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Metadynamics simulations of R–NHC reductive elimination in intermediate palladium complexes of cross-coupling and Mizoroki–Heck reactions

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Unbiased molecular dynamics simulations in gas phase

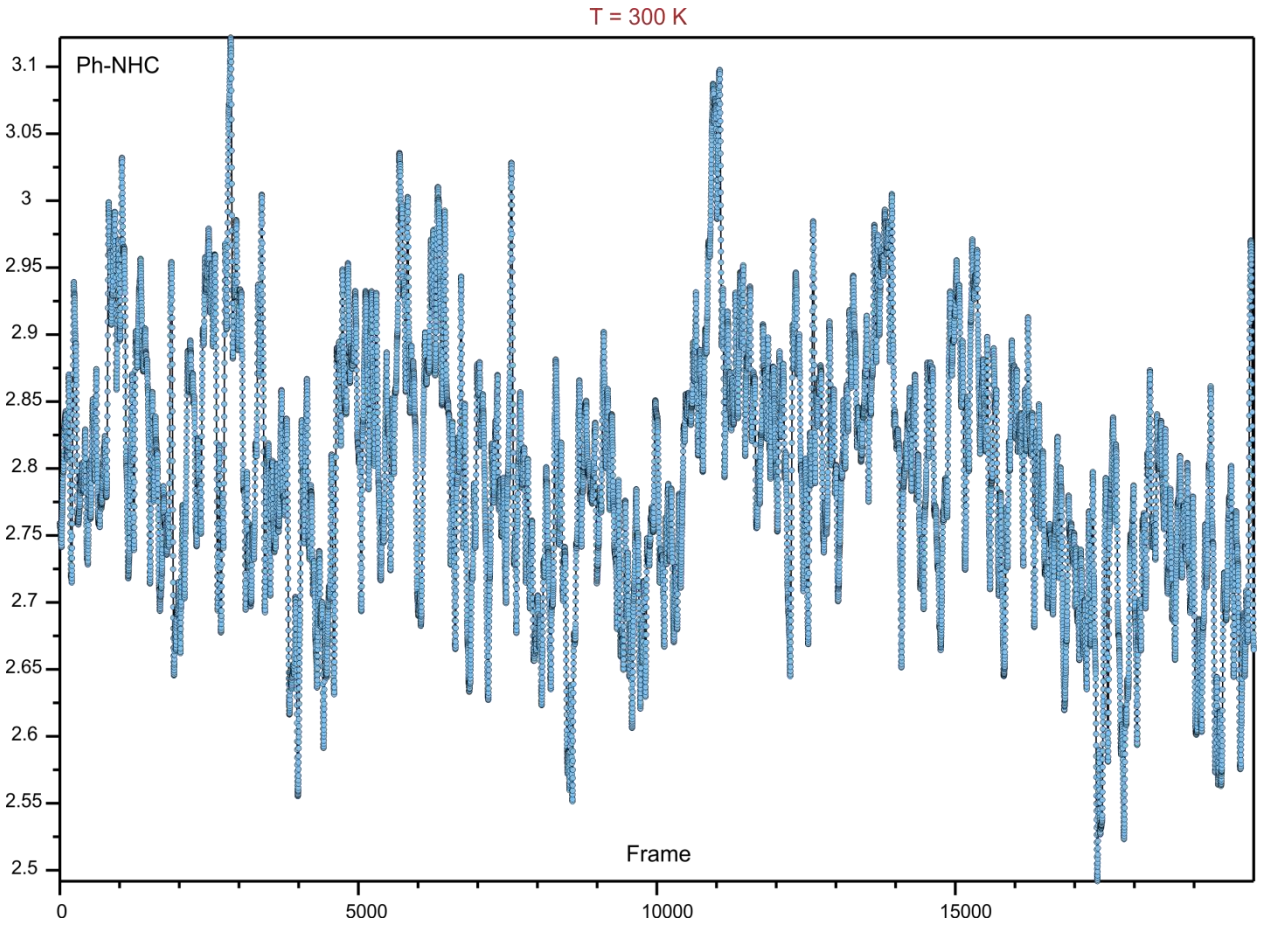

Figure S1. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 300 K.

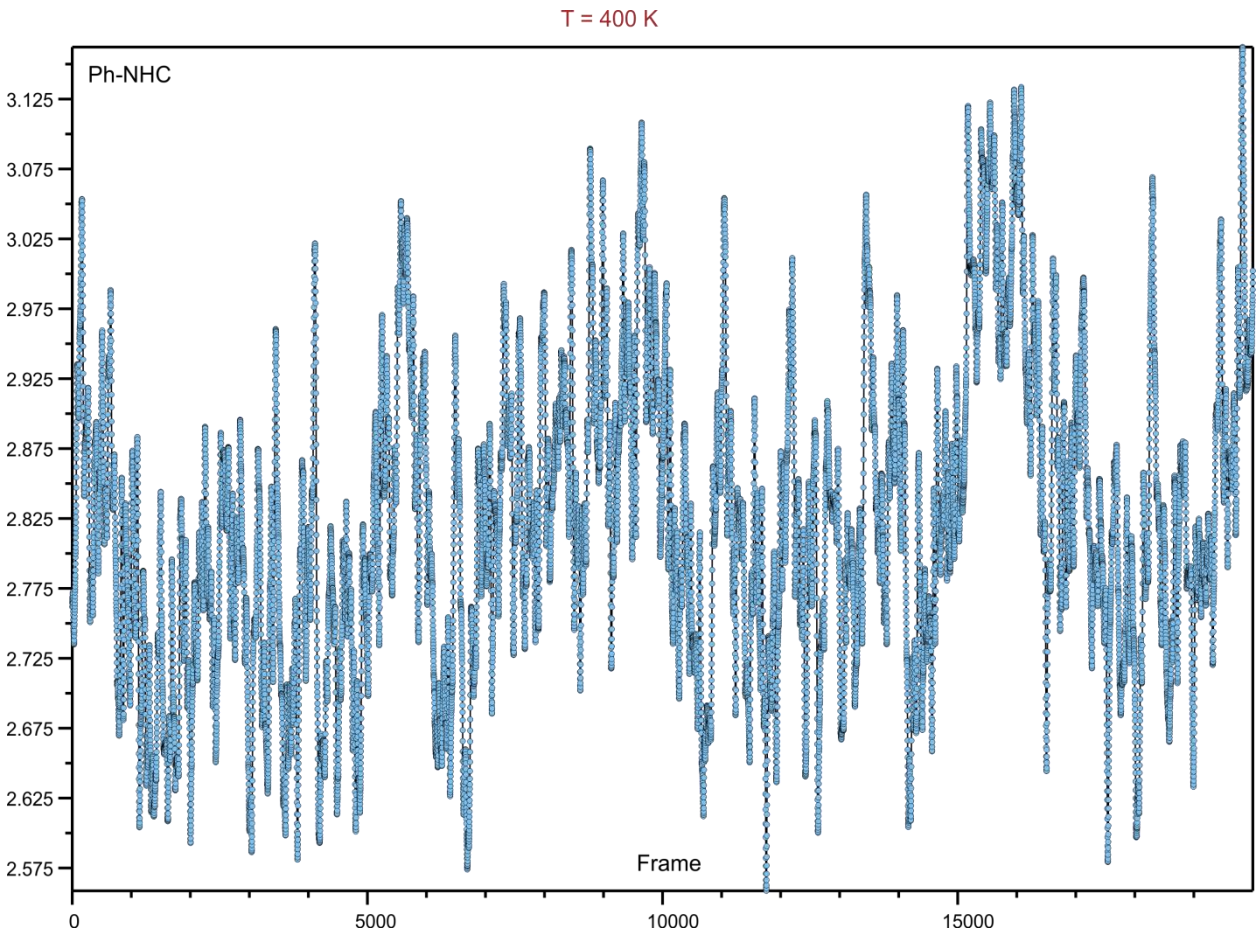

Figure S2. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 400 K.

