# 附录1

特征转换后的特征描述符与目标值OP的数据集：（其中原子序数加权平均值表示为、非键合原子半径加权平均值表示为****、共价半径加权平均值表示为、第一电离能加权平均值表示为****、第二电离能加权平均值表示为****、电子亲和能加权平均值表示为****、鲍林电负性加权平均值表示为、最外层D轨道电子数加权平均值表示为****、原子序数方差表示为*δ*AN、非键合原子半径方差表示为*δ*RA、共价半径方差表示为*δ*RC、第一电离能方差表示为*δ*FIE、第二电离能方差表示为*δ*SIE、电子亲和能方差表示为*δ*EA、鲍林电负性方差表示为*δ*EP、最外层D轨道电子数方差表示为*δ*DE、过电位表示为OP）

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |
| 2.003208 | 1.021247 | 8.589917 | 18.694707 | 1.146822 | 10.412900 | 1.910021 | 5.329400 |
| 2.003083 | 1.019081 | 8.590141 | 18.688425 | 1.150108 | 10.490000 | 1.906585 | 5.324500 |
| 2.002958 | 1.017097 | 8.591918 | 18.685668 | 1.153711 | 10.570600 | 1.903464 | 5.321100 |
| 2.002833 | 1.014997 | 8.592930 | 18.681094 | 1.157197 | 10.650400 | 1.900146 | 5.316900 |
| 2.002708 | 1.012831 | 8.593154 | 18.674812 | 1.160483 | 10.727500 | 1.896710 | 5.312000 |
| 2.002583 | 1.010847 | 8.594930 | 18.672055 | 1.164086 | 10.808100 | 1.893589 | 5.308600 |
| 2.002458 | 1.008747 | 8.595942 | 18.667482 | 1.167572 | 10.887900 | 1.890271 | 5.304400 |
| 2.002333 | 1.006581 | 8.596166 | 18.661200 | 1.170858 | 10.965000 | 1.886835 | 5.299500 |
| 2.002208 | 1.004597 | 8.597943 | 18.658443 | 1.174461 | 11.045600 | 1.883714 | 5.296100 |
| 2.002083 | 1.002497 | 8.598955 | 18.653869 | 1.177947 | 11.125400 | 1.880396 | 5.291900 |
| 2.001958 | 1.000331 | 8.599179 | 18.647587 | 1.181233 | 11.202500 | 1.876960 | 5.287000 |
| 2.001833 | 0.998347 | 8.600955 | 18.644830 | 1.184836 | 11.283100 | 1.873839 | 5.283600 |
| 2.001708 | 0.996247 | 8.601967 | 18.640257 | 1.188322 | 11.362900 | 1.870521 | 5.279400 |
| 2.001583 | 0.994081 | 8.602191 | 18.633975 | 1.191608 | 11.440000 | 1.867085 | 5.274500 |
| 2.001458 | 0.992097 | 8.603968 | 18.631218 | 1.195211 | 11.520600 | 1.863964 | 5.271100 |
| 2.001333 | 0.989997 | 8.604980 | 18.626644 | 1.198697 | 11.600400 | 1.860646 | 5.266900 |
| 2.001208 | 0.987831 | 8.605204 | 18.620362 | 1.201983 | 11.677500 | 1.857210 | 5.262000 |
| 2.001083 | 0.985847 | 8.606980 | 18.617605 | 1.205586 | 11.758100 | 1.854089 | 5.258600 |
| 2.000958 | 0.983747 | 8.607992 | 18.613032 | 1.209072 | 11.837900 | 1.850771 | 5.254400 |
| 2.000833 | 0.981581 | 8.608216 | 18.606750 | 1.212358 | 11.915000 | 1.847335 | 5.249500 |
| 2.003000 | 1.019160 | 8.590010 | 18.690960 | 1.146990 | 10.408700 | 1.910273 | 5.325200 |
| 2.002667 | 1.014956 | 8.590324 | 18.681021 | 1.150440 | 10.481700 | 1.907083 | 5.316200 |
| 2.002333 | 1.010885 | 8.592193 | 18.674518 | 1.154211 | 10.558100 | 1.904214 | 5.308600 |
| 2.002000 | 1.006697 | 8.593297 | 18.666198 | 1.157865 | 10.633700 | 1.901148 | 5.300200 |
| 2.001667 | 1.002493 | 8.593612 | 18.656259 | 1.161315 | 10.706700 | 1.897958 | 5.291200 |
| 2.001333 | 0.998422 | 8.595480 | 18.649755 | 1.165086 | 10.783100 | 1.895089 | 5.283600 |
| 2.001000 | 0.994235 | 8.596585 | 18.641435 | 1.168740 | 10.858700 | 1.892023 | 5.275200 |
| 2.000667 | 0.990031 | 8.596899 | 18.631496 | 1.172190 | 10.931700 | 1.888833 | 5.266200 |
| 2.000333 | 0.985960 | 8.598768 | 18.624993 | 1.175961 | 11.008100 | 1.885964 | 5.258600 |
| 2.000000 | 0.981772 | 8.599872 | 18.616673 | 1.179615 | 11.083700 | 1.882898 | 5.250200 |
| 1.999667 | 0.977568 | 8.600187 | 18.606734 | 1.183065 | 11.156700 | 1.879708 | 5.241200 |
| 1.999333 | 0.973497 | 8.602055 | 18.600230 | 1.186836 | 11.233100 | 1.876839 | 5.233600 |
| 1.999000 | 0.969310 | 8.603160 | 18.591910 | 1.190490 | 11.308700 | 1.873773 | 5.225200 |
| 1.998667 | 0.965106 | 8.603474 | 18.581971 | 1.193940 | 11.381700 | 1.870583 | 5.216200 |
| 1.998333 | 0.961035 | 8.605343 | 18.575468 | 1.197711 | 11.458100 | 1.867714 | 5.208600 |
| 1.998000 | 0.956847 | 8.606447 | 18.567148 | 1.201365 | 11.533700 | 1.864648 | 5.200200 |
| 1.997667 | 0.952643 | 8.606762 | 18.557209 | 1.204815 | 11.606700 | 1.861458 | 5.191200 |
| 1.997333 | 0.948572 | 8.608630 | 18.550705 | 1.208586 | 11.683100 | 1.858589 | 5.183600 |
| 1.997000 | 0.944385 | 8.609735 | 18.542385 | 1.212240 | 11.758700 | 1.855523 | 5.175200 |
| 1.996667 | 0.940181 | 8.610049 | 18.532446 | 1.215690 | 11.831700 | 1.852333 | 5.166200 |
| 2.001833 | 1.018475 | 8.588040 | 18.688659 | 1.143840 | 10.404500 | 1.913675 | 5.321000 |
| 2.000333 | 1.013603 | 8.586431 | 18.676473 | 1.144215 | 10.473400 | 1.913806 | 5.307900 |
| 1.998833 | 1.008847 | 8.586330 | 18.667668 | 1.144836 | 10.545600 | 1.914339 | 5.296100 |
| 1.997333 | 1.003975 | 8.585465 | 18.657046 | 1.145340 | 10.617000 | 1.914675 | 5.283500 |
| 1.995833 | 0.999103 | 8.583856 | 18.644860 | 1.145715 | 10.685900 | 1.914806 | 5.270400 |
| 1.994333 | 0.994347 | 8.583755 | 18.636055 | 1.146336 | 10.758100 | 1.915339 | 5.258600 |
| 1.992833 | 0.989475 | 8.582890 | 18.625434 | 1.146840 | 10.829500 | 1.915675 | 5.246000 |
| 1.991333 | 0.984603 | 8.581281 | 18.613248 | 1.147215 | 10.898400 | 1.915806 | 5.232900 |
| 1.989833 | 0.979847 | 8.581180 | 18.604443 | 1.147836 | 10.970600 | 1.916339 | 5.221100 |
| 1.988333 | 0.974975 | 8.580315 | 18.593821 | 1.148340 | 11.042000 | 1.916675 | 5.208500 |
| 1.986833 | 0.970103 | 8.578706 | 18.581635 | 1.148715 | 11.110900 | 1.916806 | 5.195400 |
| 1.985333 | 0.965347 | 8.578605 | 18.572830 | 1.149336 | 11.183100 | 1.917339 | 5.183600 |
| 1.983833 | 0.960475 | 8.577740 | 18.562209 | 1.149840 | 11.254500 | 1.917675 | 5.171000 |
| 1.982333 | 0.955603 | 8.576131 | 18.550023 | 1.150215 | 11.323400 | 1.917806 | 5.157900 |
| 1.980833 | 0.950847 | 8.576030 | 18.541218 | 1.150836 | 11.395600 | 1.918339 | 5.146100 |
| 1.979333 | 0.945975 | 8.575165 | 18.530596 | 1.151340 | 11.467000 | 1.918675 | 5.133500 |
| 1.977833 | 0.941103 | 8.573556 | 18.518410 | 1.151715 | 11.535900 | 1.918806 | 5.120400 |
| 1.976333 | 0.936347 | 8.573455 | 18.509605 | 1.152336 | 11.608100 | 1.919339 | 5.108600 |
| 1.974833 | 0.931475 | 8.572590 | 18.498984 | 1.152840 | 11.679500 | 1.919675 | 5.096000 |
| 1.973333 | 0.926603 | 8.570981 | 18.486798 | 1.153215 | 11.748400 | 1.919806 | 5.082900 |
| 2.003292 | 1.023628 | 8.589271 | 18.708197 | 1.146654 | 10.421300 | 1.910189 | 5.342000 |
| 2.003250 | 1.023787 | 8.588863 | 18.715084 | 1.149776 | 10.506600 | 1.906917 | 5.349400 |
| 2.003208 | 1.024185 | 8.589993 | 18.725818 | 1.153211 | 10.595600 | 1.903964 | 5.358600 |
| 2.003167 | 1.024466 | 8.590358 | 18.734734 | 1.156529 | 10.683800 | 1.900814 | 5.367000 |
| 2.003125 | 1.024625 | 8.589951 | 18.741622 | 1.159651 | 10.769100 | 1.897542 | 5.374400 |
| 2.003083 | 1.025022 | 8.591080 | 18.752355 | 1.163086 | 10.858100 | 1.894589 | 5.383600 |
| 2.003042 | 1.025303 | 8.591446 | 18.761272 | 1.166404 | 10.946300 | 1.891439 | 5.392000 |
| 2.003000 | 1.025462 | 8.591038 | 18.768159 | 1.169526 | 11.031600 | 1.888167 | 5.399400 |
| 2.002958 | 1.025860 | 8.592168 | 18.778893 | 1.172961 | 11.120600 | 1.885214 | 5.408600 |
| 2.002917 | 1.026141 | 8.592533 | 18.787809 | 1.176279 | 11.208800 | 1.882064 | 5.417000 |
| 2.002875 | 1.026300 | 8.592126 | 18.794697 | 1.179401 | 11.294100 | 1.878792 | 5.424400 |
| 2.002833 | 1.026697 | 8.593255 | 18.805430 | 1.182836 | 11.383100 | 1.875839 | 5.433600 |
| 2.002792 | 1.026978 | 8.593621 | 18.814347 | 1.186154 | 11.471300 | 1.872689 | 5.442000 |
| 2.002750 | 1.027137 | 8.593213 | 18.821234 | 1.189276 | 11.556600 | 1.869417 | 5.449400 |
| 2.002708 | 1.027535 | 8.594343 | 18.831968 | 1.192711 | 11.645600 | 1.866464 | 5.458600 |
| 2.002667 | 1.027816 | 8.594708 | 18.840884 | 1.196029 | 11.733800 | 1.863314 | 5.467000 |
| 2.002625 | 1.027975 | 8.594301 | 18.847772 | 1.199151 | 11.819100 | 1.860042 | 5.474400 |
| 2.002583 | 1.028372 | 8.595430 | 18.858505 | 1.202586 | 11.908100 | 1.857089 | 5.483600 |
| 2.002542 | 1.028653 | 8.595796 | 18.867422 | 1.205904 | 11.996300 | 1.853939 | 5.492000 |
| 2.002500 | 1.028812 | 8.595388 | 18.874309 | 1.209026 | 12.081600 | 1.850667 | 5.499400 |
| 2.000917 | 1.020264 | 8.583700 | 18.676059 | 1.147788 | 10.467500 | 1.911953 | 5.308400 |
| 1.998500 | 1.017139 | 8.577855 | 18.651573 | 1.152017 | 10.597900 | 1.910403 | 5.283000 |
| 1.996083 | 1.014172 | 8.573414 | 18.630168 | 1.156586 | 10.733100 | 1.909214 | 5.258600 |
| 1.993667 | 1.011089 | 8.568209 | 18.606946 | 1.161038 | 10.867500 | 1.907828 | 5.233400 |
| 1.991250 | 1.007964 | 8.562364 | 18.582460 | 1.165267 | 10.997900 | 1.906278 | 5.208000 |
| 1.988833 | 1.004997 | 8.557924 | 18.561055 | 1.169836 | 11.133100 | 1.905089 | 5.183600 |
| 1.986417 | 1.001914 | 8.552719 | 18.537834 | 1.174288 | 11.267500 | 1.903703 | 5.158400 |
| 1.984000 | 0.998789 | 8.546874 | 18.513348 | 1.178517 | 11.397900 | 1.902153 | 5.133000 |
| 1.981583 | 0.995822 | 8.542433 | 18.491943 | 1.183086 | 11.533100 | 1.900964 | 5.108600 |
| 1.979167 | 0.992739 | 8.537228 | 18.468721 | 1.187538 | 11.667500 | 1.899578 | 5.083400 |
| 1.976750 | 0.989614 | 8.531383 | 18.444235 | 1.191767 | 11.797900 | 1.898028 | 5.058000 |
| 1.974333 | 0.986647 | 8.526942 | 18.422830 | 1.196336 | 11.933100 | 1.896839 | 5.033600 |
| 1.971917 | 0.983564 | 8.521737 | 18.399609 | 1.200788 | 12.067500 | 1.895453 | 5.008400 |
| 1.969500 | 0.980439 | 8.515892 | 18.375123 | 1.205017 | 12.197900 | 1.893903 | 4.983000 |
| 1.967083 | 0.977472 | 8.511451 | 18.353718 | 1.209586 | 12.333100 | 1.892714 | 4.958600 |
| 1.964667 | 0.974389 | 8.506246 | 18.330496 | 1.214038 | 12.467500 | 1.891328 | 4.933400 |
| 1.962250 | 0.971264 | 8.500401 | 18.306010 | 1.218267 | 12.597900 | 1.889778 | 4.908000 |
| 1.959833 | 0.968297 | 8.495961 | 18.284605 | 1.222836 | 12.733100 | 1.888589 | 4.883600 |
| 1.957417 | 0.965214 | 8.490756 | 18.261384 | 1.227288 | 12.867500 | 1.887203 | 4.858400 |
| 1.955000 | 0.962089 | 8.484911 | 18.236898 | 1.231517 | 12.997900 | 1.885653 | 4.833000 |
| 2.005208 | 1.021898 | 8.590333 | 18.696975 | 1.147578 | 10.610300 | 1.911365 | 5.316800 |
| 2.007083 | 1.020368 | 8.590963 | 18.692907 | 1.151602 | 10.880100 | 1.909241 | 5.299600 |
| 2.008958 | 1.019035 | 8.593155 | 18.692418 | 1.155961 | 11.158100 | 1.907464 | 5.283600 |
| 2.010833 | 1.017586 | 8.594583 | 18.690112 | 1.160203 | 11.435300 | 1.905490 | 5.266800 |
| 2.012708 | 1.016055 | 8.595213 | 18.686044 | 1.164227 | 11.705100 | 1.903366 | 5.249600 |
| 2.014583 | 1.014722 | 8.597405 | 18.685555 | 1.168586 | 11.983100 | 1.901589 | 5.233600 |
| 2.016458 | 1.013273 | 8.598833 | 18.683250 | 1.172828 | 12.260300 | 1.899615 | 5.216800 |
| 2.018333 | 1.011743 | 8.599463 | 18.679182 | 1.176852 | 12.530100 | 1.897491 | 5.199600 |
| 2.020208 | 1.010410 | 8.601655 | 18.678693 | 1.181211 | 12.808100 | 1.895714 | 5.183600 |
