Feature combination

|  |  |
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| Feature Name | definition |
| E\_O | The adsorption energy of M1/M2 for O calculated by DFT |
| AN\_1、AN\_2 | Atomic number numbers of M1 and M2 |
| EN\_1、EN\_2 | Electronegativity of M1 and M2 |
| FE\_1、FE\_1 | The first ionization energy of M1 and M2 |
| g\_1、g\_2 | Density of M1 and M2 |
| PN\_1、PN\_2 | The cycle of M1 and M2 |
| R\_1、R\_2 | The radius of M1 and M2 |
| AN\_product、AN\_division | The atomic number quotient of M1 and M2 |
| EN\_product、EN\_division | Electronegative product quotients of M1 and M2 |
| FE\_product、FE\_division | The first ionization energy product quotient of M1 and M2 |
| g\_product、g\_division | Density quotient of M1 and M2 |
| PN\_product、PN\_division | Periodic quotient of M1 and M2 |
| R\_product、R\_division | The radius quotient of M1 and M2 |
| S\_product、S\_division | Standard molar entropy quotients for M1 and M2 |
| H\_product、H\_division | Standard moles of M1 and M2 generate enthalpy quotients |
| C\_product、C\_division | Specific heat volume quotients of M1 and M2 |
| G\_product、G\_division | Standard molar free energy quotients of M1 and M2 |
| GN\_product、GN\_division | The family number quotient of M1 and M2 |
| AE\_product、AE\_division | The first electron affinity quotient of M1 and M2 |
| E\_H | The adsorption energy of M1/M2 to H calculated by DFT |
| S\_1、S\_2 | Standard molar entropy for M1 and M2 |
| H\_1、H\_2 | Standard molar enthalpy of formation for M1 and M2 |
| C\_1、C\_2 | Specific heat capacity of M1 and M2 |
| G\_1、G\_2 | Standard molar free energy for M1 and M2 |
| GN\_1、GN\_2 | Family numbers for M1 and M2 |
| AE\_1、AE\_2 | First electron affinity of M1 and M2 |
| AN\_differ、AN\_sum | The difference in atomic number numbers of M1 and M2 is sum |
| EN\_differ、EN\_sum | The electronegativity of M1 and M2 is poor |
| FE\_differ、FE\_sum | The difference in the first ionization energy of M1 and M2 is sum |
| g\_differ、g\_sum | The density difference between M1 and M2 is sum |
| PN\_differ、PN\_sum | The period difference between M1 and M2 is sum |
| R\_differ、R\_sum | The difference between the radii of M1 and M2 is sum |
| S\_differ、S\_sum | The standard molar difference in entropy of M1 and M2 is the sum |
| H\_differ、H\_sum | The standard moles of M1 and M2 generate the sum of enthalpy differences |
| C\_differ、C\_sum | Sum of specific heat tolerances for M1 and M2 |
| G\_differ、G\_sum | Standard molar free energy difference sum for M1 and M2 |
| GN\_differ、GN\_sum | The family numbers of M1 and M2 are the sum of the differences |
| AE\_differ、AE\_sum | The first electron affinity of M1 and M2 is poor |

CO optimal characteristic combination and serial number

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| Optimal feature number combination | serial number | RMSE |
| [2] | 2 | 0.65205 |
| [2, 63] | 136 | 0.40355 |
| [2, 63, 27] | 173 | 0.35834 |
| [2, 63, 27, 62] | 279 | 0.33368 |
| [2, 63, 27, 62, 69] | 355 | 0.29882 |
| [2, 63, 27, 62, 69, 1] | 361 | 0.28046 |
| [2, 63, 27, 62, 69, 1, 45] | 471 | 0.27099 |
| [2, 63, 27, 62, 69, 1, 45, 9] | 504 | 0.26643 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57] | 616 | 0.26102 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26] | 653 | 0.25774 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21] | 713 | 0.25353 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61] | 812 | 0.24997 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3] | 823 | 0.24532 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31] | 908 | 0.2423 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72] | 1003 | 0.23979 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33] | 1030 | 0.23742 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15] | 1075 | 0.23572 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59] | 1169 | 0.23422 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39] | 1208 | 0.2337 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30] | 1257 | 0.23403 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43] | 1321 | 0.23468 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60] | 1388 | 0.23573 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35] | 1421 | 0.23696 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12] | 1457 | 0.23763 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19] | 1513 | 0.2381 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58] | 1590 | 0.23914 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32] | 1619 | 0.24069 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18] | 1659 | 0.24262 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44] | 1720 | 0.24431 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 20] | 1752 | 0.24701 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20] | 1797 | 0.24864 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7] | 1833 | 0.25179 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37] | 1891 | 0.25451 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6] | 1917 | 0.25633 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8] | 1958 | 0.25834 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48] | 2017 | 0.26063 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36] | 2050 | 0.2631 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23] | 2082 | 0.26632 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50] | 2130 | 0.26982 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25] | 2156 | 0.27411 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11] | 2184 | 0.27835 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41] | 2229 | 0.2825 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49] | 2264 | 0.28677 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73] | 2309 | 0.2914 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74] | 2340 | 0.29541 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56] | 2362 | 0.29971 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38] | 2382 | 0.30393 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24] | 2406 | 0.30796 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4] | 2425 | 0.31197 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71] | 2475 | 0.31683 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16] | 2480 | 0.32168 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5] | 2500 | 0.32722 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55] | 2538 | 0.3326 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54] | 2559 | 0.33785 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51] | 2577 | 0.34368 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70] | 2604 | 0.34967 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34] | 2612 | 0.3561 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29] | 2629 | 0.36246 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22] | 2644 | 0.36955 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46] | 2662 | 0.37661 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52] | 2678 | 0.3832 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10] | 2685 | 0.38968 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28] | 2701 | 0.39487 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47] | 2714 | 0.40103 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17] | 2723 | 0.4061 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53] | 2734 | 0.41102 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66] | 2745 | 0.41826 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40] | 2750 | 0.42506 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14] | 2756 | 0.43113 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67] | 2764 | 0.43677 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67, 13] | 2766 | 0.44325 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67, 68, 13, 65] | 2774 | 0.45851 |
| [2, 63, 27, 62, 69, 1, 45, 9, 57, 26, 21, 61, 3, 31, 72, 33, 15, 59, 39, 30, 43, 60, 35, 12, 19, 58, 32, 18, 44, 42, 20, 7, 37, 6, 8, 48, 36, 23, 50, 25, 11, 41, 49, 73, 74, 56, 38, 24, 4, 71, 16, 5, 55, 54, 51, 70, 34, 29, 22, 46, 52, 10, 28, 47, 17, 53, 66, 40, 14, 67, 68, 13, 65, 64] | 2775 | 0.46775 |

