

Supporting Information

Iron and Zinc Mediated Reductive Coupling of Styrenes and Alkyl Bromide: a Mechanistic Investigation using DFT Calculations

Guojing Pei, Wan Xu and Juan Li*

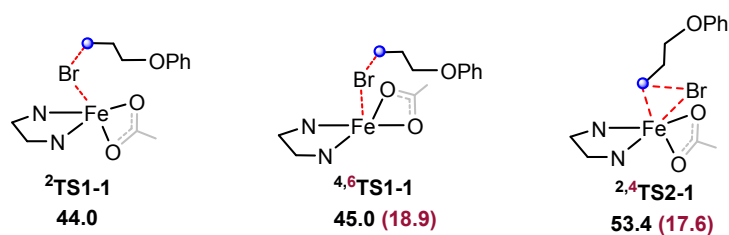
College of Chemistry and Materials Science, Guangdong Provincial Key Laboratory
of Functional Supramolecular Coordination Materials and Applications, Jinan
University, Guangzhou, Guangdong 510632, P. R. China

*Corresponding author. Email: tchjli@jnu.edu.cn (J. Li)

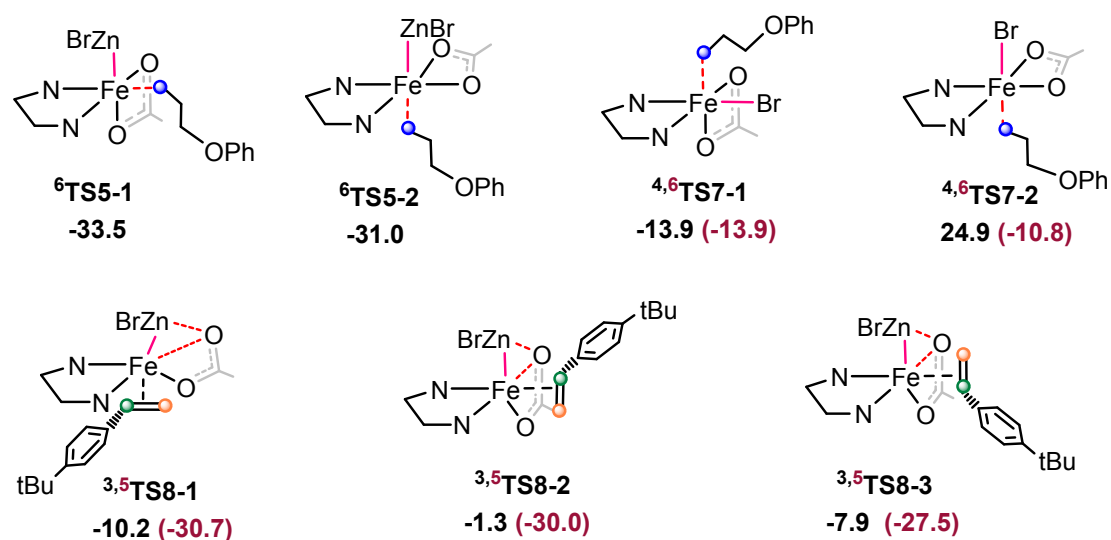
Table of Contents

| | | |
|-------------------|---|-----|
| Section 1. | Other possible isomers (Schemes S1-S4) | S2 |
| Section 2. | Other possible pathways (Figs. S1-S9) | S3 |
| Section 3. | Energies (in Hartree) for all TSs and intermediates | S7 |
| Section 4. | Calculated imaginary frequencies of all transition states species | S10 |

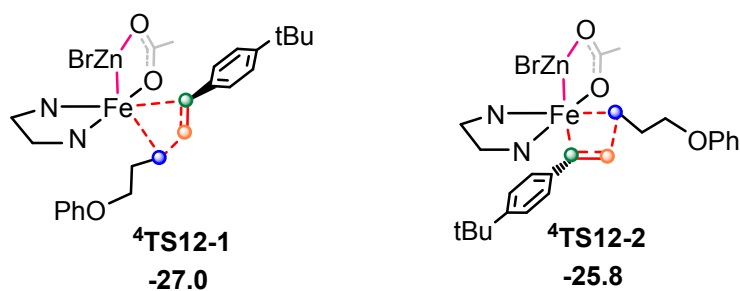
Section 1. Other possible isomers



Scheme S1 Other possible isomers of transition state **TS1** and **TS2**. Values shown are relative free energies in kcal/mol.

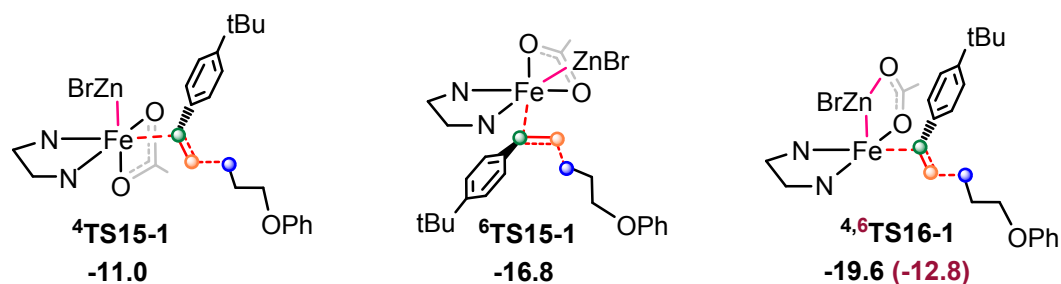


Scheme S2 Other possible isomers of transition state **TS5**, **TS7** and **TS8**. Values shown are relative free energies in kcal/mol.



Scheme S3 Other possible isomers of transition state **TS12**. Values shown are relative

free energies in kcal/mol.



Scheme S4 Other possible isomers of transition state **TS15** and **TS16**. Values shown are relative free energies in kcal/mol.