| 2.022083 | 1.008961 | 8.603083 | 18.676387 | 1.185453 | 13.085300 | 1.893740 | 5.166800 |
| 2.023958 | 1.007430 | 8.603713 | 18.672319 | 1.189477 | 13.355100 | 1.891616 | 5.149600 |
| 2.025833 | 1.006097 | 8.605905 | 18.671830 | 1.193836 | 13.633100 | 1.889839 | 5.133600 |
| 2.027708 | 1.004648 | 8.607333 | 18.669525 | 1.198078 | 13.910300 | 1.887865 | 5.116800 |
| 2.029583 | 1.003118 | 8.607963 | 18.665457 | 1.202102 | 14.180100 | 1.885741 | 5.099600 |
| 2.031458 | 1.001785 | 8.610155 | 18.664968 | 1.206461 | 14.458100 | 1.883964 | 5.083600 |
| 2.033333 | 1.000336 | 8.611583 | 18.662662 | 1.210703 | 14.735300 | 1.881990 | 5.066800 |
| 2.035208 | 0.998805 | 8.612213 | 18.658594 | 1.214727 | 15.005100 | 1.879866 | 5.049600 |
| 2.037083 | 0.997472 | 8.614405 | 18.658105 | 1.219086 | 15.283100 | 1.878089 | 5.033600 |
| 2.038958 | 0.996023 | 8.615833 | 18.655800 | 1.223328 | 15.560300 | 1.876115 | 5.016800 |
| 2.040833 | 0.994493 | 8.616463 | 18.651732 | 1.227352 | 15.830100 | 1.873991 | 4.999600 |
| 2.004375 | 1.021604 | 8.586604 | 18.690885 | 1.147536 | 10.475900 | 1.911197 | 5.321000 |
| 2.005417 | 1.019787 | 8.583593 | 18.680872 | 1.151519 | 10.614500 | 1.908909 | 5.307900 |
| 2.006458 | 1.018160 | 8.582055 | 18.674293 | 1.155836 | 10.758100 | 1.906964 | 5.296100 |
| 2.007500 | 1.016417 | 8.579754 | 18.665897 | 1.160036 | 10.900900 | 1.904822 | 5.283500 |
| 2.008542 | 1.014599 | 8.576743 | 18.655884 | 1.164019 | 11.039500 | 1.902534 | 5.270400 |
| 2.009583 | 1.012972 | 8.575205 | 18.649305 | 1.168336 | 11.183100 | 1.900589 | 5.258600 |
| 2.010625 | 1.011229 | 8.572904 | 18.640910 | 1.172536 | 11.325900 | 1.898447 | 5.246000 |
| 2.011667 | 1.009412 | 8.569893 | 18.630897 | 1.176519 | 11.464500 | 1.896159 | 5.232900 |
| 2.012708 | 1.007785 | 8.568355 | 18.624318 | 1.180836 | 11.608100 | 1.894214 | 5.221100 |
| 2.013750 | 1.006042 | 8.566054 | 18.615922 | 1.185036 | 11.750900 | 1.892072 | 5.208500 |
| 2.014792 | 1.004224 | 8.563043 | 18.605909 | 1.189019 | 11.889500 | 1.889784 | 5.195400 |
| 2.015833 | 1.002597 | 8.561505 | 18.599330 | 1.193336 | 12.033100 | 1.887839 | 5.183600 |
| 2.016875 | 1.000854 | 8.559204 | 18.590935 | 1.197536 | 12.175900 | 1.885697 | 5.171000 |
| 2.017917 | 0.999037 | 8.556193 | 18.580922 | 1.201519 | 12.314500 | 1.883409 | 5.157900 |
| 2.018958 | 0.997410 | 8.554655 | 18.574343 | 1.205836 | 12.458100 | 1.881464 | 5.146100 |
| 2.020000 | 0.995667 | 8.552354 | 18.565947 | 1.210036 | 12.600900 | 1.879322 | 5.133500 |
| 2.021042 | 0.993849 | 8.549343 | 18.555934 | 1.214019 | 12.739500 | 1.877034 | 5.120400 |
| 2.022083 | 0.992222 | 8.547805 | 18.549355 | 1.218336 | 12.883100 | 1.875089 | 5.108600 |
| 2.023125 | 0.990479 | 8.545504 | 18.540960 | 1.222536 | 13.025900 | 1.872947 | 5.096000 |
| 2.024167 | 0.988662 | 8.542493 | 18.530947 | 1.226519 | 13.164500 | 1.870659 | 5.082900 |
| 2.002167 | 1.020676 | 8.585150 | 18.684543 | 1.147116 | 10.396100 | 1.911113 | 5.312600 |
| 2.001000 | 1.017952 | 8.580721 | 18.668339 | 1.150689 | 10.456800 | 1.908743 | 5.291300 |
| 1.999833 | 1.015397 | 8.577730 | 18.655418 | 1.154586 | 10.520600 | 1.906714 | 5.271100 |
| 1.998667 | 1.012726 | 8.573975 | 18.640680 | 1.158366 | 10.583600 | 1.904488 | 5.250100 |
| 1.997500 | 1.010002 | 8.569546 | 18.624476 | 1.161939 | 10.644300 | 1.902118 | 5.228800 |
| 1.996333 | 1.007447 | 8.566555 | 18.611555 | 1.165836 | 10.708100 | 1.900089 | 5.208600 |
| 1.995167 | 1.004776 | 8.562800 | 18.596818 | 1.169616 | 10.771100 | 1.897863 | 5.187600 |
| 1.994000 | 1.002052 | 8.558371 | 18.580614 | 1.173189 | 10.831800 | 1.895493 | 5.166300 |
| 1.992833 | 0.999497 | 8.555380 | 18.567693 | 1.177086 | 10.895600 | 1.893464 | 5.146100 |
| 1.991667 | 0.996826 | 8.551625 | 18.552955 | 1.180866 | 10.958600 | 1.891238 | 5.125100 |
| 1.990500 | 0.994102 | 8.547196 | 18.536751 | 1.184439 | 11.019300 | 1.888868 | 5.103800 |
| 1.989333 | 0.991547 | 8.544205 | 18.523830 | 1.188336 | 11.083100 | 1.886839 | 5.083600 |
| 1.988167 | 0.988876 | 8.540450 | 18.509093 | 1.192116 | 11.146100 | 1.884613 | 5.062600 |
| 1.987000 | 0.986152 | 8.536021 | 18.492889 | 1.195689 | 11.206800 | 1.882243 | 5.041300 |
| 1.985833 | 0.983597 | 8.533030 | 18.479968 | 1.199586 | 11.270600 | 1.880214 | 5.021100 |
| 1.984667 | 0.980926 | 8.529275 | 18.465230 | 1.203366 | 11.333600 | 1.877988 | 5.000100 |
| 1.983500 | 0.978202 | 8.524846 | 18.449026 | 1.206939 | 11.394300 | 1.875618 | 4.978800 |
| 1.982333 | 0.975647 | 8.521855 | 18.436105 | 1.210836 | 11.458100 | 1.873589 | 4.958600 |
| 1.981167 | 0.972976 | 8.518100 | 18.421368 | 1.214616 | 11.521100 | 1.871363 | 4.937600 |
| 1.98 | 0.9702522 | 8.5136709 | 18.405163 | 1.218189 | 11.5818 | 1.868993 | 4.9163 |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **δ**EP | **δ**EA | **δ**FIE | **δ**SIE | **δ**RA | **δ**AN | **δ**RC | **δ**DE | **OP** |
| 0.017449 | 0.037825 | 1.799434 | 0.572290 | 0.004489 | 12.025814 | 0.008656 | 14.203296 | 145.6 |
| 0.017474 | 0.038275 | 1.797704 | 0.581803 | 0.007460 | 13.123296 | 0.010816 | 14.184765 | 145.3 |
| 0.017502 | 0.038731 | 1.796112 | 0.591554 | 0.010479 | 14.236216 | 0.013007 | 14.167195 | 143.1 |
| 0.017530 | 0.039177 | 1.794428 | 0.601241 | 0.013474 | 15.335780 | 0.015175 | 14.148874 | 140.7 |
| 0.017555 | 0.039601 | 1.792691 | 0.610634 | 0.016374 | 16.396136 | 0.017271 | 14.130234 | 138.4 |
| 0.017583 | 0.040031 | 1.791093 | 0.620259 | 0.019321 | 17.471274 | 0.019396 | 14.112566 | 137.6 |
| 0.017610 | 0.040450 | 1.789403 | 0.629821 | 0.022243 | 18.532934 | 0.021499 | 14.094141 | 134.9 |
| 0.017636 | 0.040849 | 1.787660 | 0.639094 | 0.025073 | 19.556152 | 0.023531 | 14.075391 | 131.6 |
| 0.017664 | 0.041253 | 1.786057 | 0.648594 | 0.027947 | 20.593521 | 0.025591 | 14.057625 | 129.4 |
| 0.017691 | 0.041646 | 1.784360 | 0.658031 | 0.030797 | 21.617275 | 0.027628 | 14.039094 | 127.1 |
| 0.017716 | 0.042018 | 1.782611 | 0.667183 | 0.033556 | 22.603344 | 0.029596 | 14.020236 | 127.3 |
| 0.017744 | 0.042396 | 1.781002 | 0.676558 | 0.036358 | 23.602954 | 0.031590 | 14.002371 | 121.7 |
| 0.017771 | 0.042763 | 1.779300 | 0.685870 | 0.039136 | 24.588804 | 0.033563 | 13.983736 | 122.4 |
| 0.017796 | 0.043109 | 1.777544 | 0.694902 | 0.041824 | 25.537713 | 0.035465 | 13.964768 | 119.3 |
| 0.017824 | 0.043461 | 1.775929 | 0.704151 | 0.044554 | 26.499576 | 0.037395 | 13.946805 | 120.4 |
| 0.017851 | 0.043802 | 1.774221 | 0.713339 | 0.047259 | 27.447520 | 0.039302 | 13.928064 | 123.4 |
| 0.017876 | 0.044123 | 1.772458 | 0.722251 | 0.049877 | 28.359257 | 0.041140 | 13.908987 | 121.7 |
| 0.017904 | 0.044448 | 1.770838 | 0.731373 | 0.052534 | 29.283384 | 0.043005 | 13.890926 | 126.1 |
| 0.017930 | 0.044763 | 1.769124 | 0.740437 | 0.055167 | 30.193424 | 0.044846 | 13.872081 | 126.9 |
| 0.017956 | 0.045058 | 1.767355 | 0.749229 | 0.057714 | 31.067978 | 0.046620 | 13.852894 | 128.0 |
| 0.017511 | 0.040367 | 1.799305 | 0.587716 | 0.004783 | 11.890664 | 0.008303 | 14.193445 | 147.2 |
| 0.017597 | 0.043272 | 1.797449 | 0.612196 | 0.008037 | 12.857479 | 0.010121 | 14.165191 | 143.7 |
| 0.017687 | 0.046217 | 1.795727 | 0.637182 | 0.011345 | 13.837824 | 0.011966 | 14.137566 | 141.6 |
| 0.017776 | 0.049126 | 1.793912 | 0.662007 | 0.014626 | 14.806124 | 0.013791 | 14.109080 | 140.0 |
| 0.017861 | 0.051929 | 1.792049 | 0.686087 | 0.017803 | 15.739612 | 0.015555 | 14.080403 | 142.7 |
| 0.017951 | 0.054771 | 1.790320 | 0.710659 | 0.021031 | 16.686054 | 0.017343 | 14.052371 | 145.9 |
| 0.018039 | 0.057575 | 1.788498 | 0.735072 | 0.024233 | 17.620334 | 0.019113 | 14.023465 | 145.9 |
| 0.018124 | 0.060275 | 1.786627 | 0.758753 | 0.027333 | 18.520485 | 0.020821 | 13.994364 | 146.7 |
| 0.018212 | 0.063013 | 1.784891 | 0.782910 | 0.030481 | 19.433034 | 0.022554 | 13.965926 | 148.1 |
| 0.018300 | 0.065713 | 1.783063 | 0.806911 | 0.033603 | 20.333294 | 0.024268 | 13.936600 | 150.4 |
| 0.018384 | 0.068311 | 1.781183 | 0.830191 | 0.036625 | 21.200098 | 0.025921 | 13.907076 | 152.7 |
| 0.018472 | 0.070945 | 1.779441 | 0.853934 | 0.039695 | 22.078764 | 0.027598 | 13.878231 | 151.3 |
| 0.018559 | 0.073540 | 1.777605 | 0.877523 | 0.042737 | 22.945004 | 0.029256 | 13.848485 | 152.8 |
| 0.018642 | 0.076036 | 1.775718 | 0.900403 | 0.045682 | 23.778451 | 0.030855 | 13.818537 | 151.3 |
| 0.018730 | 0.078566 | 1.773970 | 0.923732 | 0.048671 | 24.623244 | 0.032476 | 13.789286 | 153.7 |
| 0.018816 | 0.081057 | 1.772126 | 0.946909 | 0.051635 | 25.455464 | 0.034078 | 13.759120 | 156.8 |
| 0.018899 | 0.083451 | 1.770232 | 0.969389 | 0.054501 | 26.255544 | 0.035622 | 13.728748 | 161.5 |
| 0.018985 | 0.085877 | 1.768476 | 0.992304 | 0.057412 | 27.066474 | 0.037187 | 13.699091 | 164.7 |
| 0.019071 | 0.088263 | 1.766626 | 1.015069 | 0.060295 | 27.864674 | 0.038733 | 13.668505 | 163.8 |
| 0.019153 | 0.090554 | 1.764723 | 1.037148 | 0.063084 | 28.631376 | 0.040222 | 13.637709 | 165.8 |
| 0.018246 | 0.041650 | 1.802931 | 0.600494 | 0.001509 | 11.763880 | 0.006487 | 14.191959 | 155.8 |
| 0.019045 | 0.045796 | 1.804617 | 0.637363 | 0.001594 | 12.608123 | 0.006550 | 14.162080 | 152.1 |
| 0.019861 | 0.050001 | 1.806523 | 0.674954 | 0.001680 | 13.464121 | 0.006614 | 14.132625 | 150.7 |
| 0.020672 | 0.054155 | 1.808338 | 0.712298 | 0.001765 | 14.309311 | 0.006678 | 14.102128 | 149.2 |
| 0.021458 | 0.058163 | 1.810019 | 0.748515 | 0.001849 | 15.123822 | 0.006741 | 14.071306 | 147.8 |
| 0.022260 | 0.062227 | 1.811920 | 0.785431 | 0.001933 | 15.949584 | 0.006805 | 14.040926 | 147.1 |
| 0.023057 | 0.066240 | 1.813731 | 0.822103 | 0.002017 | 16.764430 | 0.006868 | 14.009484 | 145.1 |
| 0.023830 | 0.070110 | 1.815409 | 0.857667 | 0.002099 | 17.549200 | 0.006930 | 13.977719 | 142.0 |
| 0.024619 | 0.074033 | 1.817304 | 0.893910 | 0.002182 | 18.344736 | 0.006993 | 13.946415 | 142.1 |
| 0.025402 | 0.077905 | 1.819110 | 0.929910 | 0.002264 | 19.129236 | 0.007056 | 13.914028 | 138.4 |
| 0.026162 | 0.081636 | 1.820784 | 0.964821 | 0.002345 | 19.884256 | 0.007117 | 13.881320 | 137.1 |
| 0.026937 | 0.085418 | 1.822675 | 1.000389 | 0.002426 | 20.649574 | 0.007179 | 13.849091 | 134.6 |
| 0.027707 | 0.089149 | 1.824477 | 1.035718 | 0.002507 | 21.403730 | 0.007241 | 13.815759 | 131.9 |
| 0.028453 | 0.092741 | 1.826147 | 1.069976 | 0.002586 | 22.128991 | 0.007302 | 13.782107 | 130.2 |
| 0.029215 | 0.096383 | 1.828033 | 1.104870 | 0.002666 | 22.864101 | 0.007364 | 13.748955 | 132.4 |
| 0.029971 | 0.099973 | 1.829830 | 1.139527 | 0.002745 | 23.587911 | 0.007425 | 13.714678 | 133.1 |
