Supporting Information:

Restricted-Variance Constrained, Reaction Path, and Transition State Molecular Optimizations Using Gradient-Enhanced Kriging

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The figures in the following pages show comparisons of the performance of the RS-RFO and RVO methods for the IRC optimizations. The bars show the number of iterations needed for optimizing each step of the path (0 is the initial saddle point, negative steps go toward reactants). The circles represent the root-mean-square displacement between the corresponding optimized structures.

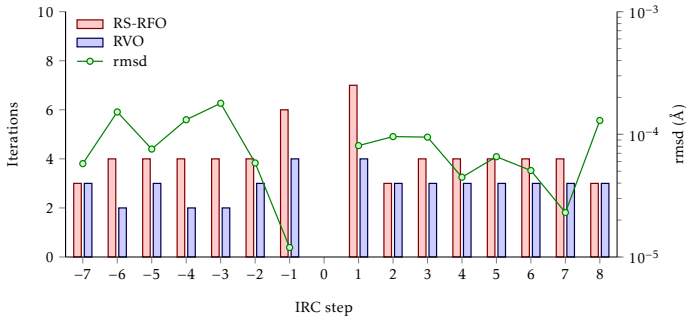

FIG. S-1. Comparison of performance for the IRC optimization of reaction #1.

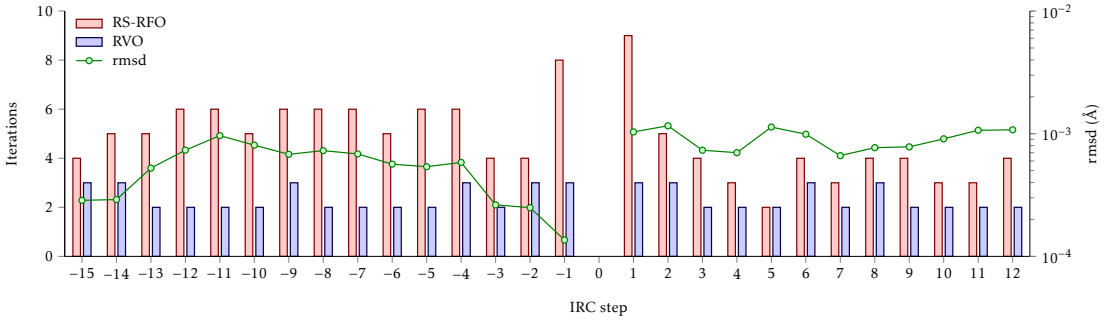

FIG. S-2. Comparison of performance for the IRC optimization of reaction #2.

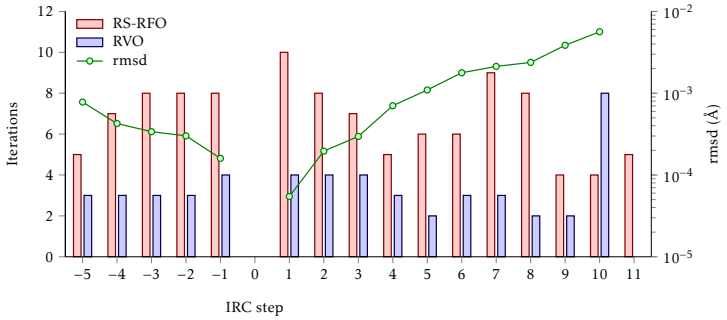

FIG. S-3. Comparison of performance for the IRC optimization of reaction #3.

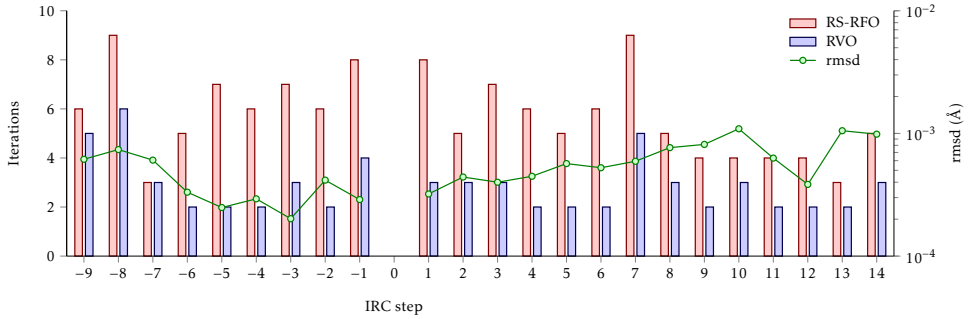

FIG. S-4. Comparison of performance for the IRC optimization of reaction #4.