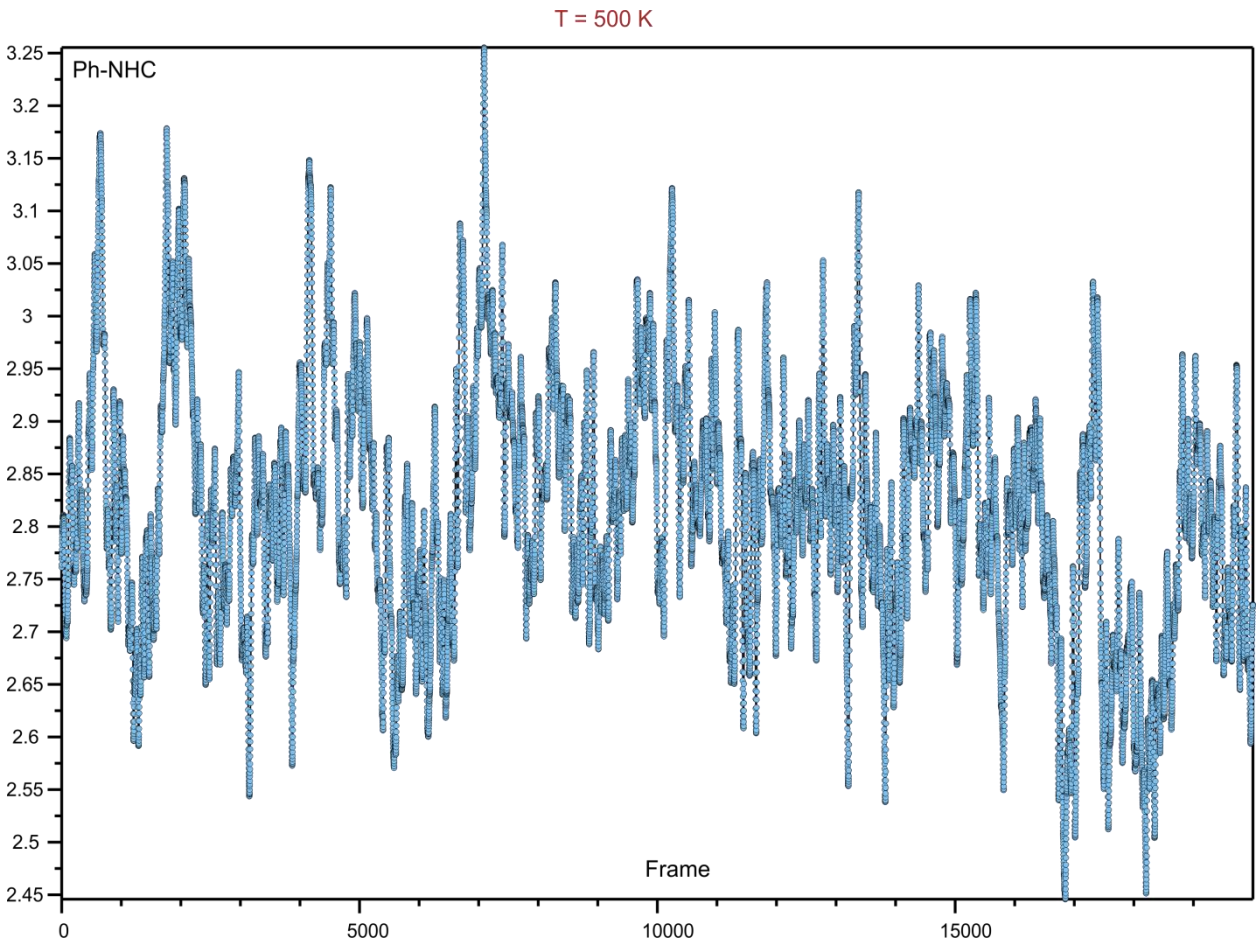

Figure S3. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 500 K.

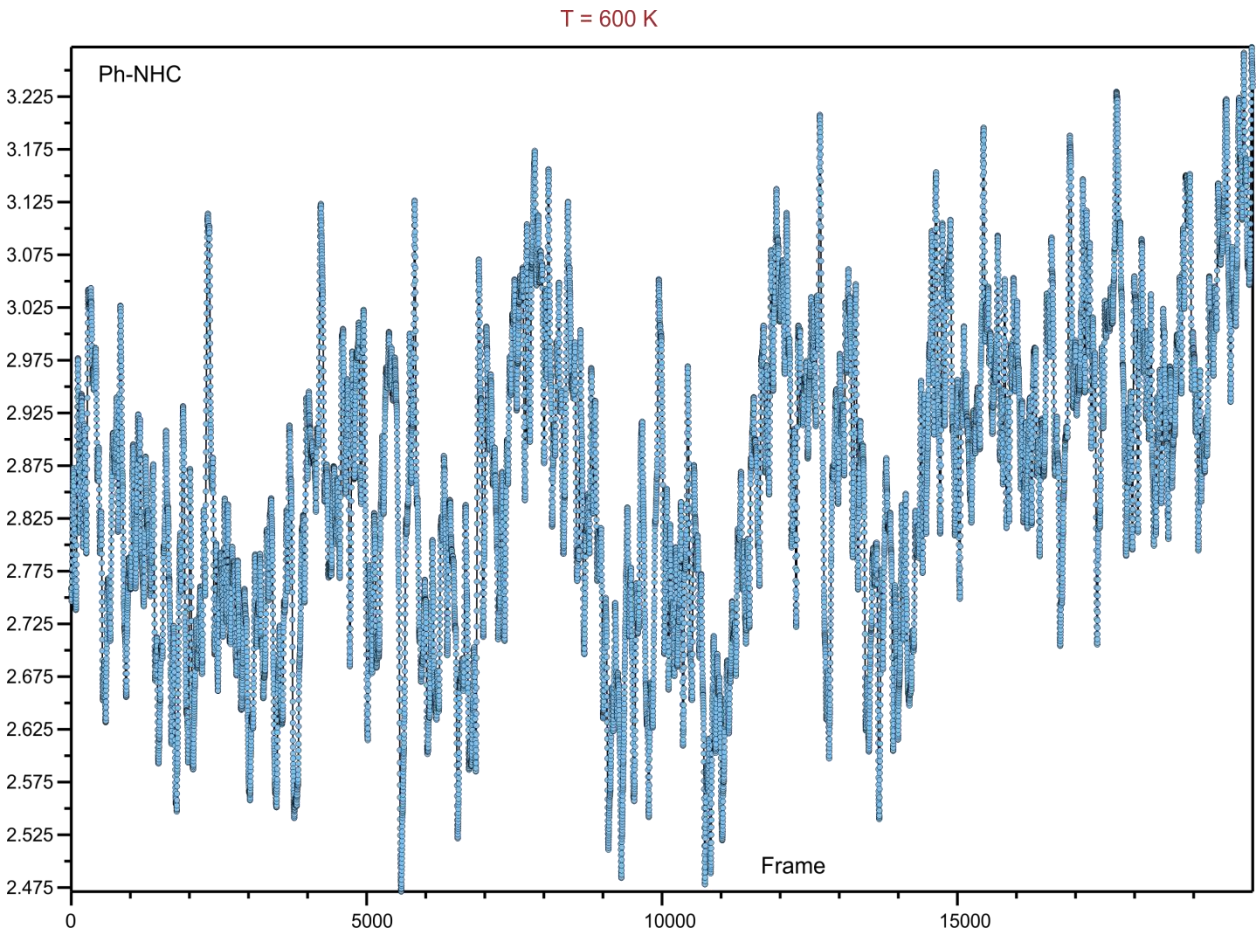

Figure S4. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 600 K.