| 0.030704 | 0.103426 | 1.831496 | 1.173132 | 0.002823 | 24.283403 | 0.007485 | 13.680082 | 138.0 |
| 0.031452 | 0.106927 | 1.833377 | 1.207352 | 0.002901 | 24.988314 | 0.007546 | 13.646006 | 137.2 |
| 0.032194 | 0.110376 | 1.835170 | 1.241337 | 0.002979 | 25.681780 | 0.007607 | 13.610784 | 139.7 |
| 0.032915 | 0.113691 | 1.836832 | 1.274289 | 0.003055 | 26.347495 | 0.007666 | 13.575244 | 142.3 |
| 0.017430 | 0.037449 | 1.800450 | 0.571873 | 0.004209 | 12.321206 | 0.008418 | 14.283036 | 165.8 |
| 0.017437 | 0.037541 | 1.799714 | 0.580863 | 0.006909 | 13.704318 | 0.010346 | 14.342258 | 165.4 |
| 0.017446 | 0.037638 | 1.799141 | 0.589969 | 0.009652 | 15.107061 | 0.012303 | 14.404206 | 163.6 |
| 0.017454 | 0.037733 | 1.798479 | 0.598890 | 0.012374 | 16.493618 | 0.014239 | 14.465311 | 154.1 |
| 0.017461 | 0.037824 | 1.797742 | 0.607415 | 0.015010 | 17.831388 | 0.016110 | 14.524136 | 151.4 |
| 0.017470 | 0.037921 | 1.797169 | 0.616051 | 0.017688 | 19.187964 | 0.018008 | 14.585651 | 155.5 |
| 0.017479 | 0.038016 | 1.796505 | 0.624498 | 0.020344 | 20.528216 | 0.019886 | 14.646336 | 144.9 |
| 0.017486 | 0.038106 | 1.795768 | 0.632558 | 0.022916 | 21.820632 | 0.021699 | 14.704764 | 145.4 |
| 0.017495 | 0.038202 | 1.795194 | 0.640724 | 0.025528 | 23.131056 | 0.023537 | 14.765846 | 143.1 |
| 0.017503 | 0.038297 | 1.794529 | 0.648698 | 0.028119 | 24.425003 | 0.025356 | 14.826111 | 140.0 |
| 0.017510 | 0.038387 | 1.793791 | 0.656293 | 0.030626 | 25.672050 | 0.027111 | 14.884142 | 140.3 |
| 0.017519 | 0.038482 | 1.793216 | 0.663989 | 0.033173 | 26.936334 | 0.028891 | 14.944791 | 142.0 |
| 0.017528 | 0.038576 | 1.792551 | 0.671490 | 0.035698 | 28.183976 | 0.030650 | 15.004636 | 145.6 |
| 0.017535 | 0.038666 | 1.791811 | 0.678619 | 0.038142 | 29.385641 | 0.032348 | 15.062270 | 147.2 |
| 0.017544 | 0.038761 | 1.791236 | 0.685845 | 0.040624 | 30.603801 | 0.034069 | 15.122486 | 147.2 |
| 0.017552 | 0.038855 | 1.790570 | 0.692873 | 0.043083 | 31.805138 | 0.035769 | 15.181911 | 149.6 |
| 0.017559 | 0.038944 | 1.789830 | 0.699537 | 0.045463 | 32.961406 | 0.037409 | 15.239148 | 151.3 |
| 0.017568 | 0.039038 | 1.789254 | 0.706293 | 0.047879 | 34.133454 | 0.039071 | 15.298931 | 152.9 |
| 0.017576 | 0.039131 | 1.788587 | 0.712847 | 0.050273 | 35.288486 | 0.040712 | 15.357936 | 152.2 |
| 0.017584 | 0.039220 | 1.787846 | 0.719046 | 0.052588 | 36.399345 | 0.042294 | 15.414775 | 154.0 |
| 0.019283 | 0.038764 | 1.817413 | 0.714961 | 0.006359 | 14.543944 | 0.006720 | 14.237689 | 187.5 |
| 0.021088 | 0.040121 | 1.833186 | 0.862752 | 0.011140 | 18.076984 | 0.007008 | 14.251520 | 183.4 |
| 0.022927 | 0.041496 | 1.849468 | 1.013123 | 0.015998 | 21.661864 | 0.007299 | 14.265926 | 180.7 |
| 0.024753 | 0.042851 | 1.865607 | 1.162396 | 0.020817 | 25.209944 | 0.007586 | 14.278324 | 178.9 |
| 0.026524 | 0.044152 | 1.881226 | 1.307060 | 0.025483 | 28.637800 | 0.007862 | 14.288424 | 178.1 |
| 0.028327 | 0.045471 | 1.897343 | 1.454215 | 0.030223 | 32.115384 | 0.008141 | 14.299091 | 179.0 |
| 0.030118 | 0.046768 | 1.913322 | 1.600277 | 0.034924 | 35.555944 | 0.008417 | 14.307709 | 175.7 |
| 0.031855 | 0.048014 | 1.928786 | 1.741813 | 0.039474 | 38.878584 | 0.008682 | 14.314076 | 177.3 |
| 0.033623 | 0.049277 | 1.944739 | 1.885753 | 0.044097 | 42.248904 | 0.008950 | 14.321006 | 171.8 |
| 0.035379 | 0.050518 | 1.960556 | 2.028606 | 0.048680 | 45.581944 | 0.009214 | 14.325844 | 173.5 |
| 0.037080 | 0.051708 | 1.975866 | 2.167013 | 0.053115 | 48.799337 | 0.009468 | 14.328478 | 168.6 |
| 0.038813 | 0.052914 | 1.991655 | 2.307738 | 0.057620 | 52.062424 | 0.009725 | 14.331671 | 163.9 |
| 0.040533 | 0.054099 | 2.007311 | 2.447381 | 0.062084 | 55.287944 | 0.009977 | 14.332729 | 165.4 |
| 0.042201 | 0.055233 | 2.022466 | 2.582658 | 0.066404 | 58.400057 | 0.010220 | 14.331628 | 163.4 |
| 0.043898 | 0.056384 | 2.038091 | 2.720170 | 0.070791 | 61.555944 | 0.010465 | 14.331086 | 163.9 |
| 0.045583 | 0.057511 | 2.053585 | 2.856603 | 0.075138 | 64.673944 | 0.010707 | 14.328364 | 165.0 |
| 0.047216 | 0.058591 | 2.068586 | 2.988749 | 0.079343 | 67.680745 | 0.010938 | 14.323527 | 171.6 |
| 0.048878 | 0.059684 | 2.084047 | 3.123049 | 0.083611 | 70.729464 | 0.011172 | 14.319251 | 173.8 |
| 0.050528 | 0.060756 | 2.099380 | 3.256273 | 0.087840 | 73.739944 | 0.011402 | 14.312749 | 176.0 |
| 0.052127 | 0.061779 | 2.114226 | 3.385286 | 0.091930 | 76.641401 | 0.011622 | 14.304175 | 180.7 |
| 0.017916 | 0.037455 | 1.798885 | 0.566185 | 0.005915 | 27.813234 | 0.007122 | 14.198838 | 165.1 |
| 0.018390 | 0.037549 | 1.796618 | 0.569768 | 0.010266 | 44.186086 | 0.007798 | 14.175431 | 163.7 |
| 0.018871 | 0.037644 | 1.794473 | 0.573477 | 0.014687 | 60.808104 | 0.008483 | 14.152371 | 162.7 |
| 0.019344 | 0.037734 | 1.792234 | 0.577152 | 0.019073 | 77.275614 | 0.009160 | 14.128018 | 159.7 |
| 0.019798 | 0.037815 | 1.789954 | 0.580705 | 0.023319 | 93.201433 | 0.009813 | 14.102944 | 157.2 |
| 0.020257 | 0.037898 | 1.787798 | 0.584382 | 0.027634 | 109.366614 | 0.010475 | 14.078231 | 152.6 |
| 0.020709 | 0.037974 | 1.785547 | 0.588024 | 0.031912 | 125.376744 | 0.011129 | 14.052198 | 150.0 |
| 0.021142 | 0.038043 | 1.783255 | 0.591547 | 0.036054 | 140.855394 | 0.011759 | 14.025456 | 148.9 |
| 0.021581 | 0.038114 | 1.781087 | 0.595192 | 0.040261 | 156.563874 | 0.012398 | 13.999091 | 147.6 |
| 0.022011 | 0.038178 | 1.778824 | 0.598803 | 0.044432 | 172.116624 | 0.013028 | 13.971378 | 144.2 |
| 0.022423 | 0.038235 | 1.776519 | 0.602296 | 0.048470 | 187.147968 | 0.013636 | 13.942968 | 144.0 |
| 0.022841 | 0.038293 | 1.774340 | 0.605908 | 0.052570 | 202.399884 | 0.014252 | 13.914951 | 142.3 |
| 0.023250 | 0.038345 | 1.772065 | 0.609487 | 0.056634 | 217.495254 | 0.014859 | 13.885558 | 141.6 |
| 0.023641 | 0.038389 | 1.769747 | 0.612950 | 0.060567 | 232.079156 | 0.015444 | 13.855479 | 140.2 |
| 0.024037 | 0.038435 | 1.767557 | 0.616529 | 0.064560 | 246.874644 | 0.016036 | 13.825811 | 143.5 |
| 0.024425 | 0.038474 | 1.765270 | 0.620077 | 0.068517 | 261.512634 | 0.016621 | 13.794738 | 143.1 |
| 0.024795 | 0.038506 | 1.762939 | 0.623510 | 0.072345 | 275.648959 | 0.017183 | 13.762990 | 146.7 |
| 0.025170 | 0.038539 | 1.760738 | 0.627057 | 0.076231 | 289.988154 | 0.017752 | 13.731671 | 148.2 |
| 0.025537 | 0.038566 | 1.758438 | 0.630573 | 0.080081 | 304.168764 | 0.018313 | 13.698918 | 149.1 |
| 0.025886 | 0.038585 | 1.756095 | 0.633975 | 0.083804 | 317.857375 | 0.018853 | 13.665500 | 153.0 |
| 0.017487 | 0.037598 | 1.806736 | 0.588096 | 0.005828 | 15.056819 | 0.007267 | 14.191959 | 119.4 |
| 0.017548 | 0.037828 | 1.812127 | 0.612944 | 0.010096 | 19.086023 | 0.008083 | 14.162080 | 116.1 |
| 0.017610 | 0.038062 | 1.817819 | 0.638305 | 0.014433 | 23.174584 | 0.008910 | 14.132625 | 115.7 |
| 0.017668 | 0.038288 | 1.823411 | 0.663503 | 0.018734 | 27.221679 | 0.009728 | 14.102128 | 112.6 |
| 0.017723 | 0.038500 | 1.828773 | 0.687944 | 0.022899 | 31.132153 | 0.010517 | 14.071306 | 113.7 |
| 0.017778 | 0.038716 | 1.834432 | 0.712883 | 0.027130 | 35.099574 | 0.011317 | 14.040926 | 115.1 |
| 0.017831 | 0.038924 | 1.839993 | 0.737661 | 0.031327 | 39.025289 | 0.012107 | 14.009484 | 118.6 |
| 0.017878 | 0.039119 | 1.845325 | 0.761694 | 0.035389 | 42.816996 | 0.012870 | 13.977719 | 117.6 |
| 0.017927 | 0.039317 | 1.850951 | 0.786212 | 0.039516 | 46.663314 | 0.013643 | 13.946415 | 119.1 |
| 0.017973 | 0.039506 | 1.856480 | 0.810570 | 0.043607 | 50.467649 | 0.014406 | 13.914028 | 119.6 |
| 0.018015 | 0.039683 | 1.861783 | 0.834196 | 0.047567 | 54.140554 | 0.015141 | 13.881320 | 121.0 |
| 0.018057 | 0.039863 | 1.867376 | 0.858292 | 0.051589 | 57.865804 | 0.015887 | 13.849091 | 121.6 |
| 0.018096 | 0.040035 | 1.872874 | 0.882230 | 0.055575 | 61.548759 | 0.016623 | 13.815759 | 123.4 |
| 0.018131 | 0.040194 | 1.878148 | 0.905450 | 0.059432 | 65.102825 | 0.017332 | 13.782107 | 126.6 |
| 0.018167 | 0.040356 | 1.883708 | 0.929123 | 0.063349 | 68.707044 | 0.018050 | 13.748955 | 127.4 |
| 0.018200 | 0.040510 | 1.889174 | 0.952642 | 0.067230 | 72.268619 | 0.018759 | 13.714678 | 129.7 |
| 0.018228 | 0.040651 | 1.894418 | 0.975454 | 0.070985 | 75.703810 | 0.019441 | 13.680082 | 131.7 |
| 0.018258 | 0.040795 | 1.899946 | 0.998706 | 0.074797 | 79.187034 | 0.020132 | 13.646006 | 135.9 |
| 0.018284 | 0.040931 | 1.905380 | 1.021805 | 0.078573 | 82.627229 | 0.020813 | 13.610784 | 135.1 |
| 0.018306 | 0.041054 | 1.910595 | 1.044209 | 0.082225 | 85.943509 | 0.021468 | 13.575244 | 137.6 |
| 0.017969 | 0.038315 | 1.811581 | 0.629607 | 0.005011 | 11.535405 | 0.007344 | 14.214081 | 145.2 |
| 0.018500 | 0.039238 | 1.821685 | 0.694696 | 0.008488 | 12.158799 | 0.008235 | 14.205245 | 142.0 |
| 0.019042 | 0.040174 | 1.832186 | 0.760987 | 0.012021 | 12.790776 | 0.009139 | 14.196805 | 138.9 |
| 0.019582 | 0.041093 | 1.842570 | 0.826822 | 0.015525 | 13.414211 | 0.010032 | 14.186750 | 140.6 |
| 0.020104 | 0.041974 | 1.852595 | 0.890654 | 0.018918 | 14.014447 | 0.010893 | 14.175317 | 137.2 |
| 0.020639 | 0.042868 | 1.863009 | 0.955648 | 0.022366 | 14.622894 | 0.011767 | 14.164286 | 134.9 |
| 0.021170 | 0.043744 | 1.873310 | 1.020190 | 0.025785 | 15.222705 | 0.012631 | 14.151606 | 131.6 |
| 0.021685 | 0.044584 | 1.883255 | 1.082763 | 0.029095 | 15.799776 | 0.013464 | 14.137575 | 130.7 |
| 0.022211 | 0.045435 | 1.893583 | 1.146461 | 0.032458 | 16.384701 | 0.014308 | 14.123955 | 127.3 |
| 0.022734 | 0.046269 | 1.903800 | 1.209710 | 0.035792 | 16.960886 | 0.015142 | 14.108650 | 124.6 |
| 0.023241 | 0.047067 | 1.913665 | 1.271024 | 0.039019 | 17.514785 | 0.015946 | 14.092021 | 121.4 |
| 0.023758 | 0.047876 | 1.923908 | 1.333425 | 0.042297 | 18.076194 | 0.016762 | 14.075811 | 120.2 |
| 0.024273 | 0.048668 | 1.934041 | 1.395382 | 0.045546 | 18.628755 | 0.017566 | 14.057881 | 121.7 |
| 0.024772 | 0.049424 | 1.943825 | 1.455437 | 0.048690 | 19.159475 | 0.018341 | 14.038653 | 124.1 |
| 0.025281 | 0.050191 | 1.953982 | 1.516543 | 0.051883 | 19.697376 | 0.019127 | 14.019855 | 126.9 |
| 0.025788 | 0.050940 | 1.964031 | 1.577206 | 0.055047 | 20.226311 | 0.019902 | 13.999300 | 130.4 |
| 0.026279 | 0.051654 | 1.973736 | 1.636002 | 0.058108 | 20.733845 | 0.020648 | 13.977472 | 133.5 |
| 0.026780 | 0.052379 | 1.983807 | 1.695812 | 0.061216 | 21.248244 | 0.021405 | 13.956086 | 134.2 |
| 0.027278 | 0.053086 | 1.993772 | 1.755183 | 0.064295 | 21.753555 | 0.022150 | 13.932906 | 132.7 |
| 0.02776095 | 0.05375844 | 2.003397038 | 1.812718562 | 0.067272432 | 22.23789495 | 0.022867702 | 13.90847731 | 138.0 |