Section 2. Other possible pathways

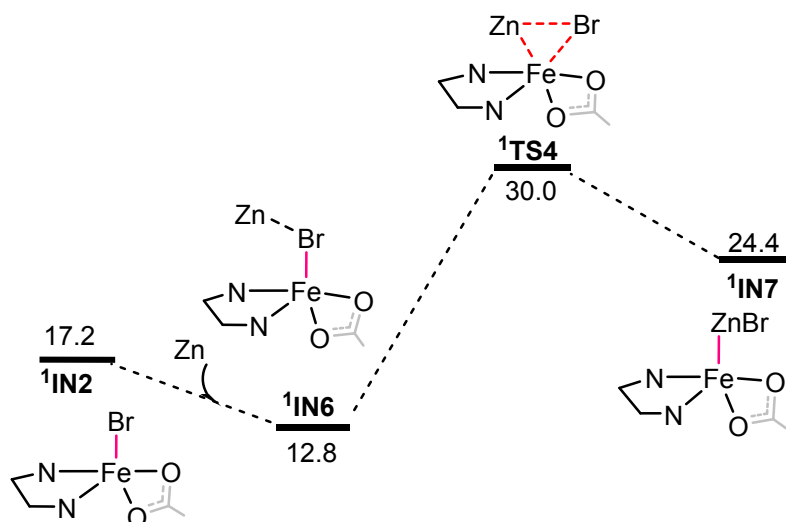


Fig. S1 Calculated energy profiles for bromide migration step from **¹IN2** along the doublet state pathway. Values shown are relative free energies in kcal/mol.

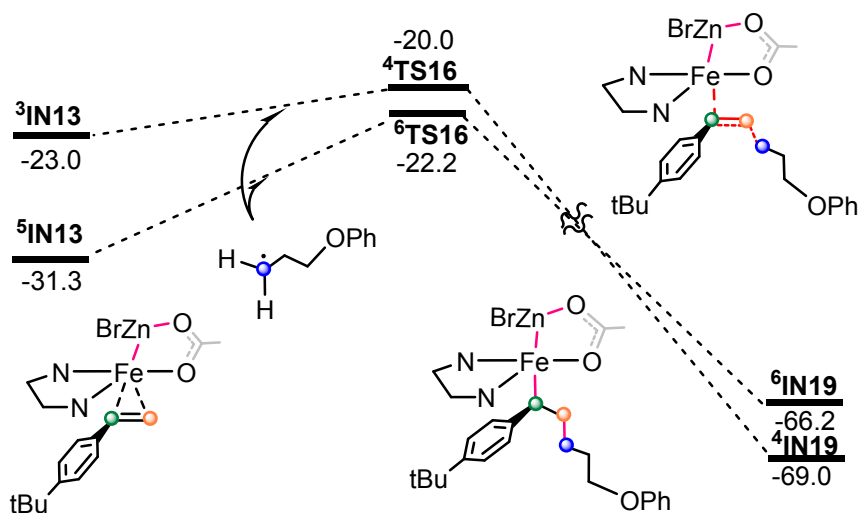


Fig. S2 Calculated energy profiles for C–C bond formation step from IN13. Values shown are relative free energies in kcal/mol.

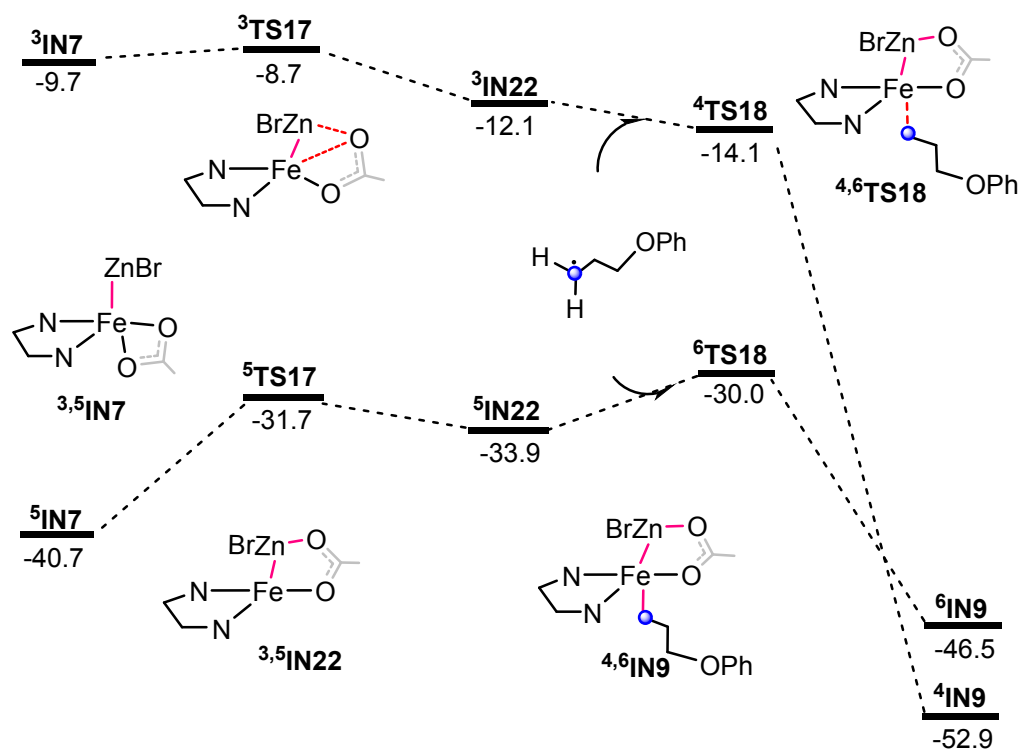


Fig. S3 Calculated energy profiles for isomerization prior to radical coordination. Values shown are relative free energies in kcal/mol.