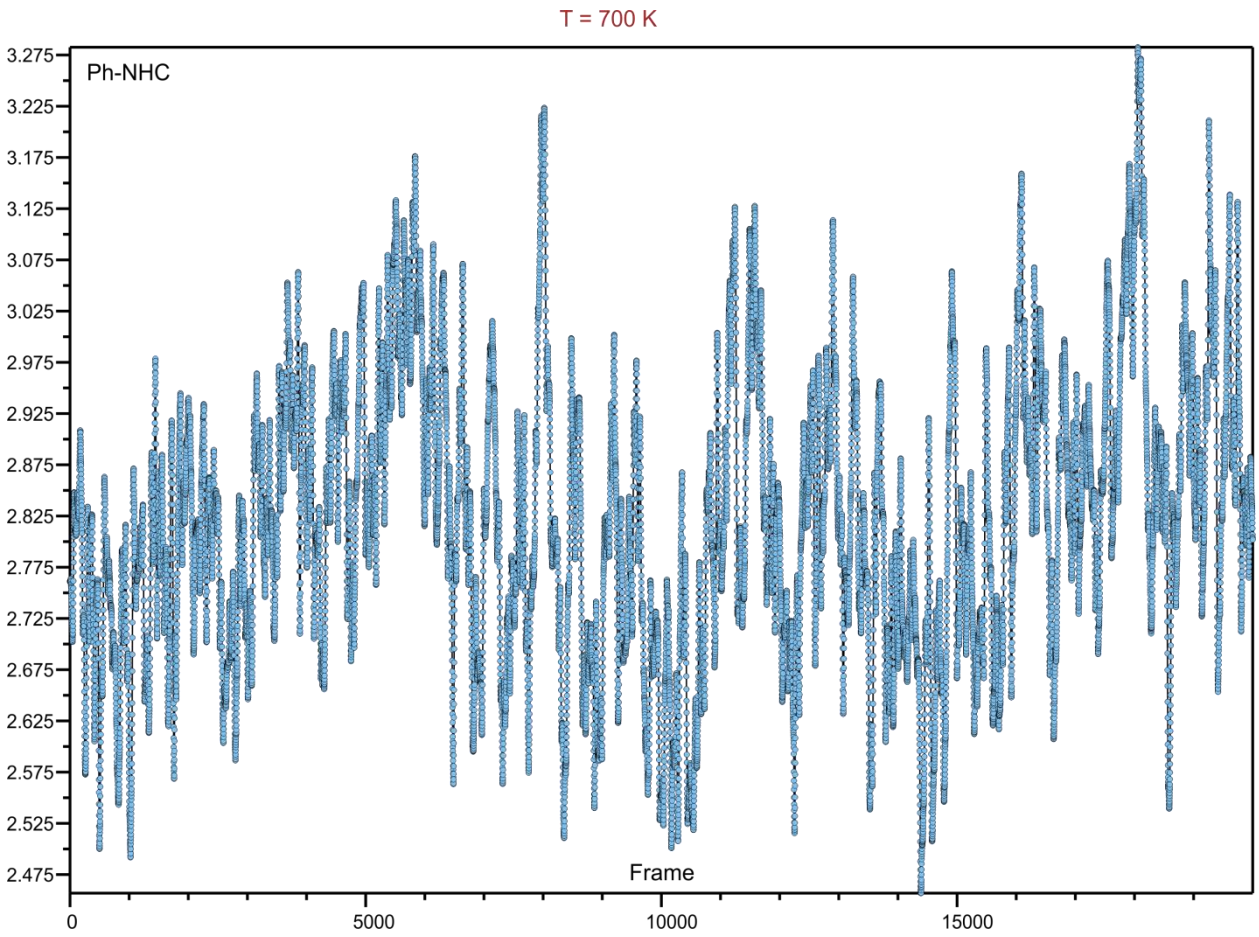

Figure S5. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 700 K.

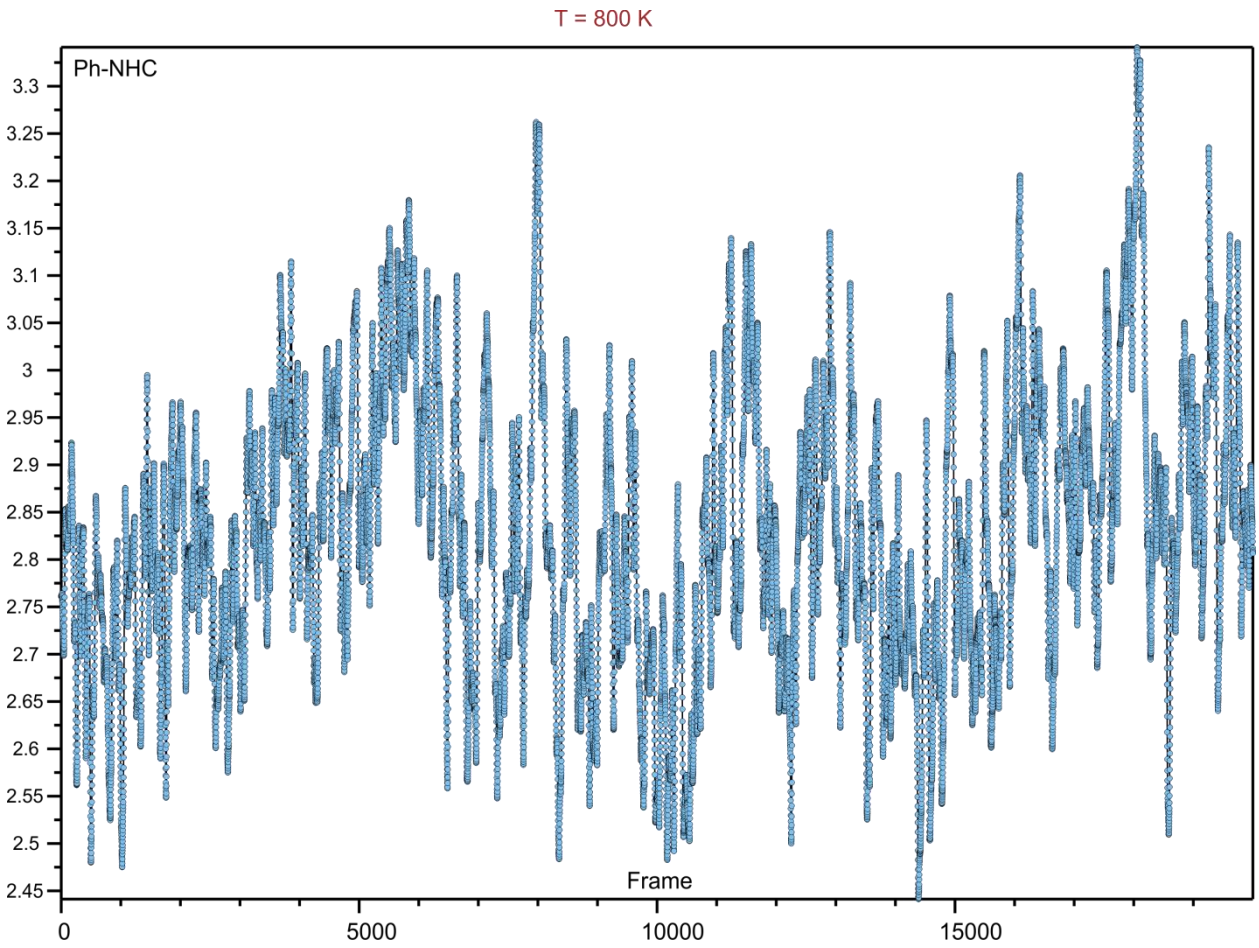

Figure S6. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 800 K.