# 附录2

实验温度和特征转换后的特征描述符与目标值OP的数据集：（其中水热温度表示为HT、磷化温度表示为PT、原子序数加权平均值表示为、非键合原子半径加权平均值表示为****、共价半径加权平均值表示为、第一电离能加权平均值表示为****、第二电离能加权平均值表示为****、电子亲和能加权平均值表示为****、鲍林电负性加权平均值表示为、最外层D轨道电子数加权平均值表示为****、原子序数方差表示为*δ*AN、非键合原子半径方差表示为*δ*RA、共价半径方差表示为*δ*RC、第一电离能方差表示为*δ*FIE、第二电离能方差表示为*δ*SIE、电子亲和能方差表示为*δ*EA、鲍林电负性方差表示为*δ*EP、最外层D轨道电子数方差表示为*δ*DE、过电位表示为OP）

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| HT | PT |  | **δ**EP |  | **δ**EA |  | **δ**FIE |  |
| 2 | 4.17 | 2.03545 | 0.023898798 | 0.7125 | 0.00504375 | 9.180385 | 1.708087837 | 18.436335 |
| 2.33 | 5 | 2.03545 | 0.023898798 | 0.7125 | 0.00504375 | 9.180385 | 1.708087837 | 18.436335 |
| 2.67 | 5.83 | 2.03545 | 0.023898798 | 0.7125 | 0.00504375 | 9.180385 | 1.708087837 | 18.436335 |
| 3 | 6.67 | 2.03545 | 0.023898798 | 0.7125 | 0.00504375 | 9.180385 | 1.708087837 | 18.436335 |
| 2 | 5 | 2.0359 | 0.02377219 | 0.72 | 0.00795 | 9.17677 | 1.718340537 | 18.45267 |
| 2.33 | 4.17 | 2.0359 | 0.02377219 | 0.72 | 0.00795 | 9.17677 | 1.718340537 | 18.45267 |
| 2.67 | 6.67 | 2.0359 | 0.02377219 | 0.72 | 0.00795 | 9.17677 | 1.718340537 | 18.45267 |
| 3 | 5.83 | 2.0359 | 0.02377219 | 0.72 | 0.00795 | 9.17677 | 1.718340537 | 18.45267 |
| 2 | 5.83 | 2.03635 | 0.023645178 | 0.7275 | 0.01074375 | 9.173155 | 1.728567101 | 18.469005 |
| 2.33 | 6.67 | 2.03635 | 0.023645178 | 0.7275 | 0.01074375 | 9.173155 | 1.728567101 | 18.469005 |
| 2.67 | 4.17 | 2.03635 | 0.023645178 | 0.7275 | 0.01074375 | 9.173155 | 1.728567101 | 18.469005 |
| 3 | 5 | 2.03635 | 0.023645178 | 0.7275 | 0.01074375 | 9.173155 | 1.728567101 | 18.469005 |
| 2 | 6.67 | 2.0368 | 0.02351776 | 0.735 | 0.013425 | 9.16954 | 1.738767528 | 18.48534 |
| 2.33 | 5.83 | 2.0368 | 0.02351776 | 0.735 | 0.013425 | 9.16954 | 1.738767528 | 18.48534 |
| 2.67 | 5 | 2.0368 | 0.02351776 | 0.735 | 0.013425 | 9.16954 | 1.738767528 | 18.48534 |
| 3 | 4.17 | 2.0368 | 0.02351776 | 0.735 | 0.013425 | 9.16954 | 1.738767528 | 18.48534 |
| 2 | 4.17 | 2.0353 | 0.02393791 | 0.713505 | 0.00600955 | 9.18169 | 1.704179264 | 18.46818 |
| 2.33 | 5 | 2.0353 | 0.02393791 | 0.713505 | 0.00600955 | 9.18169 | 1.704179264 | 18.46818 |
| 2.67 | 5.83 | 2.0353 | 0.02393791 | 0.713505 | 0.00600955 | 9.18169 | 1.704179264 | 18.46818 |
| 3 | 6.67 | 2.0353 | 0.02393791 | 0.713505 | 0.00600955 | 9.18169 | 1.704179264 | 18.46818 |
| 2 | 5 | 2.0356 | 0.02385064 | 0.72201 | 0.00984943 | 9.17938 | 1.710538856 | 18.51636 |
| 2.33 | 4.17 | 2.0356 | 0.02385064 | 0.72201 | 0.00984943 | 9.17938 | 1.710538856 | 18.51636 |
| 2.67 | 6.67 | 2.0356 | 0.02385064 | 0.72201 | 0.00984943 | 9.17938 | 1.710538856 | 18.51636 |
| 3 | 5.83 | 2.0356 | 0.02385064 | 0.72201 | 0.00984943 | 9.17938 | 1.710538856 | 18.51636 |
| 2 | 5.83 | 2.0359 | 0.02376319 | 0.730515 | 0.01354464 | 9.17707 | 1.716887775 | 18.56454 |
| 2.33 | 6.67 | 2.0359 | 0.02376319 | 0.730515 | 0.01354464 | 9.17707 | 1.716887775 | 18.56454 |
| 2.67 | 4.17 | 2.0359 | 0.02376319 | 0.730515 | 0.01354464 | 9.17707 | 1.716887775 | 18.56454 |
| 3 | 5 | 2.0359 | 0.02376319 | 0.730515 | 0.01354464 | 9.17707 | 1.716887775 | 18.56454 |
| 2 | 6.67 | 2.0362 | 0.02367556 | 0.73902 | 0.01709518 | 9.17476 | 1.723226022 | 18.61272 |
| 2.33 | 5.83 | 2.0362 | 0.02367556 | 0.73902 | 0.01709518 | 9.17476 | 1.723226022 | 18.61272 |
| 2.67 | 5 | 2.0362 | 0.02367556 | 0.73902 | 0.01709518 | 9.17476 | 1.723226022 | 18.61272 |
| 3 | 4.17 | 2.0362 | 0.02367556 | 0.73902 | 0.01709518 | 9.17476 | 1.723226022 | 18.61272 |
| 2 | 4.17 | 2.0422 | 0.02519716 | 0.707325 | 0.002170719 | 9.185485 | 1.6940839 | 18.4281 |
| 2.33 | 5 | 2.0422 | 0.02519716 | 0.707325 | 0.002170719 | 9.185485 | 1.6940839 | 18.4281 |
| 2.67 | 5.83 | 2.0422 | 0.02519716 | 0.707325 | 0.002170719 | 9.185485 | 1.6940839 | 18.4281 |
| 3 | 6.67 | 2.0422 | 0.02519716 | 0.707325 | 0.002170719 | 9.185485 | 1.6940839 | 18.4281 |
| 2 | 5 | 2.0494 | 0.02626564 | 0.70965 | 0.002305628 | 9.18697 | 1.690354389 | 18.4362 |
| 2.33 | 4.17 | 2.0494 | 0.02626564 | 0.70965 | 0.002305628 | 9.18697 | 1.690354389 | 18.4362 |
| 2.67 | 6.67 | 2.0494 | 0.02626564 | 0.70965 | 0.002305628 | 9.18697 | 1.690354389 | 18.4362 |
| 3 | 5.83 | 2.0494 | 0.02626564 | 0.70965 | 0.002305628 | 9.18697 | 1.690354389 | 18.4362 |
| 2 | 5.83 | 2.0566 | 0.02723044 | 0.711975 | 0.002429724 | 9.188455 | 1.686620468 | 18.4443 |
| 2.33 | 6.67 | 2.0566 | 0.02723044 | 0.711975 | 0.002429724 | 9.188455 | 1.686620468 | 18.4443 |
| 2.67 | 4.17 | 2.0566 | 0.02723044 | 0.711975 | 0.002429724 | 9.188455 | 1.686620468 | 18.4443 |
| 3 | 5 | 2.0566 | 0.02723044 | 0.711975 | 0.002429724 | 9.188455 | 1.686620468 | 18.4443 |
| 2 | 6.67 | 2.0638 | 0.02809156 | 0.7143 | 0.00254301 | 9.18994 | 1.682882136 | 18.4524 |
| 2.33 | 5.83 | 2.0638 | 0.02809156 | 0.7143 | 0.00254301 | 9.18994 | 1.682882136 | 18.4524 |
| 2.67 | 5 | 2.0638 | 0.02809156 | 0.7143 | 0.00254301 | 9.18994 | 1.682882136 | 18.4524 |
| 3 | 4.17 | 2.0638 | 0.02809156 | 0.7143 | 0.00254301 | 9.18994 | 1.682882136 | 18.4524 |
| 2 | 4.17 | 2.0317 | 0.02576311 | 0.70509 | 0.002017432 | 9.16729 | 1.759690976 | 18.411075 |
| 2.33 | 5 | 2.0317 | 0.02576311 | 0.70509 | 0.002017432 | 9.16729 | 1.759690976 | 18.411075 |
| 2.67 | 5.83 | 2.0317 | 0.02576311 | 0.70509 | 0.002017432 | 9.16729 | 1.759690976 | 18.411075 |
| 3 | 6.67 | 2.0317 | 0.02576311 | 0.70509 | 0.002017432 | 9.16729 | 1.759690976 | 18.411075 |
| 2 | 5 | 2.0284 | 0.02747944 | 0.70518 | 0.002009848 | 9.15058 | 1.821014504 | 18.40215 |
| 2.33 | 4.17 | 2.0284 | 0.02747944 | 0.70518 | 0.002009848 | 9.15058 | 1.821014504 | 18.40215 |
| 2.67 | 6.67 | 2.0284 | 0.02747944 | 0.70518 | 0.002009848 | 9.15058 | 1.821014504 | 18.40215 |
| 3 | 5.83 | 2.0284 | 0.02747944 | 0.70518 | 0.002009848 | 9.15058 | 1.821014504 | 18.40215 |
| 2 | 5.83 | 2.0251 | 0.02917399 | 0.70527 | 0.002002247 | 9.13387 | 1.881779583 | 18.393225 |
| 2.33 | 6.67 | 2.0251 | 0.02917399 | 0.70527 | 0.002002247 | 9.13387 | 1.881779583 | 18.393225 |
| 2.67 | 4.17 | 2.0251 | 0.02917399 | 0.70527 | 0.002002247 | 9.13387 | 1.881779583 | 18.393225 |
| 3 | 5 | 2.0251 | 0.02917399 | 0.70527 | 0.002002247 | 9.13387 | 1.881779583 | 18.393225 |
| 2 | 6.67 | 2.0218 | 0.03084676 | 0.70536 | 0.00199463 | 9.11716 | 1.941986214 | 18.3843 |
| 2.33 | 5.83 | 2.0218 | 0.03084676 | 0.70536 | 0.00199463 | 9.11716 | 1.941986214 | 18.3843 |
| 2.67 | 5 | 2.0218 | 0.03084676 | 0.70536 | 0.00199463 | 9.11716 | 1.941986214 | 18.3843 |
| 3 | 4.17 | 2.0218 | 0.03084676 | 0.70536 | 0.00199463 | 9.11716 | 1.941986214 | 18.3843 |
| 2 | 4.17 | 2.0392 | 0.02388136 | 0.706275 | 0.002016999 | 9.172165 | 1.737848758 | 18.40635 |
| 2.33 | 5 | 2.0392 | 0.02388136 | 0.706275 | 0.002016999 | 9.172165 | 1.737848758 | 18.40635 |
| 2.67 | 5.83 | 2.0392 | 0.02388136 | 0.706275 | 0.002016999 | 9.172165 | 1.737848758 | 18.40635 |
| 3 | 6.67 | 2.0392 | 0.02388136 | 0.706275 | 0.002016999 | 9.172165 | 1.737848758 | 18.40635 |
| 2 | 5 | 2.0434 | 0.02370244 | 0.70755 | 0.002005748 | 9.16033 | 1.777608381 | 18.3927 |
| 2.33 | 4.17 | 2.0434 | 0.02370244 | 0.70755 | 0.002005748 | 9.16033 | 1.777608381 | 18.3927 |
| 2.67 | 6.67 | 2.0434 | 0.02370244 | 0.70755 | 0.002005748 | 9.16033 | 1.777608381 | 18.3927 |
| 3 | 5.83 | 2.0434 | 0.02370244 | 0.70755 | 0.002005748 | 9.16033 | 1.777608381 | 18.3927 |
| 2 | 5.83 | 2.0476 | 0.02348824 | 0.708825 | 0.001991244 | 9.148495 | 1.81708787 | 18.37905 |
| 2.33 | 6.67 | 2.0476 | 0.02348824 | 0.708825 | 0.001991244 | 9.148495 | 1.81708787 | 18.37905 |
| 2.67 | 4.17 | 2.0476 | 0.02348824 | 0.708825 | 0.001991244 | 9.148495 | 1.81708787 | 18.37905 |
| 3 | 5 | 2.0476 | 0.02348824 | 0.708825 | 0.001991244 | 9.148495 | 1.81708787 | 18.37905 |
| 2 | 6.67 | 2.0518 | 0.02323876 | 0.7101 | 0.00197349 | 9.13666 | 1.856287224 | 18.3654 |
| 2.33 | 5.83 | 2.0518 | 0.02323876 | 0.7101 | 0.00197349 | 9.13666 | 1.856287224 | 18.3654 |
| 2.67 | 5 | 2.0518 | 0.02323876 | 0.7101 | 0.00197349 | 9.13666 | 1.856287224 | 18.3654 |
| 3 | 4.17 | 2.0518 | 0.02323876 | 0.7101 | 0.00197349 | 9.13666 | 1.856287224 | 18.3654 |
| 2 | 4.17 | 2.03425 | 0.024294438 | 0.697545 | 0.006345508 | 9.18433 | 1.696956171 | 18.40662 |
| 2.33 | 5 | 2.03425 | 0.024294438 | 0.697545 | 0.006345508 | 9.18433 | 1.696956171 | 18.40662 |
| 2.67 | 5.83 | 2.03425 | 0.024294438 | 0.697545 | 0.006345508 | 9.18433 | 1.696956171 | 18.40662 |
| 3 | 6.67 | 2.03425 | 0.024294438 | 0.697545 | 0.006345508 | 9.18433 | 1.696956171 | 18.40662 |
| 2 | 5 | 2.0335 | 0.02456275 | 0.69009 | 0.010554862 | 9.18466 | 1.696103124 | 18.39324 |
| 2.33 | 4.17 | 2.0335 | 0.02456275 | 0.69009 | 0.010554862 | 9.18466 | 1.696103124 | 18.39324 |
| 2.67 | 6.67 | 2.0335 | 0.02456275 | 0.69009 | 0.010554862 | 9.18466 | 1.696103124 | 18.39324 |
| 3 | 5.83 | 2.0335 | 0.02456275 | 0.69009 | 0.010554862 | 9.18466 | 1.696103124 | 18.39324 |
| 2 | 5.83 | 2.03275 | 0.024829938 | 0.682635 | 0.014653062 | 9.18499 | 1.69524986 | 18.37986 |
| 2.33 | 6.67 | 2.03275 | 0.024829938 | 0.682635 | 0.014653062 | 9.18499 | 1.69524986 | 18.37986 |
| 2.67 | 4.17 | 2.03275 | 0.024829938 | 0.682635 | 0.014653062 | 9.18499 | 1.69524986 | 18.37986 |
| 3 | 5 | 2.03275 | 0.024829938 | 0.682635 | 0.014653062 | 9.18499 | 1.69524986 | 18.37986 |
| 2 | 6.67 | 2.032 | 0.025096 | 0.67518 | 0.018640108 | 9.18532 | 1.694396378 | 18.36648 |
| 2.33 | 5.83 | 2.032 | 0.025096 | 0.67518 | 0.018640108 | 9.18532 | 1.694396378 | 18.36648 |
| 2.67 | 5 | 2.032 | 0.025096 | 0.67518 | 0.018640108 | 9.18532 | 1.694396378 | 18.36648 |
| 3 | 4.17 | 2.032 | 0.025096 | 0.67518 | 0.018640108 | 9.18532 | 1.694396378 | 18.36648 |
| 2 | 4.17 | 2.03125 | 0.026110938 | 0.70296 | 0.002481878 | 9.166975 | 1.761209674 | 18.3837 |
| 2.33 | 5 | 2.03125 | 0.026110938 | 0.70296 | 0.002481878 | 9.166975 | 1.761209674 | 18.3837 |