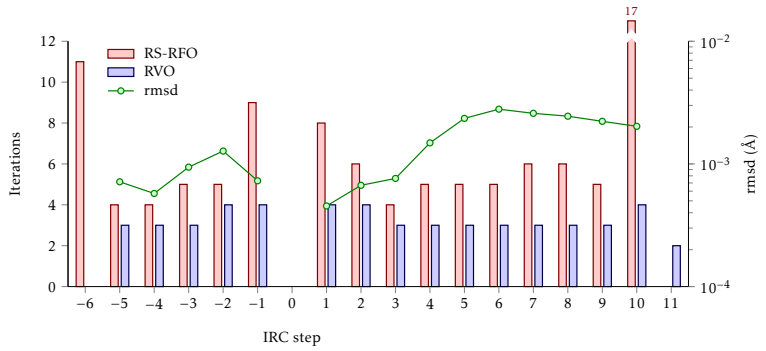

FIG. S-5. Comparison of performance for the IRC optimization of reaction #5.

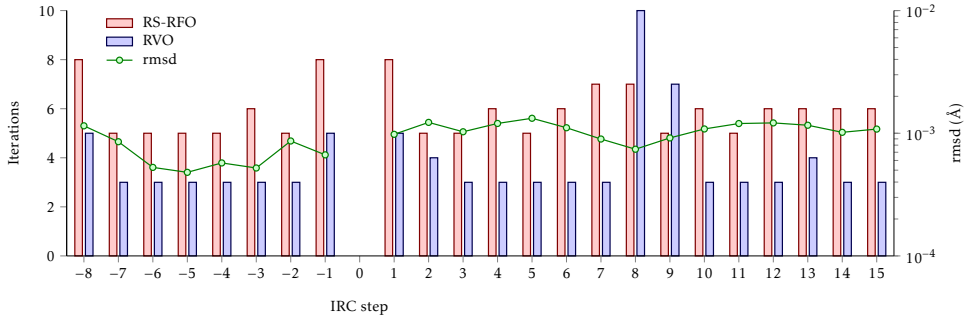

FIG. S-6. Comparison of performance for the IRC optimization of reaction #6.

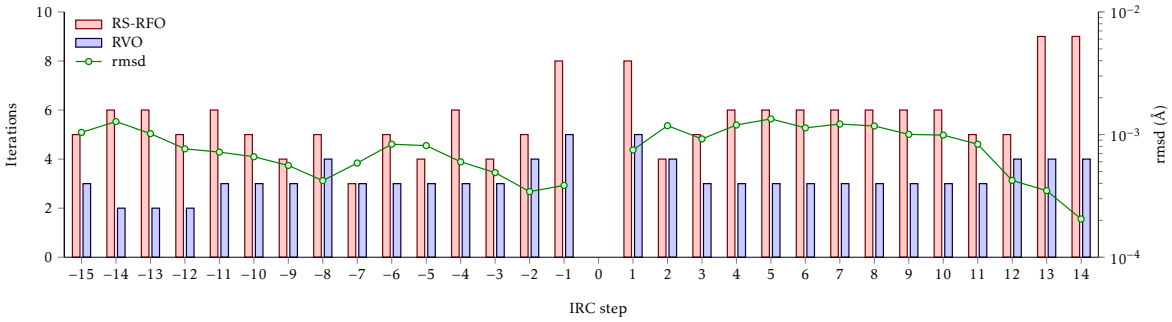

FIG. S-7. Comparison of performance for the IRC optimization of reaction #7.

