

Solvent Effect on Competition Between Weak and Strong Interactions in Phenol Solutions Studied by Near-infrared Spectroscopy

Supplementary Information

Mirosław Antoni Czarnecki,^{1} Yusuke Morisawa,^{2*} Yukiteru Katsumoto,³ Tomoyuki Takaya,⁴
Swapnil Singh,¹ Harumi Sato⁵, and Yukihiro Ozaki^{4,6*}*

¹Faculty of Chemistry, University of Wrocław, F. Joliot-Curie, 14, Wrocław 50-383, Poland.

²Department of Chemistry, School of Science and Engineering, Kindai University, Kowakae,
Higashi-Osaka, Osaka 577-8502, Japan

³Department of Chemistry, School of Science, Fukuoka University, Nanakuma, Jyonan-Ku,
Fukuoka 814-0180, Japan

⁴School of biological and Environmental Sciences, Kwansei Gakuin University, Sanda,
Hyogo 669-1337, Japan

⁵Graduate School of Human Development and Environment, Kobe University, 3-11,
Tsurukabuto, Nada-ku, Kobe 657-8501, Japan

⁶Toyota Physical and Chemical Research Institute, Yokomichi, Nagakute, Aichi 480-1192,
Japan

Corresponding authors:

Yukihiro Ozaki (yukiz89016@gmail.com)

Mirosław A. Czarnecki (mirosław.czarnecki@chem.uni.wroc.pl)

Yusuke Morisawa (morisawa@chem.kindai.ac.jp)

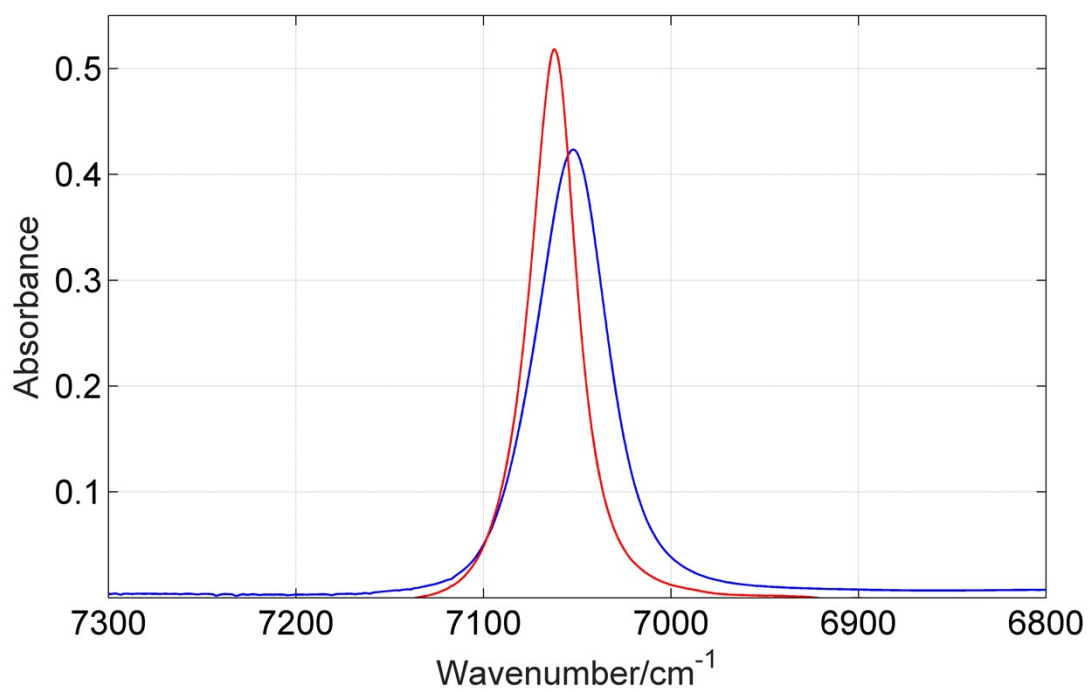


Figure SI1. NIR spectra of phenol in CCl₄ (blue line) and cyclohexane (red line) solutions at 0.05M.