| 2.67 | 5.83 | 2.03125 | 0.026110938 | 0.70296 | 0.002481878 | 9.166975 | 1.761209674 | 18.3837 |
| 3 | 6.67 | 2.03125 | 0.026110938 | 0.70296 | 0.002481878 | 9.166975 | 1.761209674 | 18.3837 |
| 2 | 5 | 2.0275 | 0.02816875 | 0.70092 | 0.002930434 | 9.14995 | 1.824030648 | 18.3474 |
| 2.33 | 4.17 | 2.0275 | 0.02816875 | 0.70092 | 0.002930434 | 9.14995 | 1.824030648 | 18.3474 |
| 2.67 | 6.67 | 2.0275 | 0.02816875 | 0.70092 | 0.002930434 | 9.14995 | 1.824030648 | 18.3474 |
| 3 | 5.83 | 2.0275 | 0.02816875 | 0.70092 | 0.002930434 | 9.14995 | 1.824030648 | 18.3474 |
| 2 | 5.83 | 2.02375 | 0.030198438 | 0.69888 | 0.003370666 | 9.132925 | 1.886271919 | 18.3111 |
| 2.33 | 6.67 | 2.02375 | 0.030198438 | 0.69888 | 0.003370666 | 9.132925 | 1.886271919 | 18.3111 |
| 2.67 | 4.17 | 2.02375 | 0.030198438 | 0.69888 | 0.003370666 | 9.132925 | 1.886271919 | 18.3111 |
| 3 | 5 | 2.02375 | 0.030198438 | 0.69888 | 0.003370666 | 9.132925 | 1.886271919 | 18.3111 |
| 2 | 6.67 | 2.02 | 0.0322 | 0.69684 | 0.003802574 | 9.1159 | 1.94793349 | 18.2748 |
| 2.33 | 5.83 | 2.02 | 0.0322 | 0.69684 | 0.003802574 | 9.1159 | 1.94793349 | 18.2748 |
| 2.67 | 5 | 2.02 | 0.0322 | 0.69684 | 0.003802574 | 9.1159 | 1.94793349 | 18.2748 |
| 3 | 4.17 | 2.02 | 0.0322 | 0.69684 | 0.003802574 | 9.1159 | 1.94793349 | 18.2748 |
| 2 | 4.17 | 2.03005 | 0.027168498 | 0.6951 | 0.00935199 | 9.177295 | 1.718234408 | 18.3984 |
| 2.33 | 5 | 2.03005 | 0.027168498 | 0.6951 | 0.00935199 | 9.177295 | 1.718234408 | 18.3984 |
| 2.67 | 5.83 | 2.03005 | 0.027168498 | 0.6951 | 0.00935199 | 9.177295 | 1.718234408 | 18.3984 |
| 3 | 6.67 | 2.03005 | 0.027168498 | 0.6951 | 0.00935199 | 9.177295 | 1.718234408 | 18.3984 |
| 2 | 5 | 2.0251 | 0.03026299 | 0.6852 | 0.01648296 | 9.17059 | 1.738569902 | 18.3768 |
| 2.33 | 4.17 | 2.0251 | 0.03026299 | 0.6852 | 0.01648296 | 9.17059 | 1.738569902 | 18.3768 |
| 2.67 | 6.67 | 2.0251 | 0.03026299 | 0.6852 | 0.01648296 | 9.17059 | 1.738569902 | 18.3768 |
| 3 | 5.83 | 2.0251 | 0.03026299 | 0.6852 | 0.01648296 | 9.17059 | 1.738569902 | 18.3768 |
| 2 | 5.83 | 2.02015 | 0.033308478 | 0.6753 | 0.02341791 | 9.163885 | 1.758815482 | 18.3552 |
| 2.33 | 6.67 | 2.02015 | 0.033308478 | 0.6753 | 0.02341791 | 9.163885 | 1.758815482 | 18.3552 |
| 2.67 | 4.17 | 2.02015 | 0.033308478 | 0.6753 | 0.02341791 | 9.163885 | 1.758815482 | 18.3552 |
| 3 | 5 | 2.02015 | 0.033308478 | 0.6753 | 0.02341791 | 9.163885 | 1.758815482 | 18.3552 |
| 2 | 6.67 | 2.0152 | 0.03630496 | 0.6654 | 0.03015684 | 9.15718 | 1.778971148 | 18.3336 |
| 2.33 | 5.83 | 2.0152 | 0.03630496 | 0.6654 | 0.03015684 | 9.15718 | 1.778971148 | 18.3336 |
| 2.67 | 5 | 2.0152 | 0.03630496 | 0.6654 | 0.03015684 | 9.15718 | 1.778971148 | 18.3336 |
| 3 | 4.17 | 2.0152 | 0.03630496 | 0.6654 | 0.03015684 | 9.15718 | 1.778971148 | 18.3336 |
| 2 | 4.17 | 2.02675 | 0.031051938 | 0.70149 | 0.00314992 | 9.165295 | 1.769529488 | 18.3612 |
| 2.33 | 5 | 2.02675 | 0.031051938 | 0.70149 | 0.00314992 | 9.165295 | 1.769529488 | 18.3612 |
| 2.67 | 5.83 | 2.02675 | 0.031051938 | 0.70149 | 0.00314992 | 9.165295 | 1.769529488 | 18.3612 |
| 3 | 6.67 | 2.02675 | 0.031051938 | 0.70149 | 0.00314992 | 9.165295 | 1.769529488 | 18.3612 |
| 2 | 5 | 2.0185 | 0.03794275 | 0.69798 | 0.0042502 | 9.14659 | 1.840550222 | 18.3024 |
| 2.33 | 4.17 | 2.0185 | 0.03794275 | 0.69798 | 0.0042502 | 9.14659 | 1.840550222 | 18.3024 |
| 2.67 | 6.67 | 2.0185 | 0.03794275 | 0.69798 | 0.0042502 | 9.14659 | 1.840550222 | 18.3024 |
| 3 | 5.83 | 2.0185 | 0.03794275 | 0.69798 | 0.0042502 | 9.14659 | 1.840550222 | 18.3024 |
| 2 | 5.83 | 2.01025 | 0.044697438 | 0.69447 | 0.005325839 | 9.127885 | 1.910871202 | 18.2436 |
| 2.33 | 6.67 | 2.01025 | 0.044697438 | 0.69447 | 0.005325839 | 9.127885 | 1.910871202 | 18.2436 |
| 2.67 | 4.17 | 2.01025 | 0.044697438 | 0.69447 | 0.005325839 | 9.127885 | 1.910871202 | 18.2436 |
| 3 | 5 | 2.01025 | 0.044697438 | 0.69447 | 0.005325839 | 9.127885 | 1.910871202 | 18.2436 |
| 2 | 6.67 | 2.002 | 0.051316 | 0.69096 | 0.006376838 | 9.10918 | 1.980492428 | 18.1848 |
| 2.33 | 5.83 | 2.002 | 0.051316 | 0.69096 | 0.006376838 | 9.10918 | 1.980492428 | 18.1848 |
| 2.67 | 5 | 2.002 | 0.051316 | 0.69096 | 0.006376838 | 9.10918 | 1.980492428 | 18.1848 |
| 3 | 4.17 | 2.002 | 0.051316 | 0.69096 | 0.006376838 | 9.10918 | 1.980492428 | 18.1848 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **δ**SIE |  | **δ**RA |  | **δ**AN |  | **δ**RC |  | **δ**DE | **OP** |
| 1.769344183 | 1.53255 | 0.205873998 | 21.015 | 36.194775 | 1.50185 | 0.097974078 | 3.515 | 12.369775 | 223.9 |
| 1.769344183 | 1.53255 | 0.205873998 | 21.015 | 36.194775 | 1.50185 | 0.097974078 | 3.515 | 12.369775 | 210.7 |
| 1.769344183 | 1.53255 | 0.205873998 | 21.015 | 36.194775 | 1.50185 | 0.097974078 | 3.515 | 12.369775 | 198.6 |
| 1.769344183 | 1.53255 | 0.205873998 | 21.015 | 36.194775 | 1.50185 | 0.097974078 | 3.515 | 12.369775 | 215.3 |
| 1.742554701 | 1.5201 | 0.20441299 | 21.03 | 36.3891 | 1.5137 | 0.09956731 | 3.53 | 12.4891 | 180.5 |
| 1.742554701 | 1.5201 | 0.20441299 | 21.03 | 36.3891 | 1.5137 | 0.09956731 | 3.53 | 12.4891 | 151.4 |
| 1.742554701 | 1.5201 | 0.20441299 | 21.03 | 36.3891 | 1.5137 | 0.09956731 | 3.53 | 12.4891 | 143 |
| 1.742554701 | 1.5201 | 0.20441299 | 21.03 | 36.3891 | 1.5137 | 0.09956731 | 3.53 | 12.4891 | 162.7 |
| 1.715231555 | 1.50765 | 0.202641978 | 21.045 | 36.582975 | 1.52555 | 0.100879698 | 3.545 | 12.607975 | 138.5 |
| 1.715231555 | 1.50765 | 0.202641978 | 21.045 | 36.582975 | 1.52555 | 0.100879698 | 3.545 | 12.607975 | 110.6 |
| 1.715231555 | 1.50765 | 0.202641978 | 21.045 | 36.582975 | 1.52555 | 0.100879698 | 3.545 | 12.607975 | 100.5 |
| 1.715231555 | 1.50765 | 0.202641978 | 21.045 | 36.582975 | 1.52555 | 0.100879698 | 3.545 | 12.607975 | 120.9 |
| 1.687374744 | 1.4952 | 0.20056096 | 21.06 | 36.7764 | 1.5374 | 0.10191124 | 3.56 | 12.7264 | 239.8 |
| 1.687374744 | 1.4952 | 0.20056096 | 21.06 | 36.7764 | 1.5374 | 0.10191124 | 3.56 | 12.7264 | 200.6 |
| 1.687374744 | 1.4952 | 0.20056096 | 21.06 | 36.7764 | 1.5374 | 0.10191124 | 3.56 | 12.7264 | 191.5 |
| 1.687374744 | 1.4952 | 0.20056096 | 21.06 | 36.7764 | 1.5374 | 0.10191124 | 3.56 | 12.7264 | 225.7 |
| 1.818910448 | 1.5444 | 0.20650264 | 21.03 | 36.4191 | 1.4906 | 0.09575164 | 3.545 | 12.697975 | 230.5 |
| 1.818910448 | 1.5444 | 0.20650264 | 21.03 | 36.4191 | 1.4906 | 0.09575164 | 3.545 | 12.697975 | 209.3 |
| 1.818910448 | 1.5444 | 0.20650264 | 21.03 | 36.4191 | 1.4906 | 0.09575164 | 3.545 | 12.697975 | 203 |
| 1.818910448 | 1.5444 | 0.20650264 | 21.03 | 36.4191 | 1.4906 | 0.09575164 | 3.545 | 12.697975 | 220.6 |
| 1.83757827 | 1.5438 | 0.20597956 | 21.06 | 36.8364 | 1.4912 | 0.09540256 | 3.59 | 13.1419 | 183.9 |
| 1.83757827 | 1.5438 | 0.20597956 | 21.06 | 36.8364 | 1.4912 | 0.09540256 | 3.59 | 13.1419 | 158.3 |
| 1.83757827 | 1.5438 | 0.20597956 | 21.06 | 36.8364 | 1.4912 | 0.09540256 | 3.59 | 13.1419 | 148.1 |
| 1.83757827 | 1.5438 | 0.20597956 | 21.06 | 36.8364 | 1.4912 | 0.09540256 | 3.59 | 13.1419 | 163 |
| 1.851603468 | 1.5432 | 0.20545576 | 21.09 | 37.2519 | 1.4918 | 0.09505276 | 3.635 | 13.581775 | 147.9 |
| 1.851603468 | 1.5432 | 0.20545576 | 21.09 | 37.2519 | 1.4918 | 0.09505276 | 3.635 | 13.581775 | 118.2 |
| 1.851603468 | 1.5432 | 0.20545576 | 21.09 | 37.2519 | 1.4918 | 0.09505276 | 3.635 | 13.581775 | 101.6 |
| 1.851603468 | 1.5432 | 0.20545576 | 21.09 | 37.2519 | 1.4918 | 0.09505276 | 3.635 | 13.581775 | 131.7 |
| 1.860986042 | 1.5426 | 0.20493124 | 21.12 | 37.6656 | 1.4924 | 0.09470224 | 3.68 | 14.0176 | 235.1 |
| 1.860986042 | 1.5426 | 0.20493124 | 21.12 | 37.6656 | 1.4924 | 0.09470224 | 3.68 | 14.0176 | 207 |
| 1.860986042 | 1.5426 | 0.20493124 | 21.12 | 37.6656 | 1.4924 | 0.09470224 | 3.68 | 14.0176 | 198.3 |
| 1.860986042 | 1.5426 | 0.20493124 | 21.12 | 37.6656 | 1.4924 | 0.09470224 | 3.68 | 14.0176 | 228 |
| 1.77820039 | 1.5477 | 0.20996071 | 21.705 | 77.097975 | 1.4948 | 0.09463696 | 3.455 | 12.067975 | 289.1 |
| 1.77820039 | 1.5477 | 0.20996071 | 21.705 | 77.097975 | 1.4948 | 0.09463696 | 3.455 | 12.067975 | 264.7 |
| 1.77820039 | 1.5477 | 0.20996071 | 21.705 | 77.097975 | 1.4948 | 0.09463696 | 3.455 | 12.067975 | 253.4 |
| 1.77820039 | 1.5477 | 0.20996071 | 21.705 | 77.097975 | 1.4948 | 0.09463696 | 3.455 | 12.067975 | 278 |
| 1.76066956 | 1.5504 | 0.21288184 | 22.41 | 117.2019 | 1.4996 | 0.09312784 | 3.41 | 11.8819 | 243.6 |
| 1.76066956 | 1.5504 | 0.21288184 | 22.41 | 117.2019 | 1.4996 | 0.09312784 | 3.41 | 11.8819 | 229.9 |
| 1.76066956 | 1.5504 | 0.21288184 | 22.41 | 117.2019 | 1.4996 | 0.09312784 | 3.41 | 11.8819 | 212 |
| 1.76066956 | 1.5504 | 0.21288184 | 22.41 | 117.2019 | 1.4996 | 0.09312784 | 3.41 | 11.8819 | 238.6 |
| 1.74300751 | 1.5531 | 0.21578839 | 23.115 | 156.311775 | 1.5044 | 0.09157264 | 3.365 | 11.691775 | 209.7 |
| 1.74300751 | 1.5531 | 0.21578839 | 23.115 | 156.311775 | 1.5044 | 0.09157264 | 3.365 | 11.691775 | 192.6 |
| 1.74300751 | 1.5531 | 0.21578839 | 23.115 | 156.311775 | 1.5044 | 0.09157264 | 3.365 | 11.691775 | 188 |
| 1.74300751 | 1.5531 | 0.21578839 | 23.115 | 156.311775 | 1.5044 | 0.09157264 | 3.365 | 11.691775 | 197.6 |
| 1.72521424 | 1.5558 | 0.21868036 | 23.82 | 194.4276 | 1.5092 | 0.08997136 | 3.32 | 11.4976 | 290.1 |
| 1.72521424 | 1.5558 | 0.21868036 | 23.82 | 194.4276 | 1.5092 | 0.08997136 | 3.32 | 11.4976 | 271.3 |
| 1.72521424 | 1.5558 | 0.21868036 | 23.82 | 194.4276 | 1.5092 | 0.08997136 | 3.32 | 11.4976 | 269 |
| 1.72521424 | 1.5558 | 0.21868036 | 23.82 | 194.4276 | 1.5092 | 0.08997136 | 3.32 | 11.4976 | 283 |
| 1.824749719 | 1.5459 | 0.20789719 | 20.955 | 35.592975 | 1.4918 | 0.09519676 | 3.47 | 12.0991 | 271.3 |
| 1.824749719 | 1.5459 | 0.20789719 | 20.955 | 35.592975 | 1.4918 | 0.09519676 | 3.47 | 12.0991 | 256.7 |
| 1.824749719 | 1.5459 | 0.20789719 | 20.955 | 35.592975 | 1.4918 | 0.09519676 | 3.47 | 12.0991 | 259 |