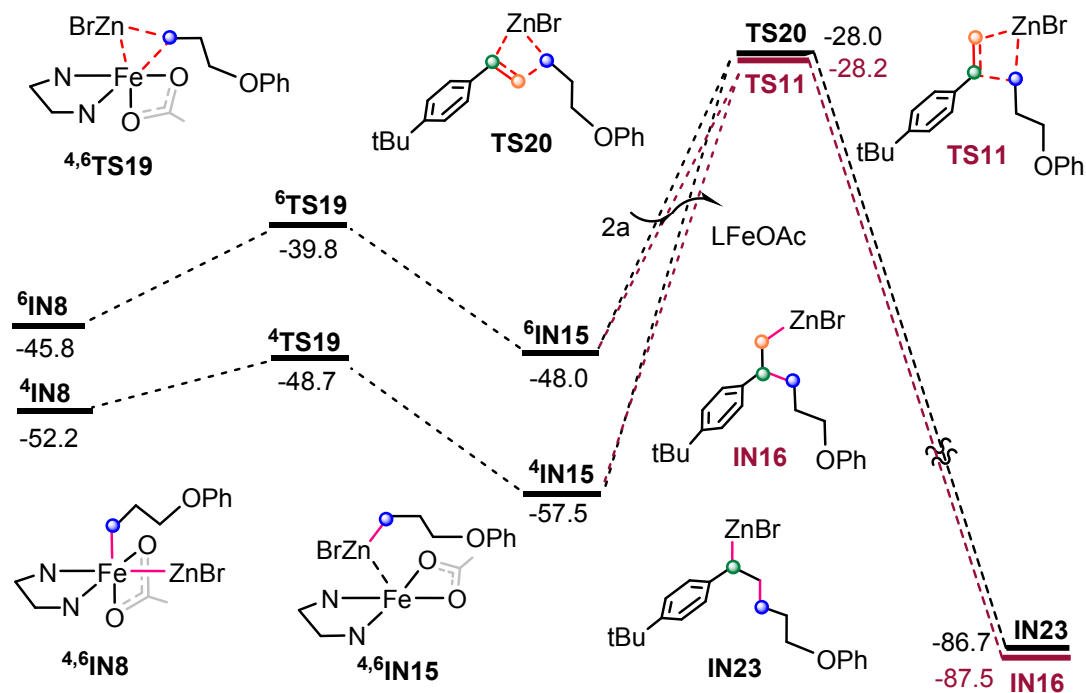


Fig. S4 Calculated energy profiles for C–C bond formation mediated by zinc started from **IN8**. Values shown are relative free energies in kcal/mol.

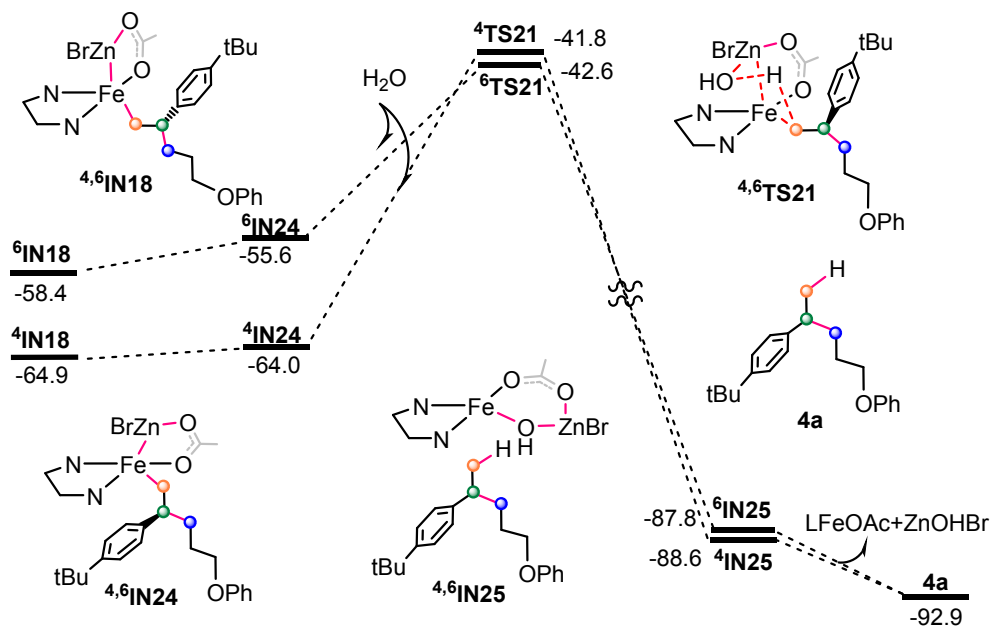


Fig. S5 Calculated energy profiles for the process **IN18** → **4a**. Values shown are relative free energies in kcal/mol.