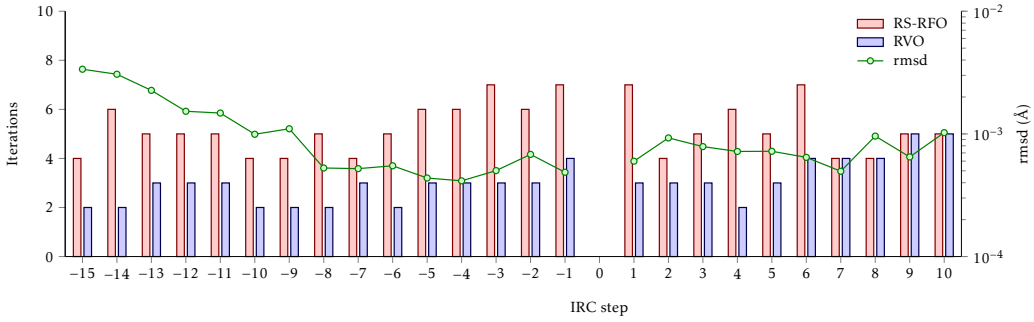

FIG. S-8. Comparison of performance for the IRC optimization of reaction #8.

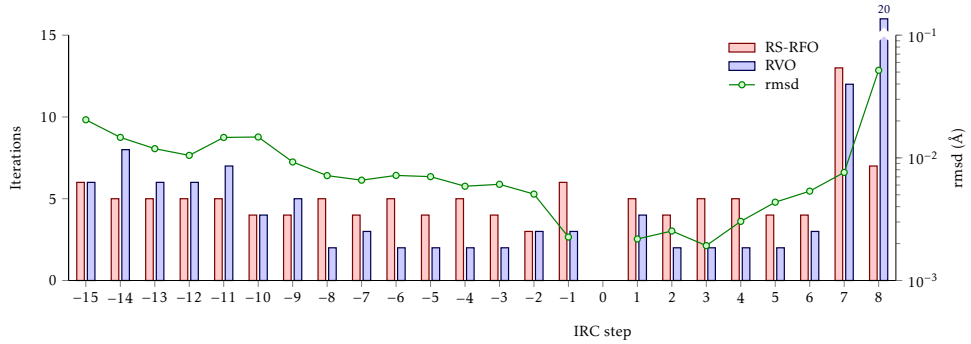

FIG. S-9. Comparison of performance for the IRC optimization of reaction #9.

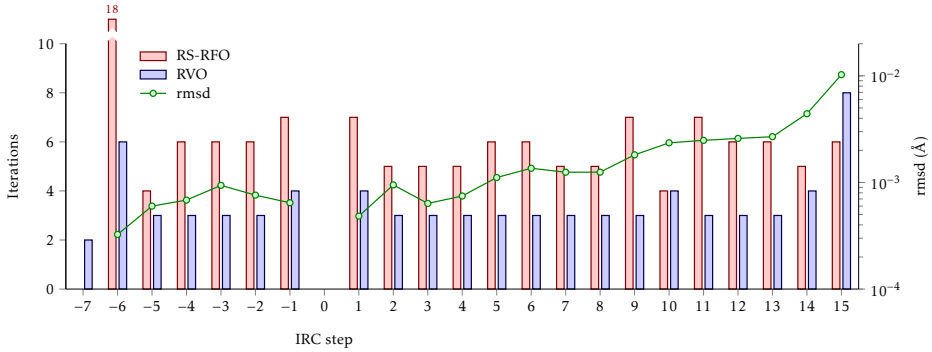

FIG. S-10. Comparison of performance for the IRC optimization of reaction #10.

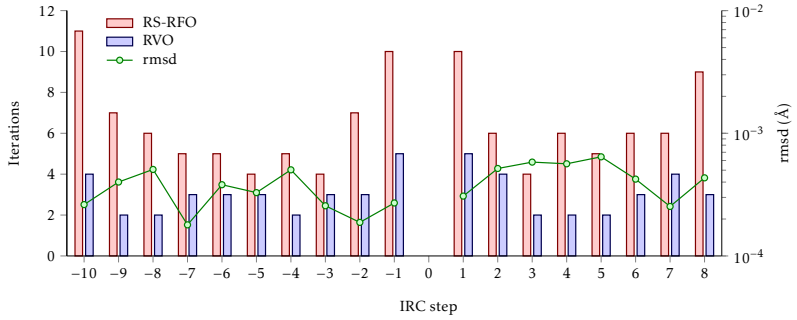

FIG. S-11. Comparison of performance for the IRC optimization of reaction #11.