| 1.824749719 | 1.5459 | 0.20789719 | 20.955 | 35.592975 | 1.4918 | 0.09519676 | 3.47 | 12.0991 | 278.1 |
| 1.853740128 | 1.5468 | 0.20876776 | 20.91 | 35.1819 | 1.4936 | 0.09428704 | 3.44 | 11.9464 | 237.9 |
| 1.853740128 | 1.5468 | 0.20876776 | 20.91 | 35.1819 | 1.4936 | 0.09428704 | 3.44 | 11.9464 | 208.4 |
| 1.853740128 | 1.5468 | 0.20876776 | 20.91 | 35.1819 | 1.4936 | 0.09428704 | 3.44 | 11.9464 | 189.9 |
| 1.853740128 | 1.5468 | 0.20876776 | 20.91 | 35.1819 | 1.4936 | 0.09428704 | 3.44 | 11.9464 | 220.8 |
| 1.882571224 | 1.5477 | 0.20963671 | 20.865 | 34.766775 | 1.4954 | 0.09337084 | 3.41 | 11.7919 | 188.3 |
| 1.882571224 | 1.5477 | 0.20963671 | 20.865 | 34.766775 | 1.4954 | 0.09337084 | 3.41 | 11.7919 | 171.5 |
| 1.882571224 | 1.5477 | 0.20963671 | 20.865 | 34.766775 | 1.4954 | 0.09337084 | 3.41 | 11.7919 | 163.2 |
| 1.882571224 | 1.5477 | 0.20963671 | 20.865 | 34.766775 | 1.4954 | 0.09337084 | 3.41 | 11.7919 | 186.6 |
| 1.91124301 | 1.5486 | 0.21050404 | 20.82 | 34.3476 | 1.4972 | 0.09244816 | 3.38 | 11.6356 | 283.4 |
| 1.91124301 | 1.5486 | 0.21050404 | 20.82 | 34.3476 | 1.4972 | 0.09244816 | 3.38 | 11.6356 | 259 |
| 1.91124301 | 1.5486 | 0.21050404 | 20.82 | 34.3476 | 1.4972 | 0.09244816 | 3.38 | 11.6356 | 248.6 |
| 1.91124301 | 1.5486 | 0.21050404 | 20.82 | 34.3476 | 1.4972 | 0.09244816 | 3.38 | 11.6356 | 276.1 |
| 1.844417178 | 1.54755 | 0.209772498 | 21.225 | 42.024375 | 1.4942 | 0.09465436 | 3.47 | 12.0991 | 228.1 |
| 1.844417178 | 1.54755 | 0.209772498 | 21.225 | 42.024375 | 1.4942 | 0.09465436 | 3.47 | 12.0991 | 213.2 |
| 1.844417178 | 1.54755 | 0.209772498 | 21.225 | 42.024375 | 1.4942 | 0.09465436 | 3.47 | 12.0991 | 196.3 |
| 1.844417178 | 1.54755 | 0.209772498 | 21.225 | 42.024375 | 1.4942 | 0.09465436 | 3.47 | 12.0991 | 201.3 |
| 1.89286171 | 1.5501 | 0.21250699 | 21.45 | 47.9475 | 1.4984 | 0.09317344 | 3.44 | 11.9464 | 171.6 |
| 1.89286171 | 1.5501 | 0.21250699 | 21.45 | 47.9475 | 1.4984 | 0.09317344 | 3.44 | 11.9464 | 147.3 |
| 1.89286171 | 1.5501 | 0.21250699 | 21.45 | 47.9475 | 1.4984 | 0.09317344 | 3.44 | 11.9464 | 135.9 |
| 1.89286171 | 1.5501 | 0.21250699 | 21.45 | 47.9475 | 1.4984 | 0.09317344 | 3.44 | 11.9464 | 153.4 |
| 1.940933598 | 1.55265 | 0.215228478 | 21.675 | 53.769375 | 1.5026 | 0.09165724 | 3.41 | 11.7919 | 129 |
| 1.940933598 | 1.55265 | 0.215228478 | 21.675 | 53.769375 | 1.5026 | 0.09165724 | 3.41 | 11.7919 | 113.7 |
| 1.940933598 | 1.55265 | 0.215228478 | 21.675 | 53.769375 | 1.5026 | 0.09165724 | 3.41 | 11.7919 | 95.3 |
| 1.940933598 | 1.55265 | 0.215228478 | 21.675 | 53.769375 | 1.5026 | 0.09165724 | 3.41 | 11.7919 | 111.1 |
| 1.98863284 | 1.5552 | 0.21793696 | 21.9 | 59.49 | 1.5068 | 0.09010576 | 3.38 | 11.6356 | 240 |
| 1.98863284 | 1.5552 | 0.21793696 | 21.9 | 59.49 | 1.5068 | 0.09010576 | 3.38 | 11.6356 | 210.3 |
| 1.98863284 | 1.5552 | 0.21793696 | 21.9 | 59.49 | 1.5068 | 0.09010576 | 3.38 | 11.6356 | 183.3 |
| 1.98863284 | 1.5552 | 0.21793696 | 21.9 | 59.49 | 1.5068 | 0.09010576 | 3.38 | 11.6356 | 209.6 |
| 1.843214336 | 1.5456 | 0.20759464 | 20.985 | 35.834775 | 1.4909 | 0.09559519 | 3.485 | 12.159775 | 281.6 |
| 1.843214336 | 1.5456 | 0.20759464 | 20.985 | 35.834775 | 1.4909 | 0.09559519 | 3.485 | 12.159775 | 248.4 |
| 1.843214336 | 1.5456 | 0.20759464 | 20.985 | 35.834775 | 1.4909 | 0.09559519 | 3.485 | 12.159775 | 260.1 |
| 1.843214336 | 1.5456 | 0.20759464 | 20.985 | 35.834775 | 1.4909 | 0.09559519 | 3.485 | 12.159775 | 278 |
| 1.890470622 | 1.5462 | 0.20816356 | 20.97 | 35.6691 | 1.4918 | 0.09508876 | 3.47 | 12.0691 | 220.9 |
| 1.890470622 | 1.5462 | 0.20816356 | 20.97 | 35.6691 | 1.4918 | 0.09508876 | 3.47 | 12.0691 | 198.3 |
| 1.890470622 | 1.5462 | 0.20816356 | 20.97 | 35.6691 | 1.4918 | 0.09508876 | 3.47 | 12.0691 | 169.4 |
| 1.890470622 | 1.5462 | 0.20816356 | 20.97 | 35.6691 | 1.4918 | 0.09508876 | 3.47 | 12.0691 | 180.1 |
| 1.93736886 | 1.5468 | 0.20873176 | 20.955 | 35.502975 | 1.4927 | 0.09458071 | 3.455 | 11.977975 | 163.6 |
| 1.93736886 | 1.5468 | 0.20873176 | 20.955 | 35.502975 | 1.4927 | 0.09458071 | 3.455 | 11.977975 | 155.2 |
| 1.93736886 | 1.5468 | 0.20873176 | 20.955 | 35.502975 | 1.4927 | 0.09458071 | 3.455 | 11.977975 | 148.7 |
| 1.93736886 | 1.5468 | 0.20873176 | 20.955 | 35.502975 | 1.4927 | 0.09458071 | 3.455 | 11.977975 | 159 |
| 1.98390905 | 1.5474 | 0.20929924 | 20.94 | 35.3364 | 1.4936 | 0.09407104 | 3.44 | 11.8864 | 273.9 |
| 1.98390905 | 1.5474 | 0.20929924 | 20.94 | 35.3364 | 1.4936 | 0.09407104 | 3.44 | 11.8864 | 231.7 |
| 1.98390905 | 1.5474 | 0.20929924 | 20.94 | 35.3364 | 1.4936 | 0.09407104 | 3.44 | 11.8864 | 216.4 |
| 1.98390905 | 1.5474 | 0.20929924 | 20.94 | 35.3364 | 1.4936 | 0.09407104 | 3.44 | 11.8864 | 268.9 |
| 1.97941231 | 1.54605 | 0.208052898 | 20.94 | 35.5164 | 1.4939 | 0.09468079 | 3.44 | 12.0664 | 278.9 |
| 1.97941231 | 1.54605 | 0.208052898 | 20.94 | 35.5164 | 1.4939 | 0.09468079 | 3.44 | 12.0664 | 265 |
| 1.97941231 | 1.54605 | 0.208052898 | 20.94 | 35.5164 | 1.4939 | 0.09468079 | 3.44 | 12.0664 | 256.7 |
| 1.97941231 | 1.54605 | 0.208052898 | 20.94 | 35.5164 | 1.4939 | 0.09468079 | 3.44 | 12.0664 | 262.8 |
| 2.16058924 | 1.5471 | 0.20907859 | 20.88 | 35.0256 | 1.4978 | 0.09323116 | 3.38 | 11.8756 | 231.2 |
| 2.16058924 | 1.5471 | 0.20907859 | 20.88 | 35.0256 | 1.4978 | 0.09323116 | 3.38 | 11.8756 | 213.2 |
| 2.16058924 | 1.5471 | 0.20907859 | 20.88 | 35.0256 | 1.4978 | 0.09323116 | 3.38 | 11.8756 | 201.6 |
| 2.16058924 | 1.5471 | 0.20907859 | 20.88 | 35.0256 | 1.4978 | 0.09323116 | 3.38 | 11.8756 | 218.7 |
| 2.33913079 | 1.54815 | 0.210102078 | 20.82 | 34.5276 | 1.5017 | 0.09175111 | 3.32 | 11.6776 | 197.1 |
| 2.33913079 | 1.54815 | 0.210102078 | 20.82 | 34.5276 | 1.5017 | 0.09175111 | 3.32 | 11.6776 | 181.3 |
| 2.33913079 | 1.54815 | 0.210102078 | 20.82 | 34.5276 | 1.5017 | 0.09175111 | 3.32 | 11.6776 | 176 |
| 2.33913079 | 1.54815 | 0.210102078 | 20.82 | 34.5276 | 1.5017 | 0.09175111 | 3.32 | 11.6776 | 183.1 |
| 2.51503696 | 1.5492 | 0.21112336 | 20.76 | 34.0224 | 1.5056 | 0.09024064 | 3.26 | 11.4724 | 287.4 |
| 2.51503696 | 1.5492 | 0.21112336 | 20.76 | 34.0224 | 1.5056 | 0.09024064 | 3.26 | 11.4724 | 268 |
| 2.51503696 | 1.5492 | 0.21112336 | 20.76 | 34.0224 | 1.5056 | 0.09024064 | 3.26 | 11.4724 | 256.7 |
| 2.51503696 | 1.5492 | 0.21112336 | 20.76 | 34.0224 | 1.5056 | 0.09024064 | 3.26 | 11.4724 | 283.1 |
| 1.88412544 | 1.53435 | 0.204781578 | 20.97 | 35.6991 | 1.50305 | 0.099192198 | 3.47 | 12.0991 | 231.2 |
| 1.88412544 | 1.53435 | 0.204781578 | 20.97 | 35.6991 | 1.50305 | 0.099192198 | 3.47 | 12.0991 | 226.1 |
| 1.88412544 | 1.53435 | 0.204781578 | 20.97 | 35.6991 | 1.50305 | 0.099192198 | 3.47 | 12.0991 | 210.3 |
| 1.88412544 | 1.53435 | 0.204781578 | 20.97 | 35.6991 | 1.50305 | 0.099192198 | 3.47 | 12.0991 | 221.4 |
| 1.97171776 | 1.5237 | 0.20231131 | 20.94 | 35.3964 | 1.5161 | 0.10194379 | 3.44 | 11.9464 | 142.9 |
| 1.97171776 | 1.5237 | 0.20231131 | 20.94 | 35.3964 | 1.5161 | 0.10194379 | 3.44 | 11.9464 | 116.5 |
| 1.97171776 | 1.5237 | 0.20231131 | 20.94 | 35.3964 | 1.5161 | 0.10194379 | 3.44 | 11.9464 | 113 |
| 1.97171776 | 1.5237 | 0.20231131 | 20.94 | 35.3964 | 1.5161 | 0.10194379 | 3.44 | 11.9464 | 133.3 |
| 2.05837696 | 1.51305 | 0.199614198 | 20.91 | 35.0919 | 1.52915 | 0.104354778 | 3.41 | 11.7919 | 191.3 |
| 2.05837696 | 1.51305 | 0.199614198 | 20.91 | 35.0919 | 1.52915 | 0.104354778 | 3.41 | 11.7919 | 153.1 |
| 2.05837696 | 1.51305 | 0.199614198 | 20.91 | 35.0919 | 1.52915 | 0.104354778 | 3.41 | 11.7919 | 152.3 |
| 2.05837696 | 1.51305 | 0.199614198 | 20.91 | 35.0919 | 1.52915 | 0.104354778 | 3.41 | 11.7919 | 170 |
| 2.14410304 | 1.5024 | 0.19669024 | 20.88 | 34.7856 | 1.5422 | 0.10642516 | 3.38 | 11.6356 | 255 |
| 2.14410304 | 1.5024 | 0.19669024 | 20.88 | 34.7856 | 1.5422 | 0.10642516 | 3.38 | 11.6356 | 239.7 |
| 2.14410304 | 1.5024 | 0.19669024 | 20.88 | 34.7856 | 1.5422 | 0.10642516 | 3.38 | 11.6356 | 210.6 |
| 2.14410304 | 1.5024 | 0.19669024 | 20.88 | 34.7856 | 1.5422 | 0.10642516 | 3.38 | 11.6356 | 251.1 |
| 2.18022256 | 1.54845 | 0.210946098 | 21.195 | 40.836975 | 1.4969 | 0.09494839 | 3.425 | 12.094375 | 293.7 |
| 2.18022256 | 1.54845 | 0.210946098 | 21.195 | 40.836975 | 1.4969 | 0.09494839 | 3.425 | 12.094375 | 270 |
| 2.18022256 | 1.54845 | 0.210946098 | 21.195 | 40.836975 | 1.4969 | 0.09494839 | 3.425 | 12.094375 | 243.6 |
| 2.18022256 | 1.54845 | 0.210946098 | 21.195 | 40.836975 | 1.4969 | 0.09494839 | 3.425 | 12.094375 | 281.3 |
| 2.55793024 | 1.5519 | 0.21484339 | 21.39 | 45.5979 | 1.5038 | 0.09370156 | 3.35 | 11.9275 | 247 |
| 2.55793024 | 1.5519 | 0.21484339 | 21.39 | 45.5979 | 1.5038 | 0.09370156 | 3.35 | 11.9275 | 231.4 |
| 2.55793024 | 1.5519 | 0.21484339 | 21.39 | 45.5979 | 1.5038 | 0.09370156 | 3.35 | 11.9275 | 216 |
| 2.55793024 | 1.5519 | 0.21484339 | 21.39 | 45.5979 | 1.5038 | 0.09370156 | 3.35 | 11.9275 | 246.9 |
| 2.92872304 | 1.55535 | 0.218716878 | 21.585 | 50.282775 | 1.5107 | 0.09235951 | 3.275 | 11.749375 | 213.7 |
| 2.92872304 | 1.55535 | 0.218716878 | 21.585 | 50.282775 | 1.5107 | 0.09235951 | 3.275 | 11.749375 | 191.6 |
| 2.92872304 | 1.55535 | 0.218716878 | 21.585 | 50.282775 | 1.5107 | 0.09235951 | 3.275 | 11.749375 | 181.3 |
| 2.92872304 | 1.55535 | 0.218716878 | 21.585 | 50.282775 | 1.5107 | 0.09235951 | 3.275 | 11.749375 | 193 |
| 3.29260096 | 1.5588 | 0.22256656 | 21.78 | 54.8916 | 1.5176 | 0.09092224 | 3.2 | 11.56 | 289.6 |
| 3.29260096 | 1.5588 | 0.22256656 | 21.78 | 54.8916 | 1.5176 | 0.09092224 | 3.2 | 11.56 | 273.6 |
| 3.29260096 | 1.5588 | 0.22256656 | 21.78 | 54.8916 | 1.5176 | 0.09092224 | 3.2 | 11.56 | 266.4 |
| 3.29260096 | 1.5588 | 0.22256656 | 21.78 | 54.8916 | 1.5176 | 0.09092224 | 3.2 | 11.56 | 274.1 |