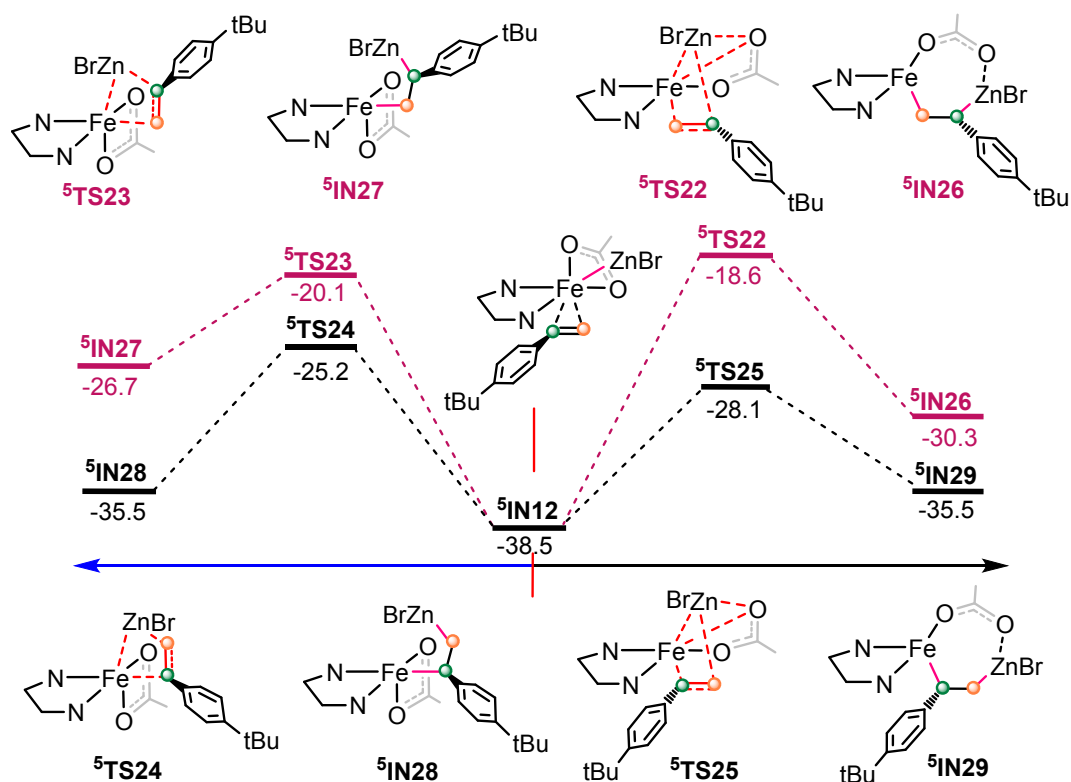


Fig. S6 Calculated energy profiles for the other mechanisms from **IN12**. Values shown are relative free energies in kcal/mol.

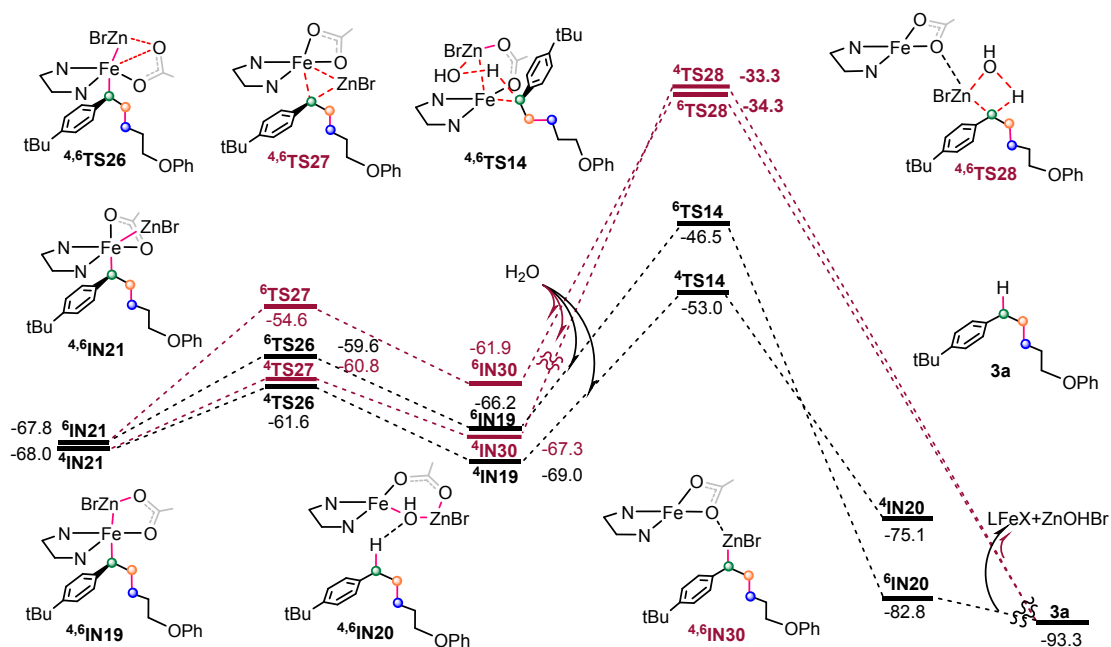


Fig. S7 Calculated energy profiles for the process **IN21** → **3a**. Values shown are relative free energies in kcal/mol.

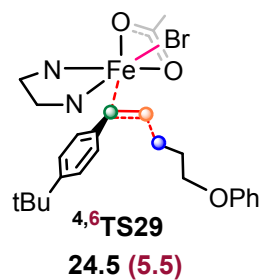


Fig. S8 Calculated TS for C–C bond formation from **IN11**. Values shown are relative free energies in kcal/mol.