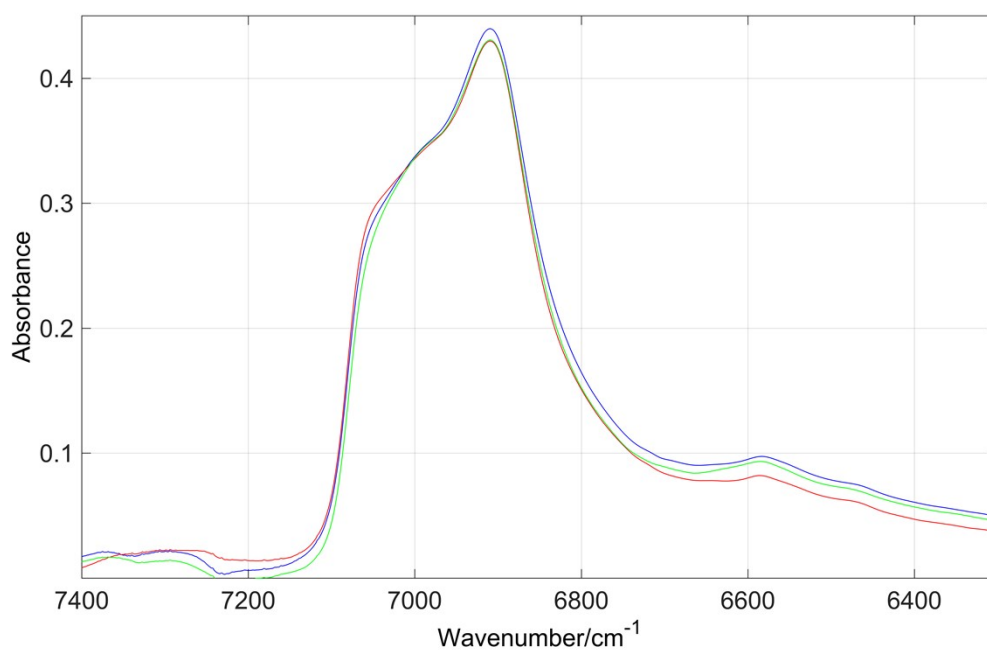


Figure SI2. NIR spectra of phenol in *o*-xylene (green), *m*-xylene (blue) and *p*-xylene (red) at the concentration of 1 M after subtraction of the spectrum of the solvent.