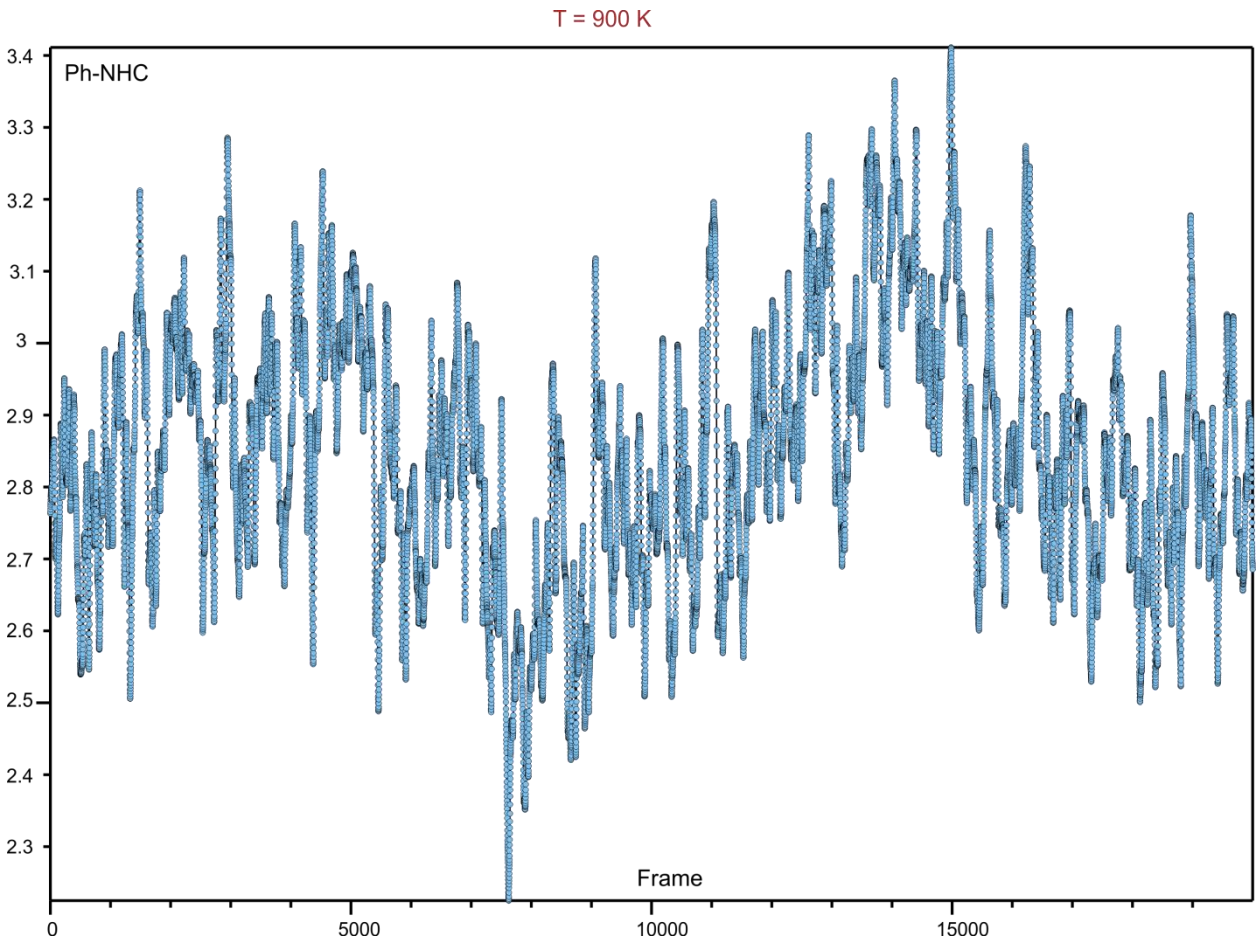

Figure S7. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 900 K.