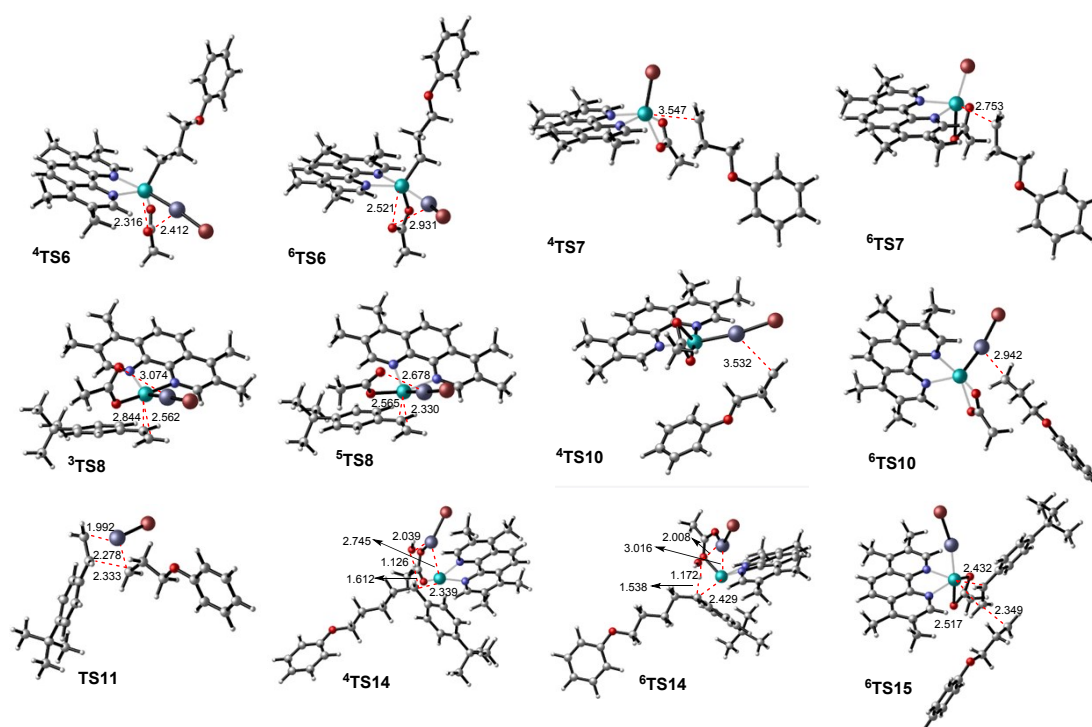


Fig. S9 Optimized structures of key transition states **4,6TS6**, **4,6TS7**, **3,5TS8**, **4,6TS10**, **4,6TS14**, **6TS15**, and **TS11**. Key bond lengths are given in Å.

Section 3. Energies (in Hartree) of All TSs and Intermediates.

| Geometry | E_0 | E | $H_{298.15}$ | $G_{298.15}$ | $E_{(sol,M06)}$ |
|----------|-------------|-------------|--------------|--------------|-----------------|
| 1a | -437.990350 | -437.979506 | -437.978562 | -438.029906 | -437.949094 |
| 2a | -466.647499 | -466.635287 | -466.634343 | -466.685549 | -466.641075 |
| 3a | -891.877175 | -891.854837 | -891.853893 | -891.932880 | -891.874621 |
| 4a | -891.875140 | -891.852820 | -891.851876 | -891.929196 | -891.875560 |
| Zn | -227.158069 | -227.156654 | -227.155710 | -227.173937 | -227.202842 |

| | | | | | |
|---------------------|--------------|--------------|--------------|--------------|--------------|
| ² LFeOAc | -1081.023413 | -1081.000856 | -1080.999912 | -1081.076706 | -1080.921637 |
| ⁴ LFeOAc | -1081.012593 | -1080.989583 | -1080.988639 | -1081.067437 | -1080.949119 |
| ⁶ LFeOAc | -1081.024566 | -1081.000779 | -1080.999835 | -1081.083258 | -1080.956813 |
| ² IN1 | -1519.014533 | -1518.978412 | -1518.977468 | -1519.096231 | -1518.876295 |
| ⁴ IN1 | -1519.028647 | -1518.991847 | -1518.990903 | -1519.109479 | -1518.925762 |
| ⁶ IN1 | -1519.019199 | -1518.983166 | -1518.982222 | -1519.099365 | -1518.928424 |
| ² TS1 | -1519.001912 | -1518.966249 | -1518.965305 | -1519.077565 | -1518.868207 |
| ⁴ TS1 | -1519.022052 | -1518.985716 | -1518.984773 | -1519.100354 | -1518.913643 |
| ⁶ TS1 | -1519.010859 | -1518.974488 | -1518.973544 | -1519.088674 | -1518.906327 |
| ¹ IN2 | -1519.022378 | -1518.985450 | -1518.984506 | -1519.097815 | -1518.901066 |
| ³ IN2 | -1519.053444 | -1519.015881 | -1519.014937 | -1519.133157 | -1518.953605 |
| ⁵ IN2 | -1094.499658 | -1094.473961 | -1094.473017 | -1094.561166 | -1094.415748 |
| ² TS2 | -1518.961394 | -1518.925821 | -1518.924877 | -1519.037081 | -1518.853442 |
| ⁴ TS2 | -1519.001936 | -1518.967261 | -1518.966317 | -1519.076412 | -1518.904960 |
| TS3 | -665.081021 | -665.067979 | -665.067035 | -665.125981 | -665.096234 |
| ² IN3 | -1519.035313 | -1519.000359 | -1518.999415 | -1519.106195 | -1518.916928 |
| ⁴ IN3 | -1519.055139 | -1519.019075 | -1519.018131 | -1519.130032 | -1518.962224 |
| ⁶ IN3 | -1519.049984 | -1519.013724 | -1519.012780 | -1519.125755 | -1518.963823 |
| IN4 | -665.148880 | -665.135286 | -665.134343 | -665.197955 | -665.159426 |
| IN5 | -665.195745 | -665.182731 | -665.181788 | -665.240030 | -665.202212 |
| ³ IN6 | -1321.627155 | -1321.600614 | -1321.599670 | -1321.688632 | -1321.566518 |
| ⁵ IN6 | -1321.659044 | -1321.631673 | -1321.630729 | -1321.724090 | -1321.627741 |
| ³ TS4 | -1321.607228 | -1321.580551 | -1321.579607 | -1321.669256 | -1321.552155 |
| ⁵ TS4 | -1321.632039 | -1321.604821 | -1321.603877 | -1321.695527 | -1321.606178 |
| ³ IN7 | -1321.624448 | -1321.596972 | -1321.596029 | -1321.688897 | -1321.574367 |
| ⁵ IN7 | -1321.649745 | -1321.621656 | -1321.620713 | -1321.716520 | -1321.620850 |
| ⁴ TS5 | -1746.171042 | -1746.132535 | -1746.131591 | -1746.252663 | -1746.106006 |
| ⁶ TS5 | -1746.186715 | -1746.147702 | -1746.146758 | -1746.274193 | -1746.154438 |
| ⁴ IN8 | -1746.228933 | -1746.190312 | -1746.189368 | -1746.309700 | -1746.191274 |
| ⁶ IN8 | -1746.206239 | -1746.167257 | -1746.166313 | -1746.290196 | -1746.178445 |
| ⁴ TS6 | -1746.225804 | -1746.187885 | -1746.186941 | -1746.306406 | -1746.182793 |
| ⁶ TS6 | -1746.206773 | -1746.168631 | -1746.167688 | -1746.288203 | -1746.179859 |
| ⁴ IN9 | -1746.239296 | -1746.200755 | -1746.199811 | -1746.321440 | -1746.190916 |
| ⁶ IN9 | -1746.218619 | -1746.179962 | -1746.179019 | -1746.301009 | -1746.180106 |
| ⁴ IN10 | -2212.885642 | -2212.834314 | -2212.833371 | -2212.980527 | -2212.857900 |
| ⁶ IN10 | -2212.864606 | -2212.813794 | -2212.812850 | -2212.959372 | -2212.838256 |
| ⁴ TS7 | -1519.048843 | -1519.011776 | -1519.010832 | -1519.129265 | -1518.949831 |
| ⁶ TS7 | -1519.042202 | -1519.005766 | -1519.004823 | -1519.118876 | -1518.950809 |
| ⁴ IN11 | -1519.058807 | -1519.022711 | -1519.021767 | -1519.133560 | -1518.965117 |
| ⁶ IN11 | -1519.049668 | -1519.013526 | -1519.012582 | -1519.124784 | -1518.963320 |
| ³ IN12 | -1788.271568 | -1788.230382 | -1788.229438 | -1788.352222 | -1788.255733 |
| ⁵ IN12 | -1788.303264 | -1788.261654 | -1788.260710 | -1788.388319 | -1788.278952 |
| ³ TS8 | -1788.269697 | -1788.228897 | -1788.227953 | -1788.351096 | -1788.240963 |