CO2 optimal characteristic combination and serial number

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| Optimal feature number combination | serial number | RMSE |
| [1] | 1 | 0.27957 |
| [1, 69] | 142 | 0.22727 |
| [1, 69, 57] | 203 | 0.19097 |
| [1, 69, 57, 2] | 220 | 0.16572 |
| [1, 69, 57, 2, 63] | 350 | 0.15109 |
| [1, 69, 57, 2, 63, 58] | 415 | 0.14759 |
| [1, 69, 57, 2, 63, 58, 61] | 486 | 0.13944 |
| [1, 69, 57, 2, 63, 58, 61, 6] | 501 | 0.13963 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60] | 619 | 0.13352 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37] | 664 | 0.13085 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27] | 719 | 0.12372 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59] | 811 | 0.12266 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62] | 874 | 0.11824 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45] | 924 | 0.12258 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36] | 977 | 0.1169 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26] | 1028 | 0.11674 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34] | 1093 | 0.11536 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38] | 1152 | 0.11391 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35] | 1208 | 0.1147 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3] | 1236 | 0.11259 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23] | 1309 | 0.1173 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24] | 1363 | 0.11474 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22] | 1415 | 0.11408 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9] | 1454 | 0.1228 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21] | 1516 | 0.116 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33] | 1572 | 0.11204 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18] | 1612 | 0.11173 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19] | 1660 | 0.11203 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49] | 1723 | 0.11372 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55] | 1774 | 0.11182 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48] | 1813 | 0.1141 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8] | 1833 | 0.12334 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4] | 1873 | 0.128 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7] | 1916 | 0.12081 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5] | 1956 | 0.12876 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15] | 2001 | 0.11545 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54] | 2061 | 0.11645 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16] | 2078 | 0.11555 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31] | 2121 | 0.11537 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30] | 2156 | 0.11552 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32] | 2191 | 0.11535 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50] | 2233 | 0.11671 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17] | 2253 | 0.11617 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25] | 2286 | 0.11608 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20] | 2316 | 0.11681 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52] | 2357 | 0.11838 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51] | 2385 | 0.1187 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47] | 2412 | 0.11899 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56] | 2440 | 0.12001 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53] | 2465 | 0.12045 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46] | 2489 | 0.12116 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74] | 2522 | 0.12059 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72] | 2543 | 0.13031 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73] | 2565 | 0.12167 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71] | 2585 | 0.12227 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28] | 2591 | 0.1226 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29] | 2610 | 0.12515 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70] | 2639 | 0.13357 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41] | 2647 | 0.12958 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42] | 2663 | 0.13122 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43] | 2678 | 0.13329 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44] | 2692 | 0.13489 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39] | 2703 | 0.13786 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11] | 2711 | 0.14113 |
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| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68] | 2747 | 0.15202 |
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| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40] | 2768 | 0.16519 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40, 13] | 2771 | 0.16892 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40, 13, 10] | 2773 | 0.17373 |
| [1, 69, 57, 2, 63, 58, 61, 6, 60, 37, 27, 59, 62, 45, 36, 26, 34, 38, 35, 3, 23, 24, 22, 9, 21, 33, 18, 19, 49, 55, 48, 8, 4, 7, 5, 15, 54, 16, 31, 30, 32, 50, 17, 25, 20, 52, 51, 47, 56, 53, 46, 74, 72, 73, 71, 28, 29, 70, 41, 42, 43, 44, 39, 11, 12, 14, 68, 65, 66, 67, 40, 13, 10, 64] | 2775 | 0.1791 |