# 附录3

import numpy as np

import pandas as pd

import matplotlib.pyplot as plt

import seaborn as sns

from sklearn.metrics import mean\_squared\_error

from sklearn.model\_selection import cross\_val\_score

from sklearn.feature\_selection import SelectKBest, f\_regression

from sklearn.metrics import r2\_score, mean\_squared\_error

from collections import Counter

dataset=pd.read\_csv(r'文件位置.csv')

features.head()

X= dataset.iloc[:, 0:11].values#输入和输出数据集划分

y = dataset.iloc[:,11].values.reshape(-1,1)

corr = dataset.corr()#相关系数矩阵，即给出了任意两个变量之间的相关系数

import matplotlib.pyplot as plt

import seaborn as sns

plt.xticks(range(len(corr.columns)), corr.columns)

plt.yticks(range(len(corr.columns)), corr.columns)

plt.savefig('皮尔逊.png', dpi=500, bbox\_inches='tight') plt.show()

from sklearn.model\_selection import train\_test\_split#划分数据集

X\_train, X\_test, y\_train, y\_test = train\_test\_split(X, y, test\_size = 0.3, random\_state = 42)

1.线性模型

from sklearn.linear\_model import LinearRegression

regressor\_linear = LinearRegression()

regressor\_linear.fit(X\_train, y\_train)

from sklearn.metrics import r2\_score

cv\_linear = cross\_val\_score(estimator = regressor\_linear, X = X\_train, y = y\_train, cv = 10)

var\_linear=np.var(cv\_linear)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_linear), np.std(cv\_linear)))

print("Variance:",var\_linear )

print("每次交叉验证后的准确率结果：\n",cv\_linear)

y\_pred\_linear\_train = regressor\_linear.predict(X\_train)

r2\_score\_linear\_train = r2\_score(y\_train, y\_pred\_linear\_train)

y\_pred\_linear\_test = regressor\_linear.predict(X\_test)

r2\_score\_linear\_test = r2\_score(y\_test, y\_pred\_linear\_test)

rmse\_linear\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_linear\_train)))

rmse\_linear\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_linear\_test)))

print('R2\_score (train): ', r2\_score\_linear\_train)

print('R2\_score (test): ', r2\_score\_linear\_test)

print("RMSE(train): ", rmse\_linear\_train)

print("RMSE(test): ", rmse\_linear\_test)

plt.figure(figsize=(5,5))

plt.plot([0,300], [0, 300], 'r--')

plt.scatter(y\_train, y\_pred\_linear\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7)

plt.scatter(y\_test,y\_pred\_linear\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7)

plt.legend()

plt.xlim([80,300])#坐标轴范围

plt.ylim([80,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

2.脊回归

from sklearn.linear\_model import Ridge

from sklearn.preprocessing import StandardScaler

from sklearn.pipeline import Pipeline

from sklearn.preprocessing import PolynomialFeatures

steps=[('scalar',StandardScaler()),('poly',PolynomialFeatures(degree=2)),('model',Ridge(alpha=3.8, fit\_intercept=True))]

ridge\_pipe = Pipeline(steps)

ridge\_pipe.fit(X\_train, y\_train)

from sklearn.metrics import r2\_score

cv\_ridge = cross\_val\_score(estimator = ridge\_pipe, X = X\_train, y = y\_train, cv = 10)

var\_ridge=np.var(cv\_ridge)

print("每次交叉验证后的准确率结果：\n",cv\_ridge)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_ridge), np.std(cv\_ridge)))

print("Variance:",var\_ridge )

y\_pred\_ridge\_train = ridge\_pipe.predict(X\_train)

r2\_score\_ridge\_train = r2\_score(y\_train, y\_pred\_ridge\_train)

y\_pred\_ridge\_test = ridge\_pipe.predict(X\_test)

r2\_score\_ridge\_test = r2\_score(y\_test, y\_pred\_ridge\_test)

rmse\_ridge\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_ridge\_train)))

rmse\_ridge\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_ridge\_test)))

print('CV: ', cv\_ridge.mean())

print('R2\_score (train): ', r2\_score\_ridge\_train)

print('R2\_score (test): ', r2\_score\_ridge\_test)

print("RMSE(train): ", rmse\_ridge\_train)

print("RMSE(test): ", rmse\_ridge\_test)

plt.figure(figsize=(5,5))

plt.plot([0,300], [0, 300], 'r--')

plt.scatter(y\_train, y\_pred\_ridge\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7,c = None)

plt.scatter(y\_test,y\_pred\_ridge\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7,c = None)

plt.legend()

plt.xlim([80,300])

plt.ylim([80,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

3.K近邻回归

from sklearn.neighbors import KNeighborsRegressor

param\_grid = [{'weights':['uniform'],'n\_neighbors':[k for k in range(1,8)]},{'weights':['distance'],