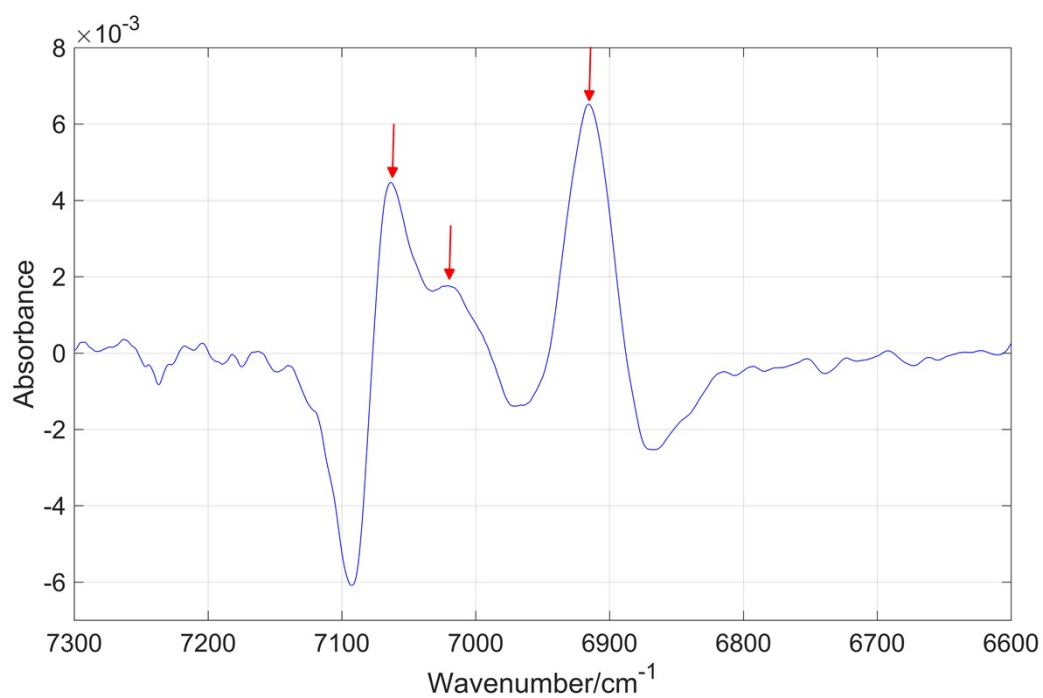


Fig. SI3. Second derivative NIR spectrum (multiplied by -1) of phenol in toluene at concentration of 0.5 M. The red arrows indicate peak positions.

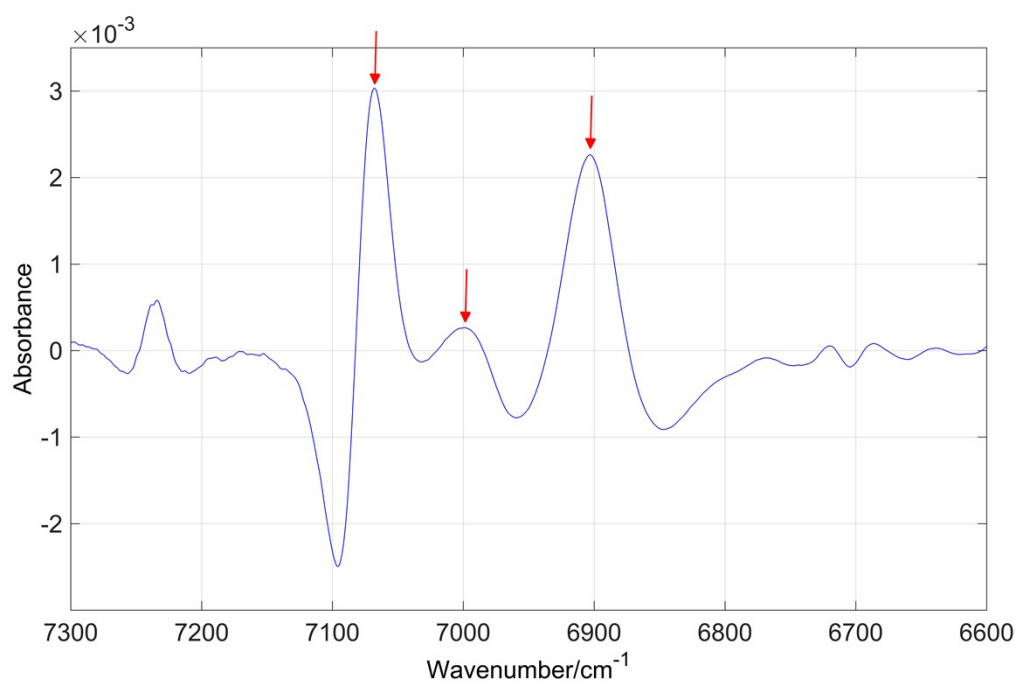


Fig. SI4. Second derivative NIR spectrum (multiplied by -1) of phenol in o-xylene at concentration of 1 M after subtraction of the spectrum of the solvent. The red arrows indicate peak positions.