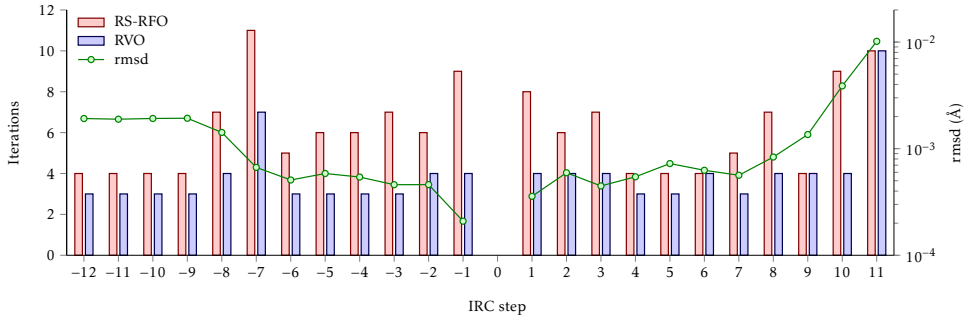

FIG. S-12. Comparison of performance for the IRC optimization of reaction #12.

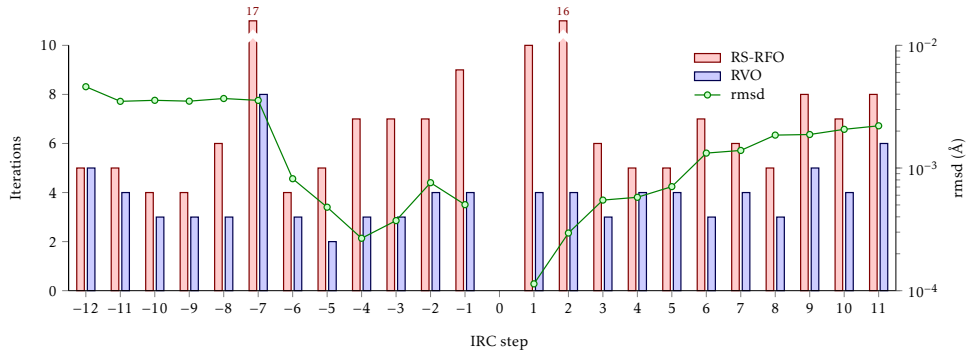

FIG. S-13. Comparison of performance for the IRC optimization of reaction #13.

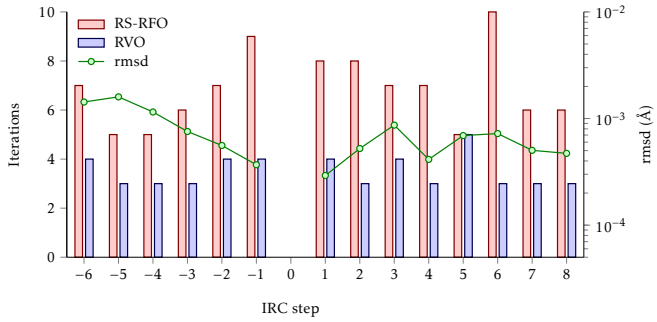

FIG. S-14. Comparison of performance for the IRC optimization of reaction #14.

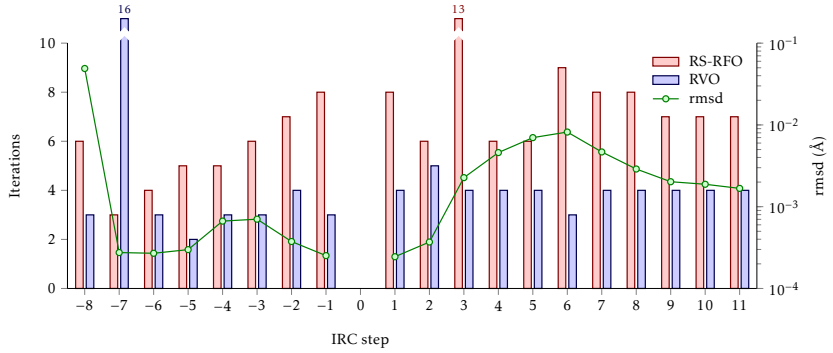

FIG. S-15. Comparison of performance for the IRC optimization of reaction #15.