'n\_neighbors':[k for k in range(1,8)],'p':[p for p in range(1,8)] }]

KNR=GridSearchCV(estimator=KNeighborsRegressor(), param\_grid=param\_grid,cv=10)

KNR.fit(X\_train, y\_train)

print(KNR.best\_params\_)

regressor\_KNR=KNR.best\_estimator\_

regressor\_KNR.fit(X\_train,y\_train)

from sklearn.metrics import r2\_score

cv\_KNR = cross\_val\_score(estimator = regressor\_KNR, X = X\_train, y = y\_train, cv = 10)

var\_KNR=np.var(cv\_KNR)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_KNR), np.std(cv\_KNR)))

print("Variance:",var\_KNR )

y\_pred\_KNR\_train = regressor\_KNR.predict(X\_train)

r2\_score\_KNR\_train = r2\_score(y\_train, y\_pred\_KNR\_train)

y\_pred\_KNR\_test = regressor\_KNR.predict(X\_test)

r2\_score\_KNR\_test = r2\_score(y\_test, y\_pred\_KNR\_test)

rmse\_KNR\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_KNR\_train)))

rmse\_KNR\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_KNR\_test)))

print('CV: ', cv\_KNR.mean())

print('R2\_score (train): ', r2\_score\_KNR\_train)

print('R2\_score (test): ', r2\_score\_KNR\_test)

print("RMSE(train): ", rmse\_KNR\_train)

print("RMSE(test): ", rmse\_KNR\_test)

plt.figure(figsize=(5,5))

plt.plot([0,300], [0, 300], 'r--')

plt.scatter(y\_train, y\_pred\_KNR\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7)

plt.scatter(y\_test,y\_pred\_KNR\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7)

plt.legend()

plt.xlim([100,300])

plt.ylim([100,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

4.Lasso回归

from sklearn.linear\_model import Lasso

from sklearn.preprocessing import StandardScaler

from sklearn.pipeline import Pipeline

from sklearn.preprocessing import PolynomialFeatures

lasso\_pipe = Pipeline(steps)

lasso\_pipe.fit(X\_train, y\_train)

from sklearn.metrics import r2\_score

from sklearn.linear\_model import Lasso

from sklearn.preprocessing import StandardScaler

from sklearn.pipeline import Pipeline

from sklearn.preprocessing import PolynomialFeatures

cv\_lasso = cross\_val\_score(estimator = lasso\_pipe, X = X\_train, y = y\_train, cv = 10)

var\_lasso=np.var(cv\_lasso)

print("每次交叉验证后的准确率结果：\n",cv\_lasso)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_lasso), np.std(cv\_lasso)))

print("Variance:",var\_lasso )

# Predicting R2 Score the Test set results

y\_pred\_lasso\_train = lasso\_pipe.predict(X\_train)

r2\_score\_lasso\_train = r2\_score(y\_train, y\_pred\_lasso\_train)

y\_pred\_lasso\_test = lasso\_pipe.predict(X\_test)

r2\_score\_lasso\_test = r2\_score(y\_test, y\_pred\_lasso\_test)

rmse\_lasso\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_lasso\_train)))

rmse\_lasso\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_lasso\_test)))

print('CV: ', cv\_lasso.mean())

print('R2\_score (train): ', r2\_score\_lasso\_train)

print('R2\_score (test): ', r2\_score\_lasso\_test)

print("RMSE(train): ", rmse\_lasso\_train)

print("RMSE(test): ", rmse\_lasso\_test)

plt.figure(figsize=(5,5))

plt.plot([80,300], [80, 300], 'r--')

y = np.arange(1,1,1)

x = np.arange(1,1,1)

plt.scatter(y\_train, y\_pred\_lasso\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7,c = None)

plt.scatter(y\_test,y\_pred\_lasso\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7)

plt.legend()

plt.xlim([80,300])

plt.ylim([80,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

5.随机森林回归

from sklearn.ensemble import RandomForestRegressor

from sklearn.model\_selection import GridSearchCV

param\_grid={'n\_estimators':[50,100,200,300],'max\_depth':[10,20, 30, None],'min\_samples\_split': [2, 5, 10],'min\_samples\_leaf': [1, 2, 4]}

rf = RandomForestRegressor()

rf\_random=GridSearchCV(estimator=rf,param\_grid=param\_grid,cv=5)

rf\_random.fit(X\_train,y\_train)

print(rf\_random .best\_params\_)

regressor\_rf=rf\_random.best\_estimator\_

from sklearn.metrics import r2\_score

cv\_rf = cross\_val\_score(estimator = regressor\_rf, X = X\_train, y = y\_train, cv = 10)

var\_rf=np.var(cv\_rf)

print("每次交叉验证后的准确率结果：\n",cv\_rf)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_rf), np.std(cv\_rf)))

print("Variance:",var\_rf )

# Predicting R2 Score the Train set results

y\_pred\_rf\_train = regressor\_rf.predict(X\_train)

r2\_score\_rf\_train = r2\_score(y\_train, y\_pred\_rf\_train)

# Predicting R2 Score the Test set results

y\_pred\_rf\_test = regressor\_rf.predict(X\_test)

r2\_score\_rf\_test = r2\_score(y\_test, y\_pred\_rf\_test)

rmse\_rf\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_rf\_train)))

rmse\_rf\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_rf\_test)))

print('CV: ', cv\_rf.mean())

print('R2\_score (train): ', r2\_score\_rf\_train)

print('R2\_score (test): ', r2\_score\_rf\_test)

print("RMSE(train): ", rmse\_rf\_train)

print("RMSE(test): ", rmse\_rf\_test)

plt.figure(figsize=(5,5))

plt.plot([80,300], [80, 300], 'r--')

plt.scatter(y\_train, y\_pred\_rf\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7)

plt.scatter(y\_test,y\_pred\_rf\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7)

plt.legend()

plt.xlim([80,300])

plt.ylim([80,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

6.自适应增强回归

from sklearn.ensemble import AdaBoostRegressor

adaboost = AdaBoostRegressor()

param\_grid = {'n\_estimators': [50, 100, 150],'learning\_rate': [0.01, 0.05, 0.1]}

grid\_search = GridSearchCV(adaboost, param\_grid, cv=10, scoring='r2')

grid\_search.fit(X\_train, y\_train)

print("Best parameters:", grid\_search.best\_params\_)

regressor\_ada= grid\_search.best\_estimator\_

regressor\_ada.fit(X\_train, y\_train)

import warnings

warnings.filterwarnings("ignore")

from sklearn.metrics import r2\_score

cv\_ada = cross\_val\_score(estimator = regressor\_ada, X = X\_train, y = y\_train, cv = 10)

var\_ada=np.var(cv\_ada)

print("每次交叉验证后的准确率结果：\n",cv\_ada)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_ada), np.std(cv\_ada)))

print("Variance:",var\_ada )

y\_pred\_ada\_train = regressor\_ada.predict(X\_train)

r2\_score\_ada\_train = r2\_score(y\_train, y\_pred\_ada\_train)

y\_pred\_ada\_test = regressor\_ada.predict(X\_test)

r2\_score\_ada\_test = r2\_score(y\_test, y\_pred\_ada\_test)

rmse\_ada\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_ada\_train)))

rmse\_ada\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_ada\_test)))

print('CV: ', cv\_ada.mean())

print('R2\_score (train): ', r2\_score\_ada\_train)

print('R2\_score (test): ', r2\_score\_ada\_test)

print("RMSE(train): ", rmse\_ada\_train)

print("RMSE(test): ", rmse\_ada\_test)

plt.figure(figsize=(5,5))

plt.plot([0,300], [0, 300], 'r--')

plt.scatter(y\_train, y\_pred\_ada\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7)

plt.scatter(y\_test,y\_pred\_ada\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7)

plt.legend()

plt.xlim([80,300])

plt.ylim([80,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

6.极致梯度提升回归

import xgboost as xgb

from xgboost import plot\_importance

reg = xgb.XGBRegressor()

param\_grid = {"learning\_rate": [0.05, 0.1, 0.2],"n\_estimators": [100, 200, 300],"max\_depth": [3, 4, 5]}

grid\_search = GridSearchCV(reg, param\_grid, cv=5, scoring="neg\_mean\_squared\_error")

grid\_search.fit(X\_train, y\_train)

best\_params = grid\_search.best\_params\_

print("Best parameters:", best\_params)

regressor\_xgb = xgb.XGBRegressor(\*\*best\_params)

regressor\_xgb.fit(X\_train, y\_train)

from sklearn.metrics import r2\_score

cv\_xgb = cross\_val\_score(estimator = regressor\_xgb, X = X\_train, y = y\_train, cv = 10)

var\_xgb=np.var(cv\_xgb)

print("每次交叉验证后的准确率结果：\n",cv\_xgb)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_xgb), np.std(cv\_xgb)))

print("Variance:",var\_xgb )

y\_pred\_xgb\_train = regressor\_xgb.predict(X\_train)

r2\_score\_xgb\_train = r2\_score(y\_train, y\_pred\_xgb\_train)

y\_pred\_xgb\_test = regressor\_xgb.predict(X\_test)

r2\_score\_xgb\_test = r2\_score(y\_test, y\_pred\_xgb\_test)

rmse\_xgb\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_xgb\_train)))

rmse\_xgb\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_xgb\_test)))

print('CV: ', cv\_xgb.mean())

print('R2\_score (train): ', r2\_score\_xgb\_train)

print('R2\_score (test): ', r2\_score\_xgb\_test)

print("RMSE(train): ", rmse\_xgb\_train)

print("RMSE(test): ", rmse\_xgb\_test)

#极致梯度提升回归重要性排序

plot\_importance(regressor\_xgb)

plt.show()

7.梯度提升回归

from sklearn.ensemble import GradientBoostingRegressor

param=[{'learning\_rate':[1.0,1e-1,1e-2,1e-3,1e-4,1e-5]},

{'n\_estimators':[100,250,500]},

{'max\_depth':[4,6,8,10]}]

gbr=GridSearchCV(estimator=GradientBoostingRegressor(),param\_grid=param,cv=10)

gbr.fit(X\_train,y\_train)

print(gbr.best\_params\_)

regressor\_gbr=gbr.best\_estimator\_

regressor\_gbr.fit(X\_train,y\_train)

from sklearn.metrics import r2\_score

cv\_gbr = cross\_val\_score(estimator = regressor\_gbr, X = X\_train, y = y\_train, cv = 10)

var\_gbr=np.var(cv\_gbr)

print("每次交叉验证后的准确率结果：\n",cv\_gbr)

print('R2 mean: %.3f +/- %.3f' % (np.mean(cv\_gbr), np.std(cv\_gbr)))

print("Variance:",var\_gbr )

y\_pred\_gbr\_train = regressor\_gbr.predict(X\_train)

r2\_score\_gbr\_train = r2\_score(y\_train, y\_pred\_gbr\_train)

y\_pred\_gbr\_test = regressor\_gbr.predict(X\_test)

r2\_score\_gbr\_test = r2\_score(y\_test, y\_pred\_gbr\_test)

rmse\_gbr\_train = (np.sqrt(mean\_squared\_error(y\_train, y\_pred\_gbr\_train)))

rmse\_gbr\_test = (np.sqrt(mean\_squared\_error(y\_test, y\_pred\_gbr\_test)))

print('CV: ', cv\_gbr.mean())

print('R2\_score (train): ', r2\_score\_gbr\_train)

print('R2\_score (test): ', r2\_score\_gbr\_test)

print("RMSE(train): ", rmse\_gbr\_train)

print("RMSE(test): ", rmse\_gbr\_test)

plt.figure(figsize=(5,5))

plt.plot([0,300], [0, 300], 'r--')

plt.scatter(y\_train, y\_pred\_gbr\_train , color = 'blue', label = 'train',s = 80, edgecolor = 'k', alpha = 0.7)

plt.scatter(y\_test,y\_pred\_gbr\_test,color='r',label='test',s = 80, edgecolor = 'k', alpha = 0.7)

plt.legend()

plt.xlim([100,300])

plt.ylim([100,300])

plt.xlabel('True/eV')

plt.ylabel('Predicted/eV')

from sklearn.inspection import permutation\_importance#梯度提升回归模型重要性排序

feature\_importance = regressor\_gbr.feature\_importances\_

sorted\_idx = np.argsort(feature\_importance)

pos = np.arange(sorted\_idx.shape[0]) + .5

fig = plt.figure(figsize=(12, 6))

plt.subplot(1, 2, 1)

plt.barh(pos, feature\_importance[sorted\_idx], align='center')

plt.yticks(pos, np.array(dataset.columns)[sorted\_idx])

plt.title('Feature Importance (MDI)')

**joblib库调用**

import joblib

joblib.dump(调参后定义的模型,'model\_filename.pkl')

model=joblib.load('model\_filename.pkl')

#模型预测

input\_data=np.array([[需要预测的数据]])

predictions=model.predict(input\_data)

print(predictions)