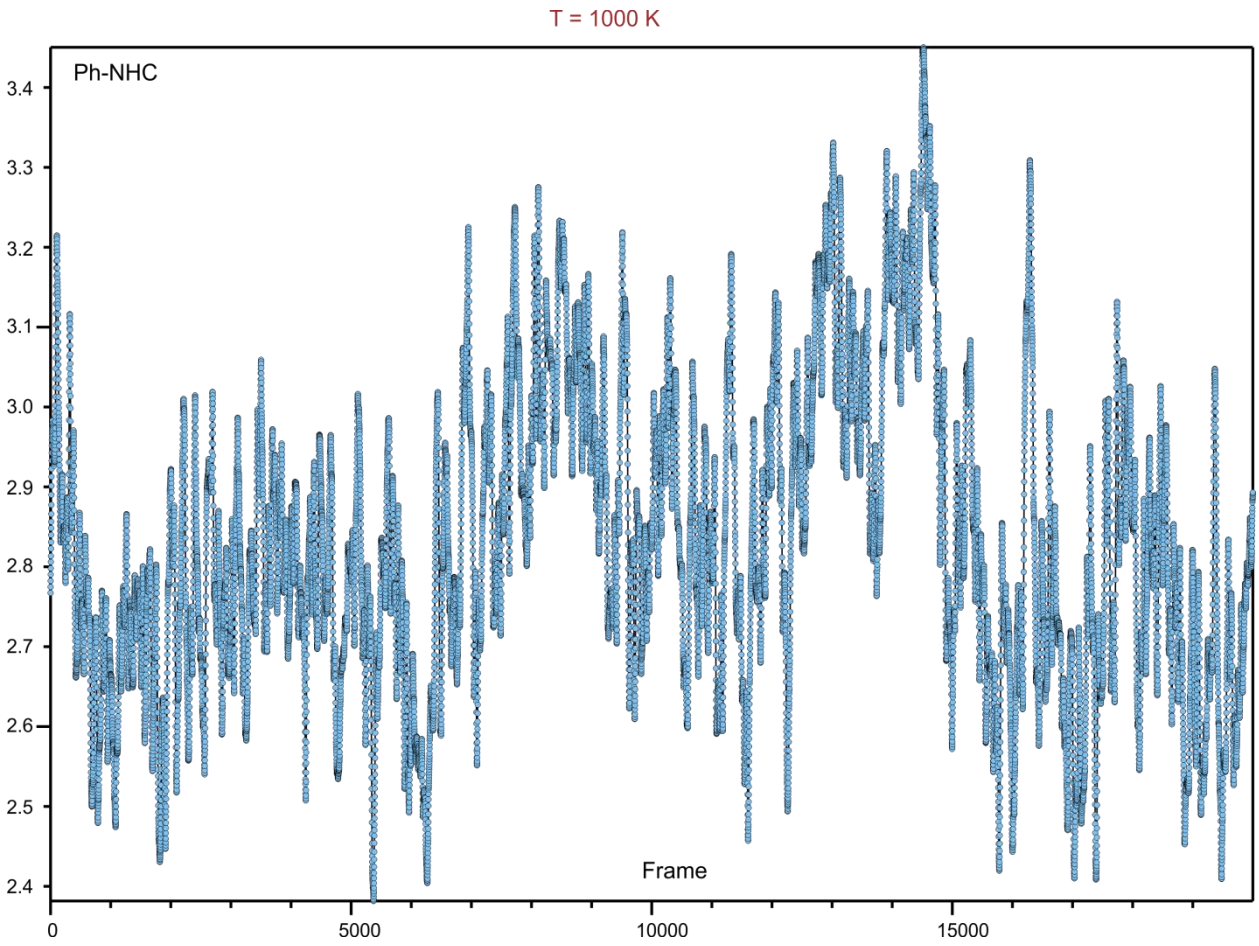

Figure S8. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 1000 K.

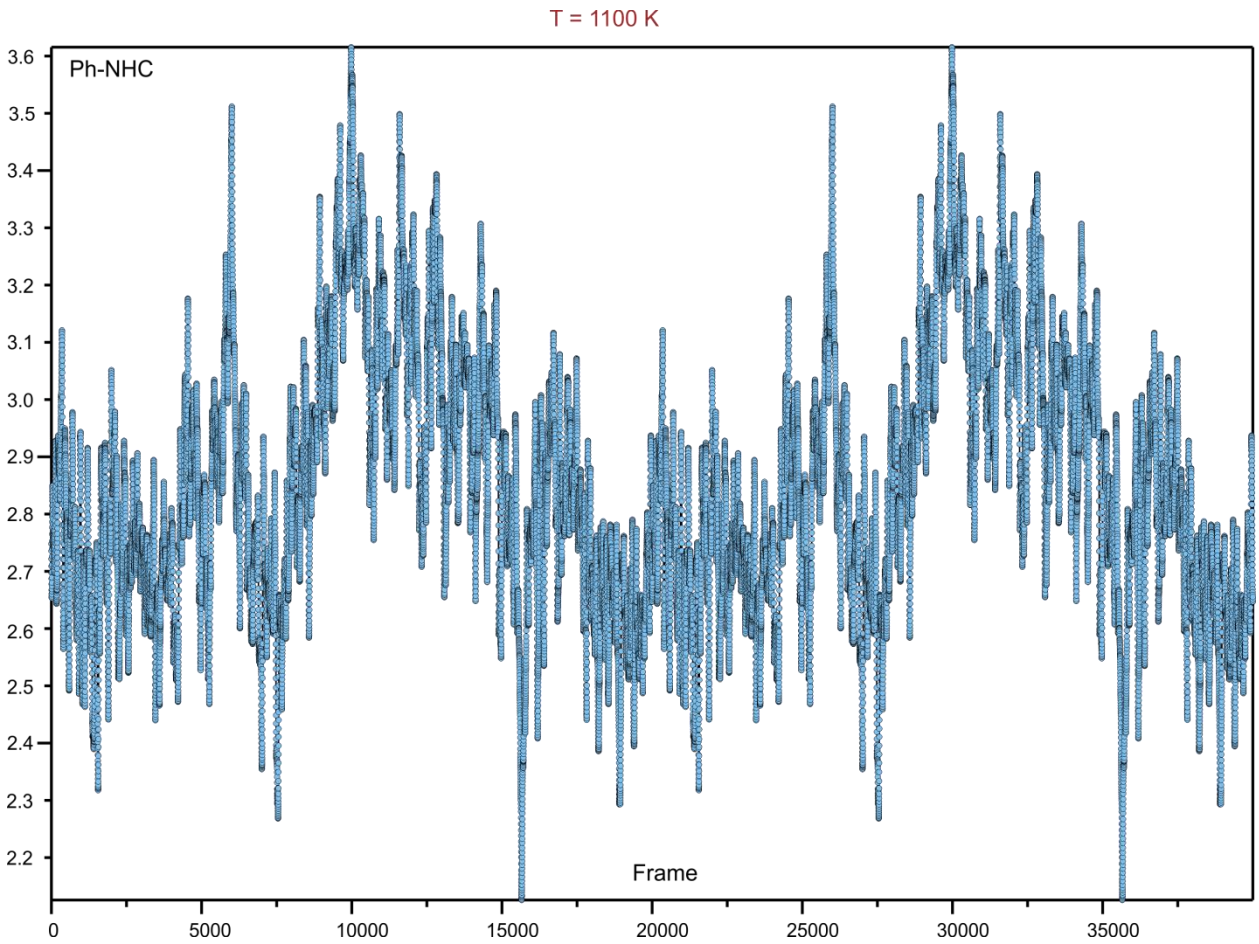

Figure S9. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 1100 K.