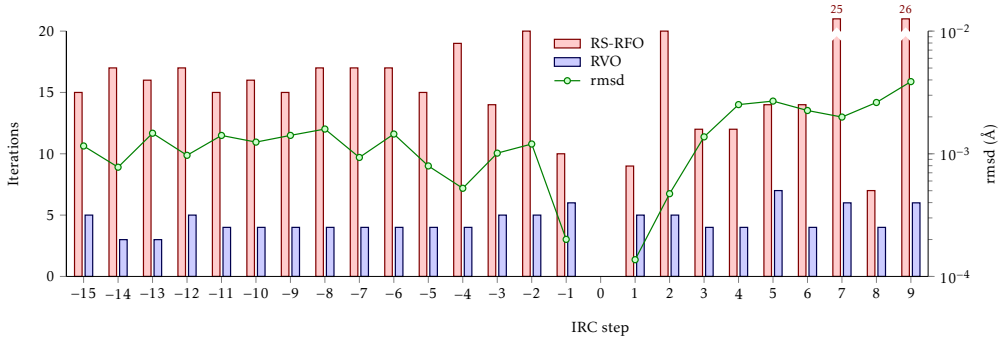

FIG. S-16. Comparison of performance for the IRC optimization of reaction #16.

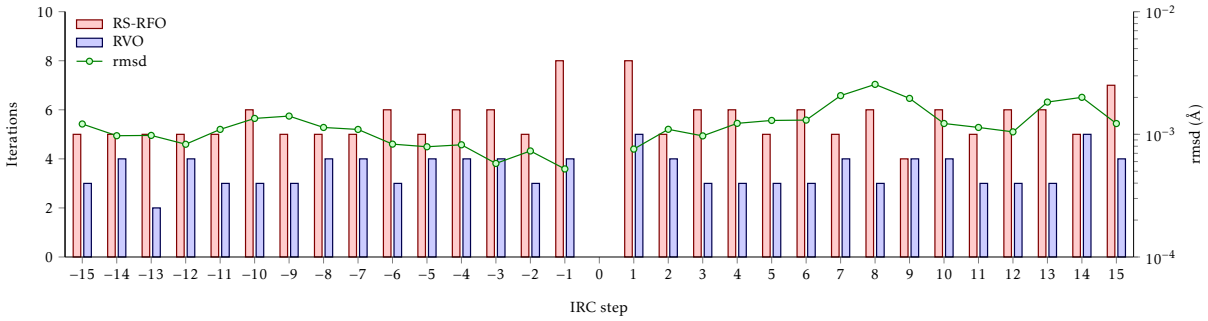

FIG. S-17. Comparison of performance for the IRC optimization of reaction #17.

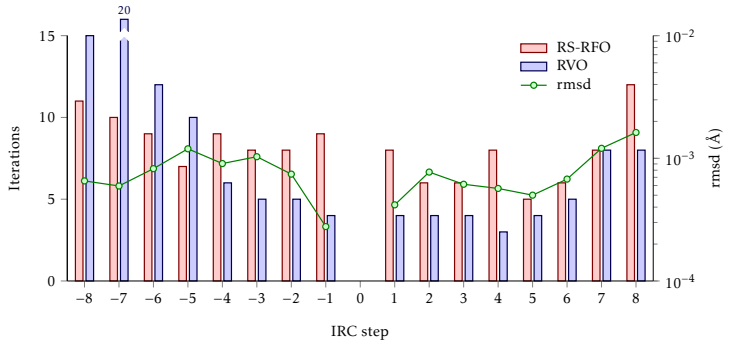

FIG. S-18. Comparison of performance for the IRC optimization of reaction #18.