| | | | | | |
|-------------------|--------------|--------------|--------------|--------------|--------------|
| ⁵ TS8 | -1788.283576 | -1788.242467 | -1788.241523 | -1788.366735 | -1788.271185 |
| ³ IN13 | -1788.294261 | -1788.253932 | -1788.252988 | -1788.371476 | -1788.263082 |
| ⁵ IN13 | -1788.286793 | -1788.245311 | -1788.244367 | -1788.368611 | -1788.270882 |
| ³ IN14 | -1788.284167 | -1788.242832 | -1788.241888 | -1788.366045 | -1788.266222 |
| ⁵ IN14 | -1788.280952 | -1788.239410 | -1788.238466 | -1788.363838 | -1788.270015 |
| ⁴ TS9 | -2212.828911 | -2212.777670 | -2212.776726 | -2212.924687 | -2212.797383 |
| ⁶ TS9 | -2212.817723 | -2212.766928 | -2212.765984 | -2212.913328 | -2212.803205 |
| ⁴ TS10 | -1746.170614 | -1746.132037 | -1746.131093 | -1746.253009 | -1746.120033 |
| ⁶ TS10 | -1746.201095 | -1746.163627 | -1746.162684 | -1746.281597 | -1746.152838 |
| ⁴ IN15 | -1746.234518 | -1746.195620 | -1746.194677 | -1746.318137 | -1746.195870 |
| ⁶ IN15 | -1746.221770 | -1746.183191 | -1746.182247 | -1746.304559 | -1746.182237 |
| TS11 | -1131.776726 | -1131.750930 | -1131.749986 | -1131.838209 | -1131.787857 |
| IN16 | -1131.867305 | -1131.841543 | -1131.840599 | -1131.930054 | -1131.885310 |
| ⁴ TS12 | -2212.849253 | -2212.799011 | -2212.798067 | -2212.941448 | -2212.829674 |
| ⁶ TS12 | -2212.824036 | -2212.773384 | -2212.772440 | -2212.917825 | -2212.814999 |
| ⁴ IN17 | -2212.914088 | -2212.862678 | -2212.861735 | -2213.013602 | -2212.884489 |
| ⁶ IN17 | -2212.894248 | -2212.842735 | -2212.841792 | -2212.993486 | -2212.874688 |
| ⁴ TS13 | -2212.847965 | -2212.797345 | -2212.796402 | -2212.942097 | -2212.821107 |
| ⁶ TS13 | -2212.821954 | -2212.771098 | -2212.770155 | -2212.917326 | -2212.798913 |
| ⁴ IN18 | -2212.909188 | -2212.857789 | -2212.856846 | -2213.009547 | -2212.875218 |
| ⁶ IN18 | -2212.886072 | -2212.834660 | -2212.833716 | -2212.984588 | -2212.866736 |
| ⁴ IN19 | -2212.912821 | -2212.861422 | -2212.860478 | -2213.012197 | -2212.883489 |
| ⁶ IN19 | -2212.896770 | -2212.845179 | -2212.844235 | -2212.996191 | -2212.878380 |
| ⁴ TS14 | -2289.300653 | -2289.247821 | -2289.246878 | -2289.398726 | -2289.307764 |
| ⁶ TS14 | -2289.293606 | -2289.240967 | -2289.240024 | -2289.389407 | -2289.297840 |
| ⁴ IN20 | -2289.383571 | -2289.329532 | -2289.328588 | -2289.491064 | -2289.337414 |
| ⁶ IN20 | -2289.370060 | -2289.315969 | -2289.315025 | -2289.475878 | -2289.350600 |
| ⁴ TS15 | -2212.811689 | -2212.759236 | -2212.758292 | -2212.910188 | -2212.792316 |
| ⁶ TS15 | -2212.824770 | -2212.773442 | -2212.772498 | -2212.922267 | -2212.808289 |
| ⁴ IN21 | -2212.900041 | -2212.848366 | -2212.847422 | -2212.999055 | -2212.881700 |
| ⁶ IN21 | -2212.886961 | -2212.835082 | -2212.834138 | -2212.986903 | -2212.880230 |
| ¹ IN6 | -1321.605266 | -1321.578149 | -1321.577205 | -1321.665828 | -1321.543362 |
| ¹ TS4 | -1321.589591 | -1321.563429 | -1321.562486 | -1321.648195 | -1321.517907 |
| ¹ IN7 | -1321.593417 | -1321.566563 | -1321.565619 | -1321.654347 | -1321.524864 |
| ⁴ TS16 | -2212.828637 | -2212.776586 | -2212.775643 | -2212.926960 | -2212.800122 |
| ⁶ TS16 | -2212.822313 | -2212.771676 | -2212.770732 | -2212.920121 | -2212.803644 |
| ³ TS17 | -1321.616303 | -1321.589625 | -1321.588681 | -1321.679251 | -1321.574262 |
| ⁵ TS17 | -1321.636306 | -1321.609939 | -1321.608995 | -1321.699133 | -1321.610092 |
| ³ IN22 | -1321.629665 | -1321.602461 | -1321.601517 | -1321.692356 | -1321.580312 |
| ⁵ IN22 | -1321.636196 | -1321.608071 | -1321.607127 | -1321.704215 | -1321.608446 |
| ⁴ TS18 | -1746.179675 | -1746.142826 | -1746.141882 | -1746.257713 | -1746.130815 |
| ⁶ TS18 | -1746.184716 | -1746.145672 | -1746.144729 | -1746.269491 | -1746.149035 |
| ⁴ TS19 | -1746.226718 | -1746.188843 | -1746.187899 | -1746.306635 | -1746.185759 |