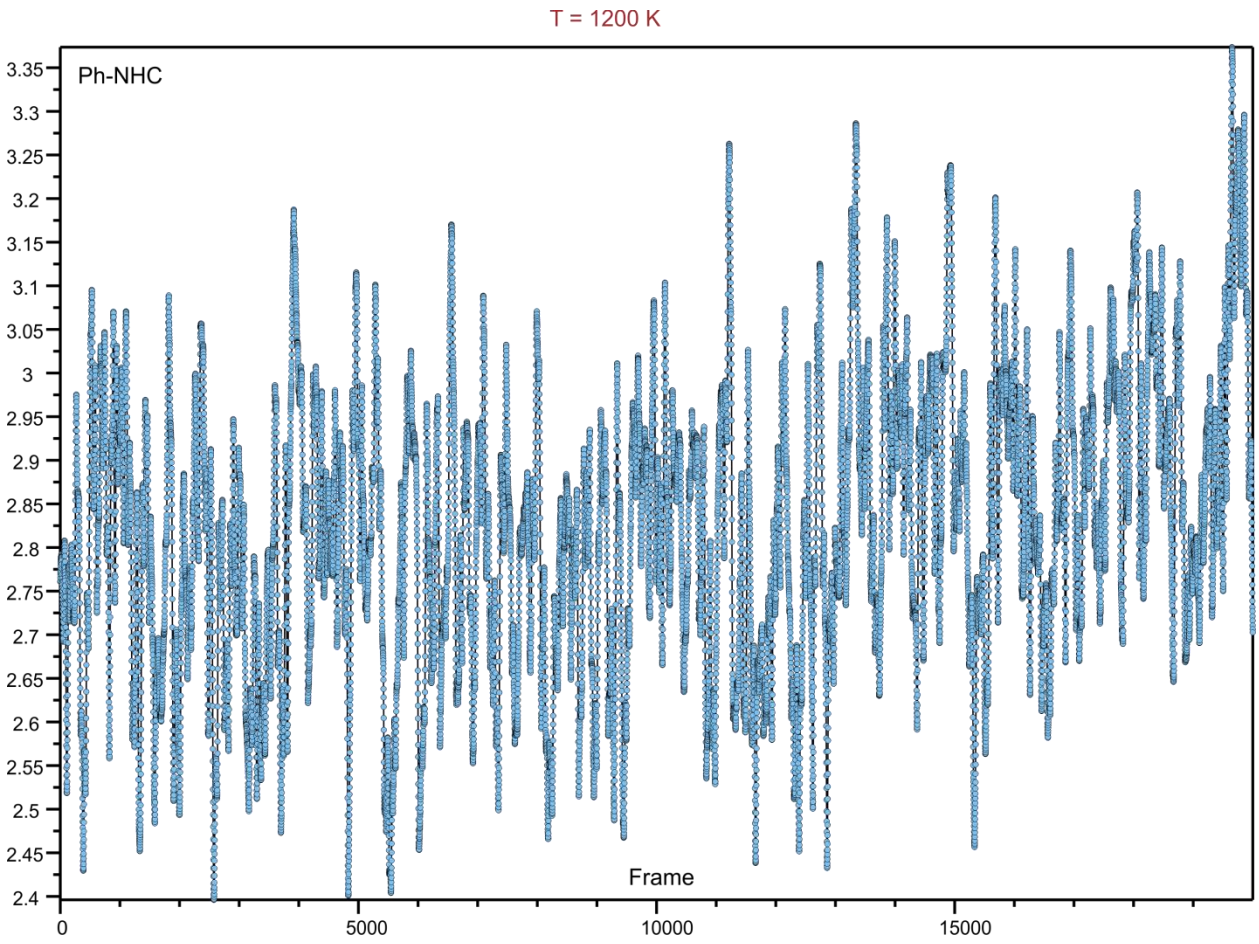

Figure S10. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 1200 K.

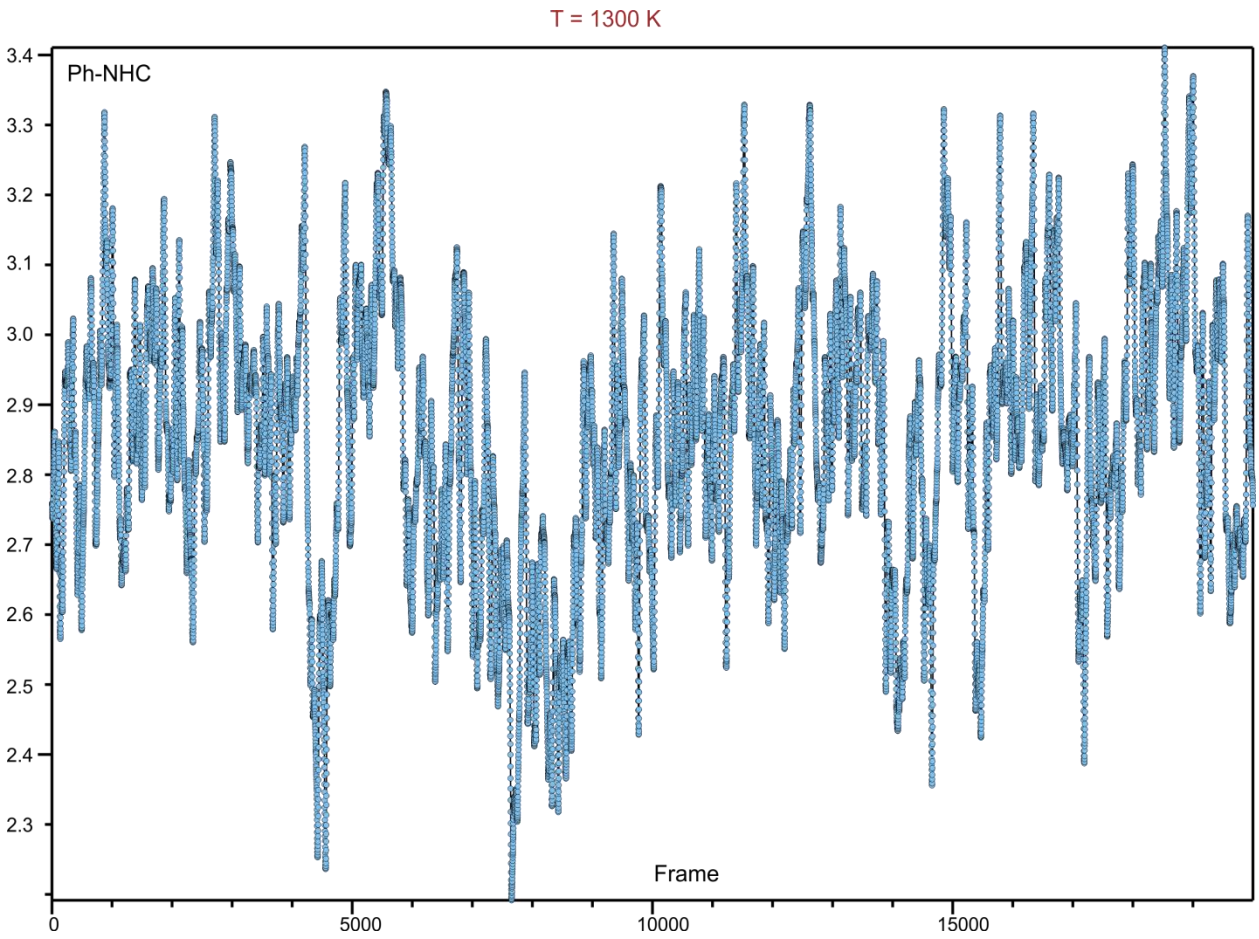

Figure S11. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 1300 K.

