

Fig. 1 Vapor pressure estimation method for metal complexes by the COSMO-SAC method. Black arrows show the conventional calculation method, blue arrows show the improved method by non-regressive method to calculate ϵ_{dsp} , red arrows show the method to modify the activity coefficient due to dispersion interaction based on molecular polarizability, and green arrow shows the method to modify the activity coefficient due to molecular branching.

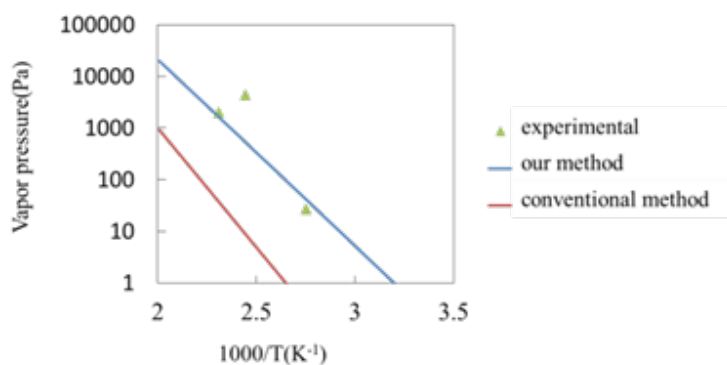


Fig. 2 Comparison between the measured (experimental) and estimated vapor pressures of Titanium tetraisopropoxide using conventional and improved COSMO-SAC methods.

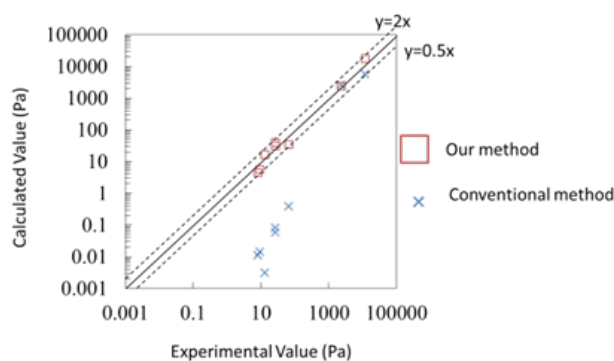


Fig. 3 Verification of the accuracy of the conventional and improved COSMO-SAC method.

References

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