| | | | | | |
|---------------------|--------------|--------------|--------------|--------------|--------------|
| ⁶ TS19 | -1746.200149 | -1746.162018 | -1746.161074 | -1746.281039 | -1746.169647 |
| TS20 | -1131.774711 | -1131.748884 | -1131.747941 | -1131.836339 | -1131.787743 |
| IN23 | -1131.867199 | -1131.841310 | -1131.840367 | -1131.930472 | -1131.883640 |
| ⁴ IN24 | -2212.909752 | -2212.858555 | -2212.857611 | -2213.006999 | -2212.877173 |
| ⁶ IN24 | -2212.888274 | -2212.837702 | -2212.836758 | -2212.984357 | -2212.864287 |
| ⁴ TS21 | -2289.299315 | -2289.246238 | -2289.245294 | -2289.400729 | -2289.285434 |
| ⁶ TS21 | -2289.285977 | -2289.233120 | -2289.232177 | -2289.385214 | -2289.287698 |
| ⁴ IN25 | -2289.380908 | -2289.326815 | -2289.325871 | -2289.485079 | -2289.361767 |
| ⁶ IN25 | -2289.373874 | -2289.319646 | -2289.318702 | -2289.479878 | -2289.357992 |
| ⁵ TS22 | -1788.267703 | -1788.226723 | -1788.225779 | -1788.349511 | -1788.249546 |
| ⁵ TS23 | -1788.266803 | -1788.225801 | -1788.224858 | -1788.349418 | -1788.250763 |
| ⁵ TS24 | -1788.274697 | -1788.234652 | -1788.233709 | -1788.355336 | -1788.261537 |
| ⁵ TS25 | -1788.274811 | -1788.233826 | -1788.232882 | -1788.357447 | -1788.263948 |
| ⁵ IN26 | -1788.297942 | -1788.257032 | -1788.256089 | -1788.379438 | -1788.269270 |
| ⁵ IN27 | -1788.285750 | -1788.244403 | -1788.243459 | -1788.370389 | -1788.259772 |
| ⁵ IN28 | -1788.291096 | -1788.250082 | -1788.249138 | -1788.372563 | -1788.277380 |
| ⁵ IN29 | -1788.301021 | -1788.260074 | -1788.259131 | -1788.381887 | -1788.277864 |
| ⁴ TS26 | -2212.898943 | -2212.848126 | -2212.847182 | -2212.995705 | -2212.873683 |
| ⁶ TS26 | -2212.880795 | -2212.831488 | -2212.830544 | -2212.975344 | -2212.872090 |
| ⁴ TS27 | -2212.895342 | -2212.844503 | -2212.843559 | -2212.991391 | -2212.873340 |
| ⁶ TS27 | -2212.875994 | -2212.824599 | -2212.823655 | -2212.974855 | -2212.859775 |
| ⁴ IN30 | -2212.921945 | -2212.870550 | -2212.869606 | -2213.021643 | -2212.879459 |
| ⁶ IN30 | -2212.910168 | -2212.859491 | -2212.858548 | -2213.007992 | -2212.871697 |
| ⁴ TS28 | -2289.285637 | -2289.232476 | -2289.231533 | -2289.385830 | -2289.272977 |
| ⁶ TS28 | -2289.272984 | -2289.219864 | -2289.218921 | -2289.375871 | -2289.271130 |
| ² TS1-1 | -1518.986121 | -1518.951396 | -1518.950453 | -1519.058407 | -1518.862294 |
| ⁴ TS1-1 | -1518.995983 | -1518.961017 | -1518.960073 | -1519.071042 | -1518.857612 |
| ⁶ TS1-1 | -1519.008556 | -1518.974136 | -1518.973192 | -1519.081525 | -1518.900376 |
| ² TS2-1 | -1518.961344 | -1518.926116 | -1518.925173 | -1519.034334 | -1518.847919 |
| ⁴ TS2-1 | -1518.998883 | -1518.964196 | -1518.963252 | -1519.072682 | -1518.901369 |
| ⁶ TS5-1 | -1746.192340 | -1746.153592 | -1746.152648 | -1746.274512 | -1746.157908 |
| ⁶ TS5-2 | -1746.189336 | -1746.150577 | -1746.149633 | -1746.271870 | -1746.153556 |
| ⁴ TS7-1 | -1519.007391 | -1518.971512 | -1518.970569 | -1519.081566 | -1518.952725 |
| ⁴ TS7-2 | -1519.011177 | -1518.975246 | -1518.974303 | -1519.086479 | -1518.889372 |
| ⁶ TS7-1 | -1519.041695 | -1519.005312 | -1519.004368 | -1519.118362 | -1518.949279 |
| ⁶ TS7-2 | -1519.035572 | -1518.999316 | -1518.998372 | -1519.111829 | -1518.944938 |
| ³ TS8-1 | -1788.268362 | -1788.228138 | -1788.227195 | -1788.349334 | -1788.238213 |
| ³ TS8-2 | -1788.259318 | -1788.219428 | -1788.218485 | -1788.336778 | -1788.227421 |
| ³ TS8-3 | -1788.264005 | -1788.224158 | -1788.223214 | -1788.340824 | -1788.238464 |
| ⁵ TS8-1 | -1788.281190 | -1788.240064 | -1788.239120 | -1788.363359 | -1788.269567 |
| ⁵ TS8-2 | -1788.279448 | -1788.238488 | -1788.237544 | -1788.360029 | -1788.269862 |
| ⁵ TS8-3 | -1788.279250 | -1788.238416 | -1788.237472 | -1788.360282 | -1788.265385 |
| ⁴ TS12-1 | -2212.845874 | -2212.795182 | -2212.794239 | -2212.939884 | -2212.819213 |