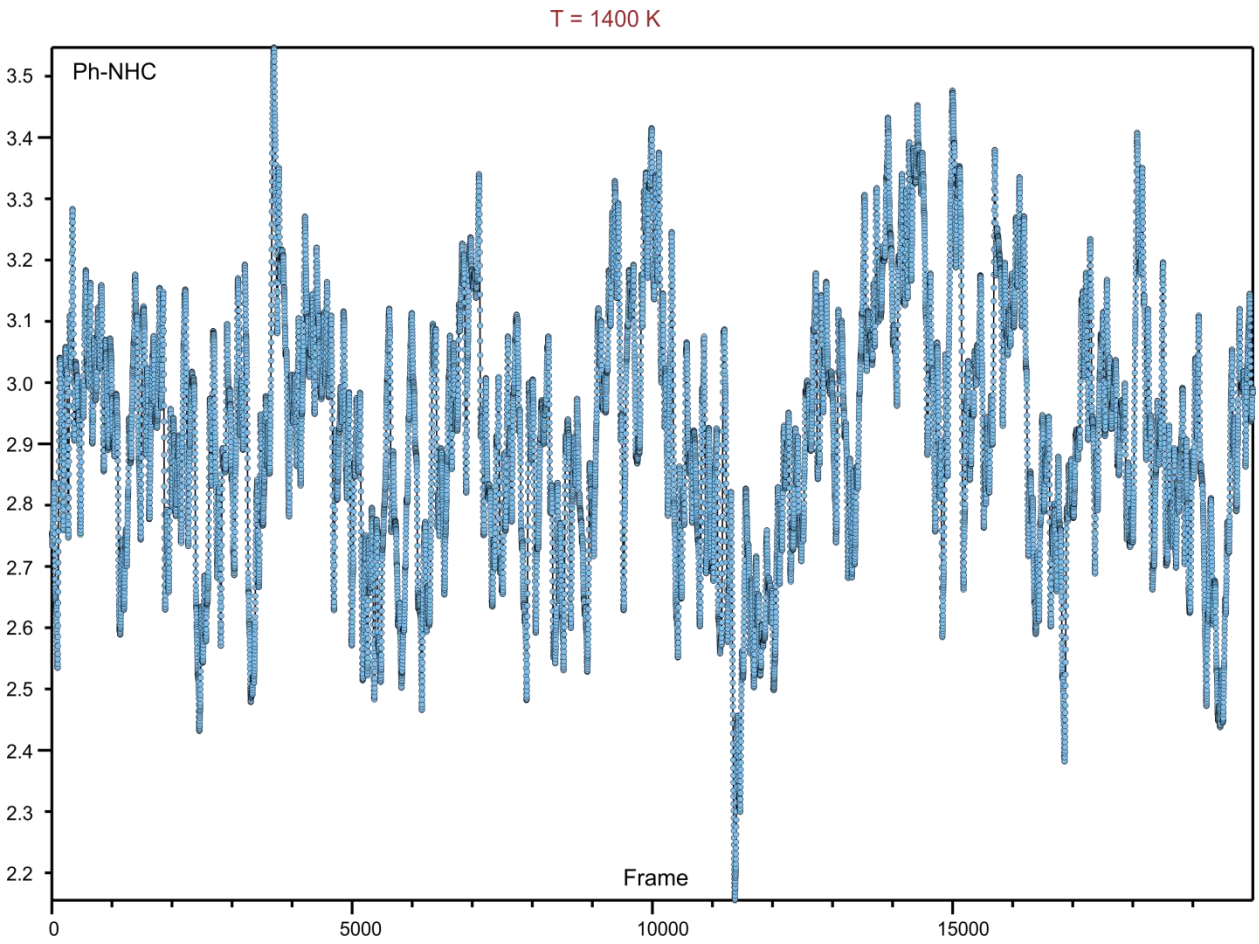

Figure S12. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 1400 K.

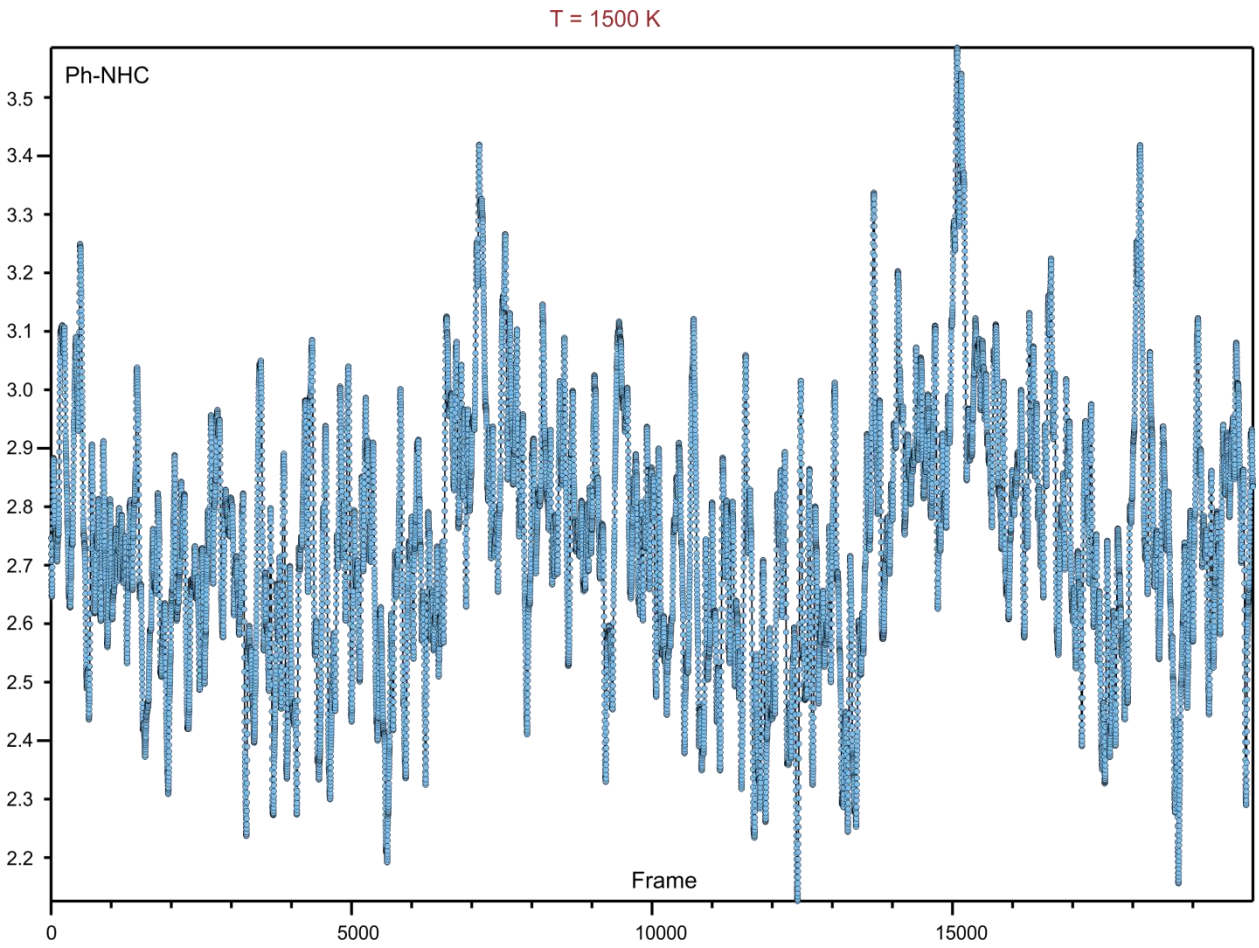

Figure S13. The dependence of the Ph-NHC distance on the time of the MD simulation of complex **1**. Temperature = 1500 K.