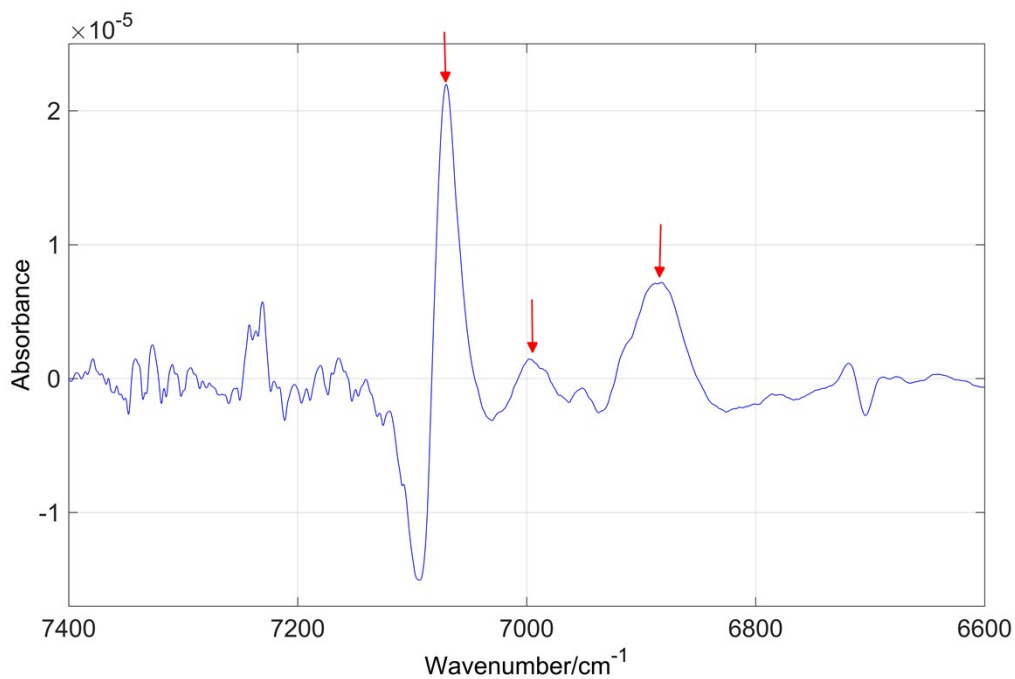


Fig. SI5. Second derivative NIR spectrum (multiplied by -1) of phenol in mesitylene at concentration of 1 M after subtraction of the spectrum of the solvent. The red arrows indicate peak positions.

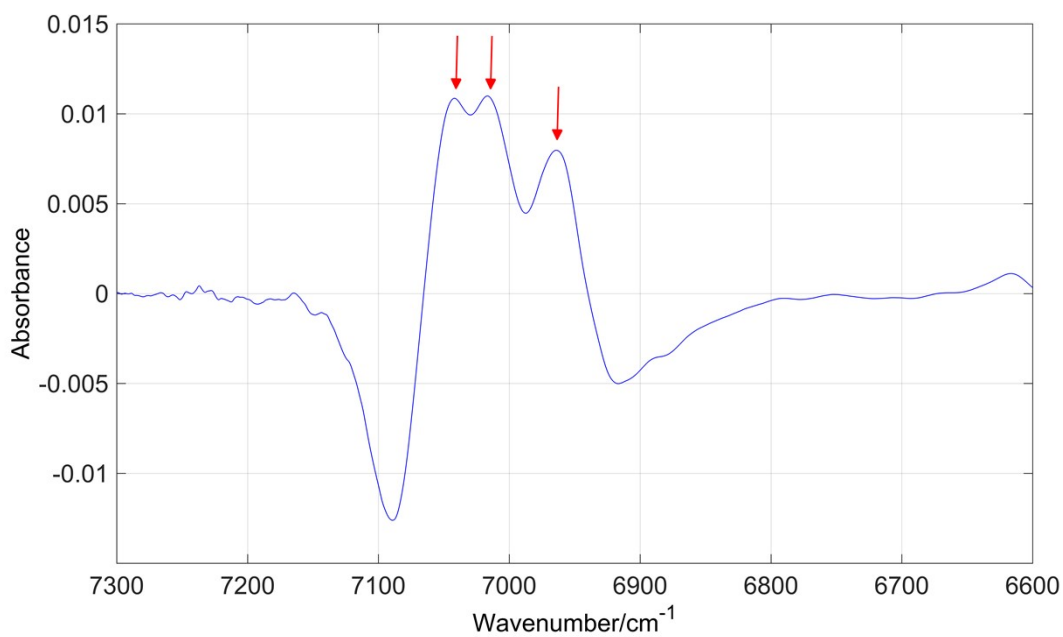


Fig. SI6. Second derivative NIR spectrum (multiplied by -1) of phenol in chlorobenzene at concentration of 0.5 M. The red arrows indicate peak positions.

