-----------|-----------|-----------|
| Atomic Number              | x         | y         | z         |
| 30                         | 11.102311 | 11.633725 | 9.973335  |
| 17                         | 10.463825 | 12.634412 | 11.831423 |
| 17                         | 11.451350 | 12.557184 | 7.998624  |
| 7                          | 9.770738  | 9.988307  | 9.960991  |
| 7                          | 12.492227 | 9.989061  | 9.982155  |
| 6                          | 8.459764  | 10.078697 | 10.240347 |
| 6                          | 7.656173  | 8.950631  | 10.369349 |
| 6                          | 8.246347  | 7.693402  | 10.227705 |
| 6                          | 9.612872  | 7.606032  | 9.964666  |
| 6                          | 10.352020 | 8.785271  | 9.831555  |
| 6                          | 11.824034 | 8.783343  | 9.453725  |
| 6                          | 11.936278 | 8.767220  | 7.913468  |
| 6                          | 13.759713 | 9.950949  | 10.183774 |
| 6                          | 14.677230 | 8.739134  | 10.050575 |
| 6                          | 16.065334 | 9.362787  | 10.275535 |
| 6                          | 16.357065 | 10.214304 | 9.018928  |
| 6                          | 15.381879 | 11.412159 | 9.183592  |
| 6                          | 14.640272 | 11.135231 | 10.536870 |
| 6                          | 13.972587 | 12.354026 | 11.133651 |
| 6                          | 15.773707 | 10.429358 | 11.375015 |
| 6                          | 16.970678 | 11.332718 | 11.683393 |
| 6                          | 15.256645 | 9.860109  | 12.703852 |
| 1                          | 8.076972  | 11.090134 | 10.374862 |
| 1                          | 6.594579  | 9.060290  | 10.588758 |
| 1                          | 7.647502  | 6.788157  | 10.328231 |
| 1                          | 10.103416 | 6.637140  | 9.862709  |
| 1                          | 12.282714 | 7.870550  | 9.870800  |
| 1                          | 11.394284 | 7.905696  | 7.500690  |
| 1                          | 12.987532 | 8.703803  | 7.605205  |
| 1                          | 11.514835 | 9.696496  | 7.508372  |
| 1                          | 14.583122 | 8.236059  | 9.077950  |
| 1                          | 14.424253 | 7.995654  | 10.822483 |
| 1                          | 16.846128 | 8.630044  | 10.525819 |
| 1                          | 16.169270 | 9.643366  | 8.099365  |
| 1                          | 17.403801 | 10.540109 | 8.978382  |
| 1                          | 14.665535 | 11.531654 | 8.359393  |
| 1                          | 15.914394 | 12.369166 | 9.276497  |
| 1                          | 13.358489 | 12.877211 | 10.387695 |
| 1                          | 14.729150 | 13.075522 | 11.473190 |
| 1                          | 13.324118 | 12.107755 | 11.984392 |
| 1                          | 16.659668 | 12.204622 | 12.276622 |
| 1                          | 17.484610 | 11.705526 | 10.789440 |
| 1                          | 17.709532 | 10.781154 | 12.282330 |
| 1                          | 16.006290 | 9.198765  | 13.160995 |
| 1                          | 14.319855 | 9.294891  | 12.608631 |
| 1                          | 15.060814 | 10.67646  | 13.412704 |

| SE-PIC-Zn (in a unit cell) |           |           |           |
|----------------------------|-----------|-----------|-----------|
| Atomic Number              | x         | y         | z         |
| 30                         | 11.111755 | 11.631293 | 10.071852 |
| 17                         | 11.012488 | 12.527551 | 12.074516 |
| 17                         | 10.934019 | 12.547301 | 8.067657  |
| 7                          | 9.763748  | 9.997402  | 10.009563 |
| 7                          | 12.489597 | 9.996544  | 10.008998 |
| 6                          | 8.437054  | 10.096724 | 9.820616  |
| 6                          | 7.609561  | 8.979741  | 9.792804  |
| 6                          | 8.191178  | 7.719150  | 9.940733  |
| 6                          | 9.570193  | 7.620385  | 10.120312 |
| 6                          | 10.334671 | 8.793442  | 10.159904 |
| 6                          | 11.830470 | 8.750479  | 10.430998 |
| 6                          | 12.083158 | 8.561095  | 11.942063 |
| 6                          | 13.678886 | 9.936840  | 9.523362  |
| 6                          | 14.471928 | 8.680278  | 9.182419  |
| 6                          | 15.737136 | 9.269333  | 8.537017  |
| 6                          | 15.307206 | 9.859635  | 7.174398  |
| 6                          | 14.482700 | 11.114822 | 7.577995  |
| 6                          | 14.542077 | 11.127232 | 9.142301  |
| 6                          | 14.213642 | 12.453985 | 9.801614  |
| 6                          | 15.982697 | 10.532819 | 9.410494  |
| 6                          | 17.128641 | 11.412087 | 8.897278  |
| 6                          | 16.243345 | 10.242765 | 10.896065 |
| 1                          | 8.054509  | 11.108904 | 9.682063  |
| 1                          | 6.535009  | 9.099316  | 9.653875  |
| 1                          | 7.577778  | 6.817839  | 9.909598  |
| 1                          | 10.055544 | 6.650939  | 10.233679 |
| 1                          | 12.236562 | 7.881588  | 9.887838  |
| 1                          | 11.689454 | 9.425636  | 12.494427 |
| 1                          | 13.161972 | 8.488983  | 12.133070 |
| 1                          | 11.598376 | 7.645231  | 12.305298 |
| 1                          | 14.699512 | 8.100826  | 10.089201 |
| 1                          | 13.909173 | 8.020898  | 8.504336  |
| 1                          | 16.574923 | 8.561070  | 8.482129  |
| 1                          | 16.176115 | 10.127107 | 6.559635  |
| 1                          | 14.713095 | 9.138769  | 6.596365  |
| 1                          | 13.443142 | 11.106807 | 7.226322  |
| 1                          | 14.928510 | 12.042871 | 7.196249  |
| 1                          | 13.327058 | 12.920496 | 9.351298  |
| 1                          | 14.024093 | 12.340032 | 10.877647 |
| 1                          | 15.410984 | 9.731314  | 11.398022 |
| 1                          | 16.408861 | 11.182250 | 11.441980 |
| 1                          | 17.145634 | 9.624711  | 11.019057 |
| 1                          | 15.045857 | 13.159566 | 9.668613  |
| 1                          | 18.075880 | 10.852057 | 8.951024  |
| 1                          | 17.245127 | 12.308313 | 9.524070  |
| 1                          | 16.999224 | 11.746405 | 7.860480  |

| CHCl <sub>3</sub> (in a unit cell) |           |           |           |  |
|------------------------------------|-----------|-----------|-----------|--|
| Atomic Number                      | x         | y         | z         |  |
| 17                                 | 10.383901 | 11.627309 | 11.463075 |  |
| 17                                 | 10.383901 | 11.627309 | 8.536925  |  |
| 17                                 | 7.994194  | 10.781902 | 10.000000 |  |
| 6                                  | 9.765860  | 10.840021 | 10.000000 |  |
| 1                                  | 10.130147 | 9.810160  | 10.000000 |  |