Metadynamics simulation in vacuum

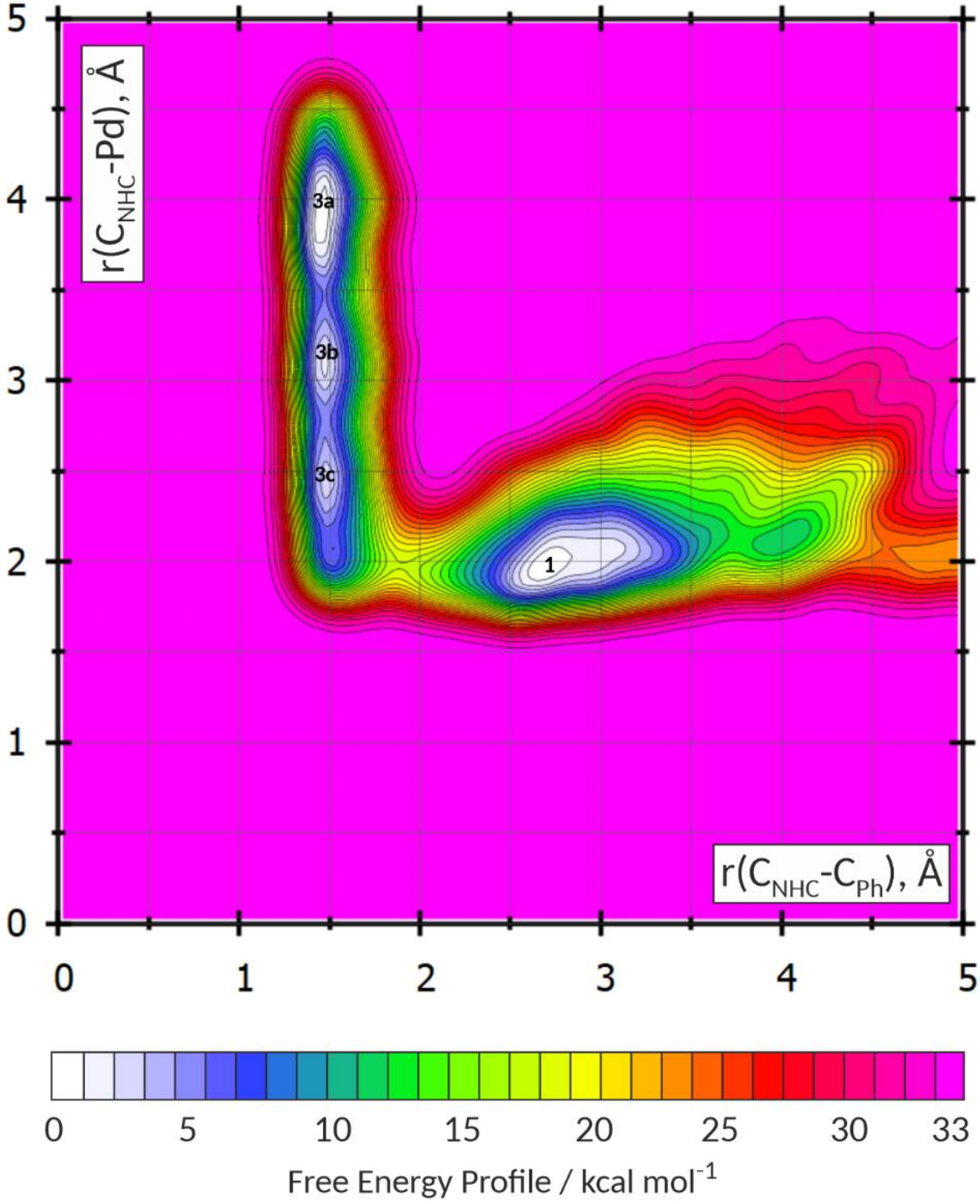

Figure S14. Free energy profile (kcal/mol) of R-NHC coupling reaction, obtained as result of the metadynamics modeling in vacuum using CV1 and CV2 collective variables; RI PBE D3 def2-SVP.

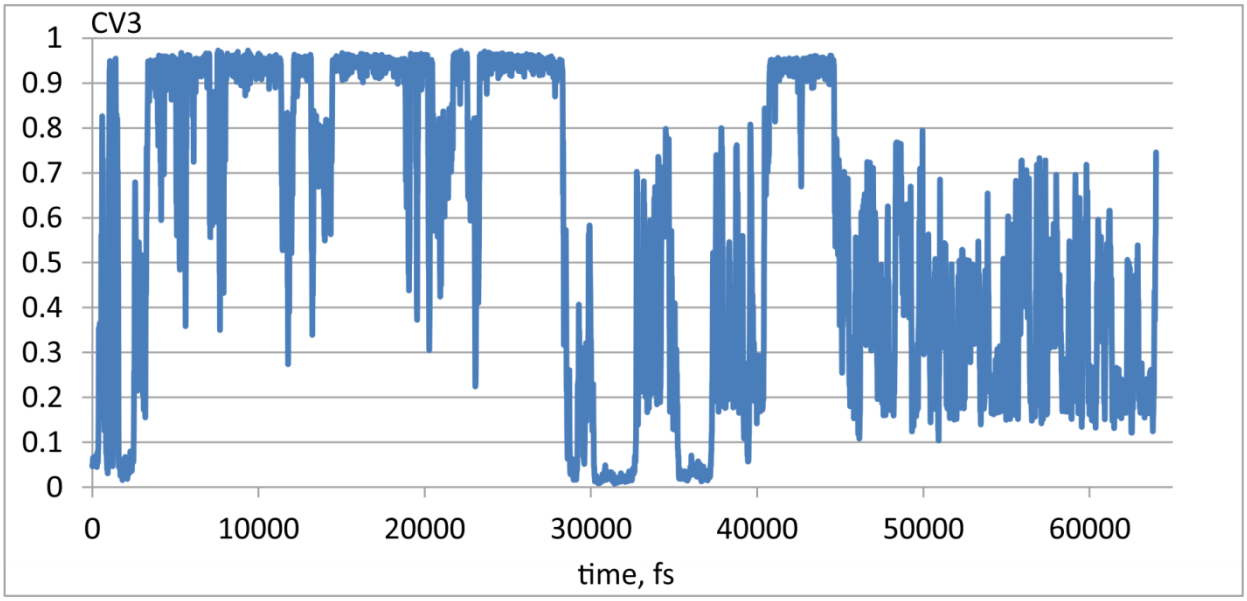

Figure S15. The dependence of the collective variable CV3 on the time of the metadynamic simulation.

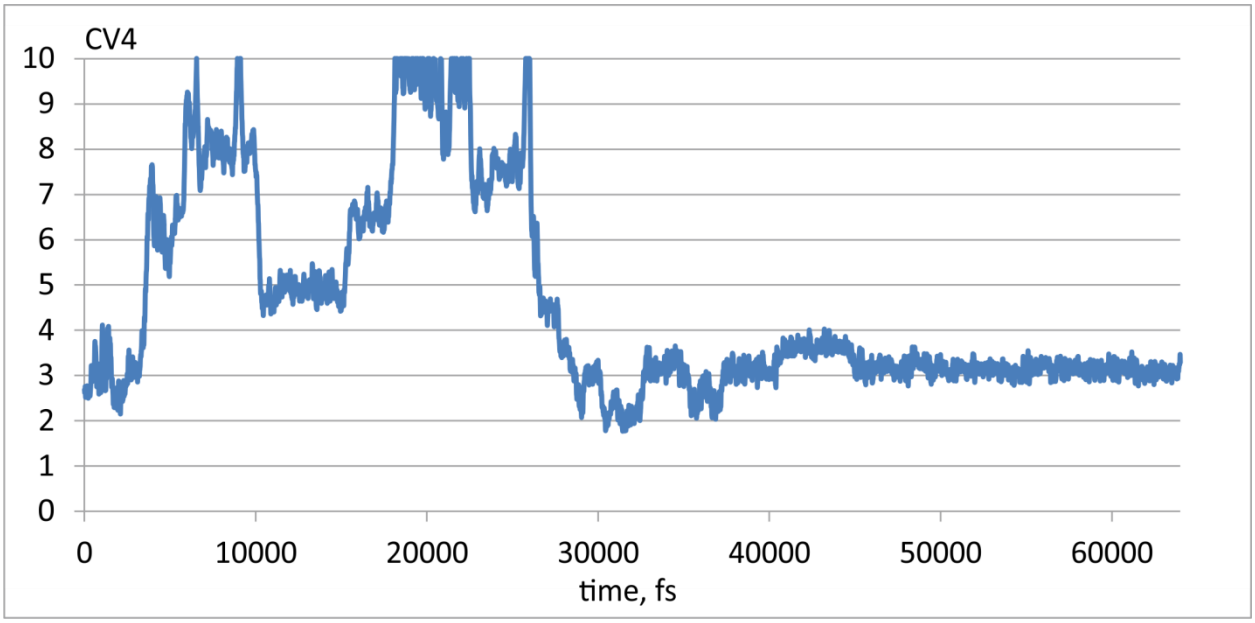

Figure S16. The dependence of the collective variable CV4 on the time of the metadynamic simulation.