| | | | | | |
|---------------------|--------------|--------------|--------------|--------------|--------------|
| ⁴ TS12-2 | -2212.833977 | -2212.782745 | -2212.781801 | -2212.929831 | -2212.813757 |
| ⁴ TS15-1 | -2212.812961 | -2212.760766 | -2212.759822 | -2212.910906 | -2212.785560 |
| ⁶ TS15-1 | -2212.818093 | -2212.769053 | -2212.768109 | -2212.912983 | -2212.799233 |
| ⁴ TS16-1 | -2212.821919 | -2212.771593 | -2212.770649 | -2212.915564 | -2212.803014 |
| ⁶ TS16-1 | -2212.813965 | -2212.763637 | -2212.762694 | -2212.909061 | -2212.791538 |
| ⁴ TS29 | -1985.640662 | -1985.591160 | -1985.590217 | -1985.732847 | -1985.554305 |
| ⁶ TS29 | -1985.665789 | -1985.619413 | -1985.618470 | -1985.750724 | -1985.590992 |

E_0 = Sum of electronic and zero-point energies calculated by B3LYP in gas phase

E = Sum of electronic and thermal energies calculated by B3LYP in gas phase

$H_{298.15}$ = Sum of electronic and thermal enthalpies calculated by B3LYP in gas phase

$G_{298.15}$ = Sum of electronic and thermal free energies calculated by B3LYP in gas phase

$E_{(M06)}$ = Single point energies calculated by M06 in solvent

Section 4. Calculated imaginary frequencies of all transition states species.

| Species | Frequency |
|------------------|-----------|
| ² TS1 | -245.45 |
| ⁴ TS1 | -250.23 |
| ⁶ TS1 | -323.13 |
| ² TS2 | -293.98 |
| ⁴ TS2 | -335.11 |
| TS3 | -327.22 |
| ³ TS4 | -61.11 |
| ⁵ TS4 | -60.44 |
| ⁴ TS5 | -90.05 |
| ⁶ TS5 | -106.86 |
| ⁴ TS6 | -62.65 |
| ⁶ TS6 | -12.30 |
| ⁴ TS7 | -32.78 |
| ⁶ TS7 | -72.09 |
| ³ TS8 | -38.63 |
| ⁵ TS8 | -64.59 |
| ⁴ TS9 | -59.93 |

| | |
|--------------------|----------|
| ⁶ TS9 | -349.05 |
| ⁴ TS10 | -27.86 |
| ⁶ TS10 | -39.80 |
| TS11 | -389.05 |
| ⁴ TS12 | -426.00 |
| ⁶ TS12 | -296.01 |
| ⁴ TS13 | -386.06 |
| ⁶ TS13 | -257.84 |
| ⁴ TS14 | -482.52 |
| ⁶ TS14 | -887.74 |
| ⁴ TS15 | -335.61 |
| ⁶ TS15 | -402.88 |
| ¹ TS4 | -39.33 |
| ⁴ TS16 | -474.59 |
| ⁶ TS16 | -541.42 |
| ³ TS17 | -54.22 |
| ⁵ TS17 | -20.39 |
| ⁴ TS18 | -89.32 |
| ⁶ TS18 | -51.43 |
| ⁴ TS19 | -49.74 |
| ⁶ TS19 | -41.45 |
| TS20 | -437.22 |
| ⁴ TS21 | -308.45 |
| ⁶ TS21 | -1067.51 |
| ⁵ TS22 | -131.45 |
| ⁵ TS23 | -146.41 |
| ⁵ TS24 | -147.18 |
| ⁵ TS25 | -138.52 |
| ⁴ TS26 | -62.49 |
| ⁶ TS26 | -83.70 |
| ⁴ TS27 | -57.68 |
| ⁶ TS27 | -42.13 |
| ⁴ TS28 | -1367.48 |
| ⁶ TS28 | -1412.77 |
| ² TS1-1 | -323.52 |
| ⁴ TS1-1 | -254.52 |
| ⁶ TS1-1 | -227.15 |
| ² TS2-1 | -352.84 |
| ⁴ TS2-1 | -415.46 |
| ⁶ TS5-1 | -121.03 |
| ⁶ TS5-2 | -91.92 |
| ⁴ TS7-1 | -92.32 |
| ⁴ TS7-2 | -123.03 |

| | |
|---------------------|---------|
| ⁶ TS7-1 | -70.57 |
| ⁶ TS7-2 | -110.39 |
| ³ TS8-1 | -54.41 |
| ³ TS8-2 | -59.48 |
| ³ TS8-3 | -59.05 |
| ⁵ TS8-1 | -47.68 |
| ⁵ TS8-2 | -28.34 |
| ⁵ TS8-3 | -39.82 |
| ⁴ TS12-1 | -378.36 |
| ⁴ TS12-2 | -400.13 |
| ⁴ TS15-1 | -338.85 |
| ⁶ TS15-1 | -358.03 |
| ⁴ TS16-1 | -355.08 |
| ⁶ TS16-1 | -409.05 |
| ⁴ TS29 | -401.64 |
| ⁶ TS29 | -405.49 |