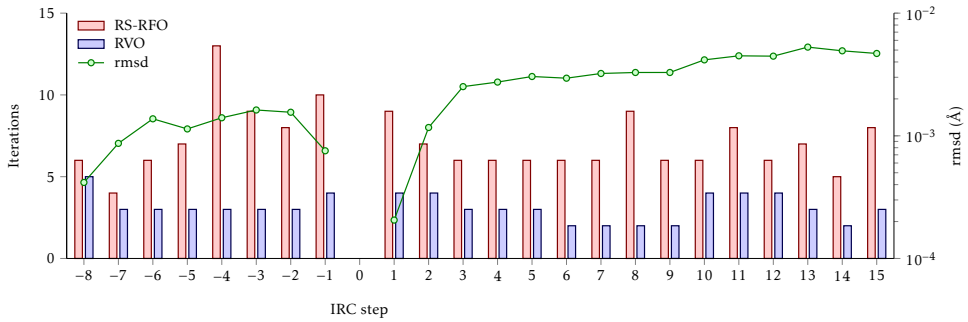

FIG. S-19. Comparison of performance for the IRC optimization of reaction #19.

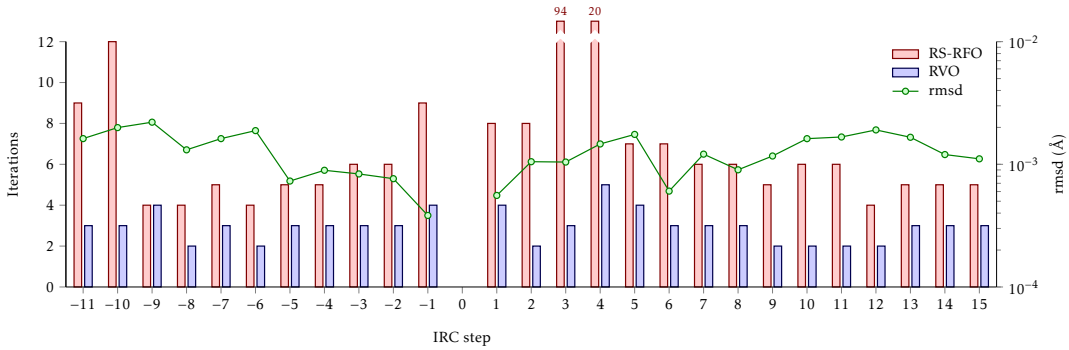

FIG. S-20. Comparison of performance for the IRC optimization of reaction #20.

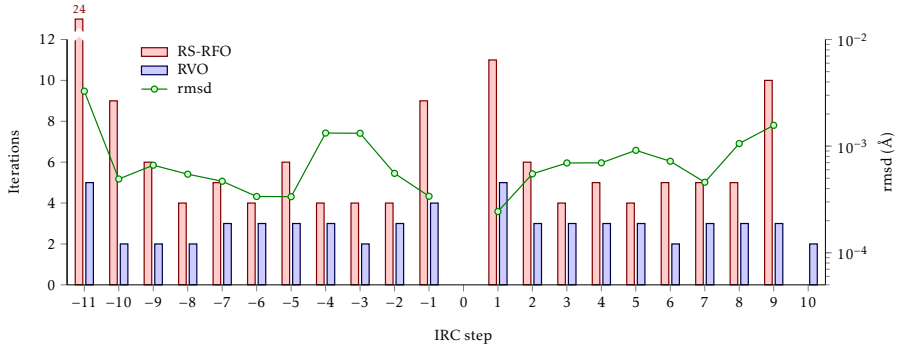

FIG. S-21. Comparison of performance for the IRC optimization of reaction #21.

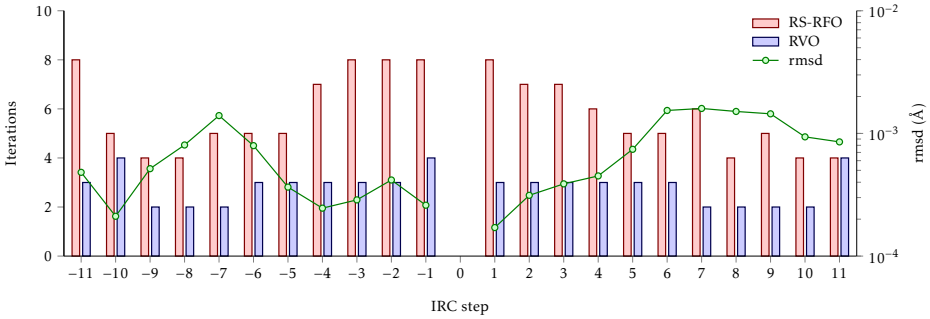

FIG. S-22. Comparison of performance for the IRC optimization of reaction #22.

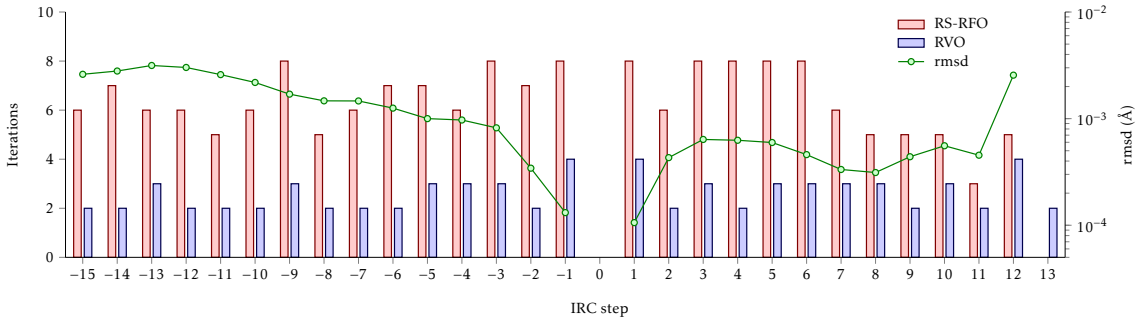

FIG. S-23. Comparison of performance for the IRC optimization of reaction #23.

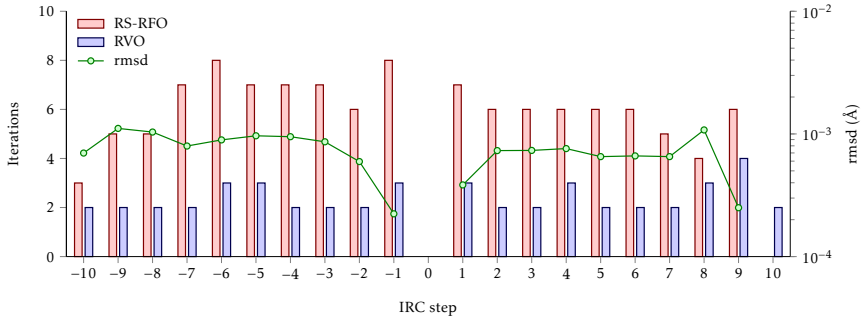

FIG. S-24. Comparison of performance for the IRC optimization of reaction #24.

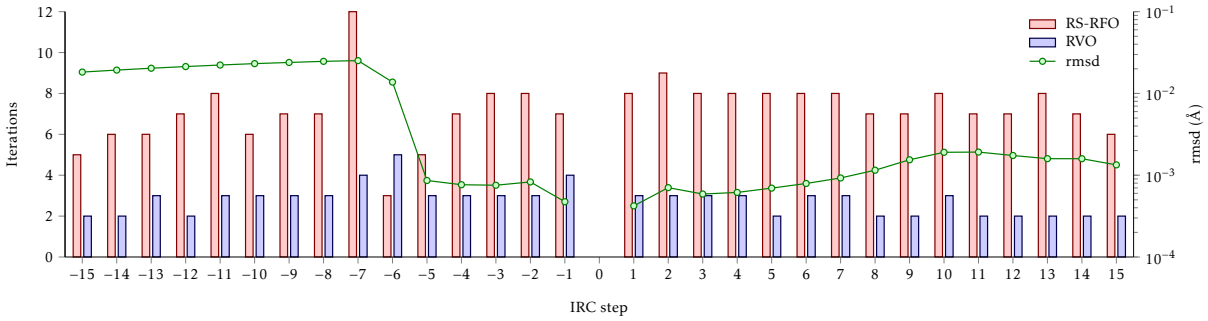

FIG. S-25. Comparison of performance for the IRC optimization of reaction #25.