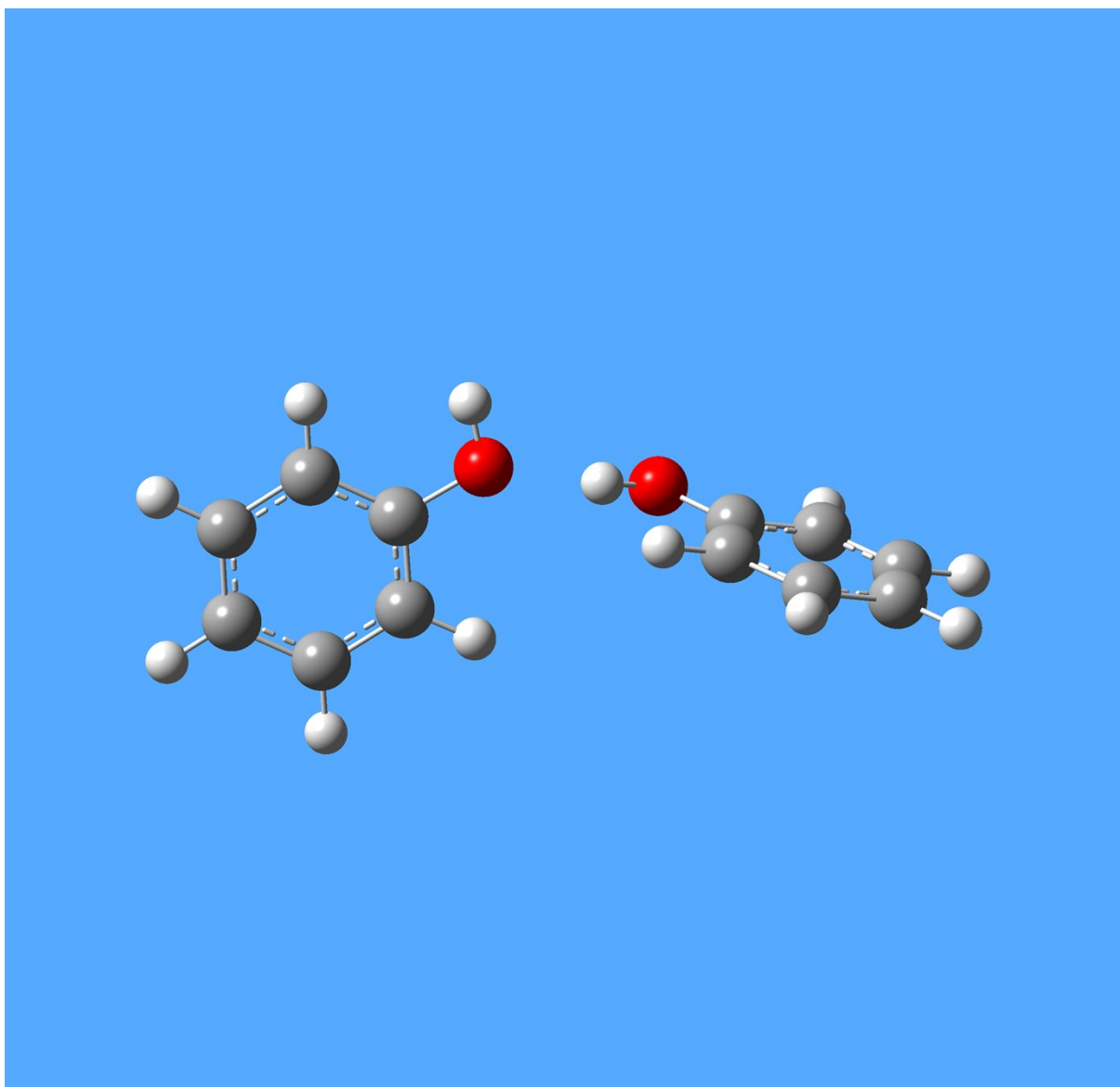


Figure S7. Optimized (B3LYP/6-311++G(2df,2pd)) structure of dimer of phenol.

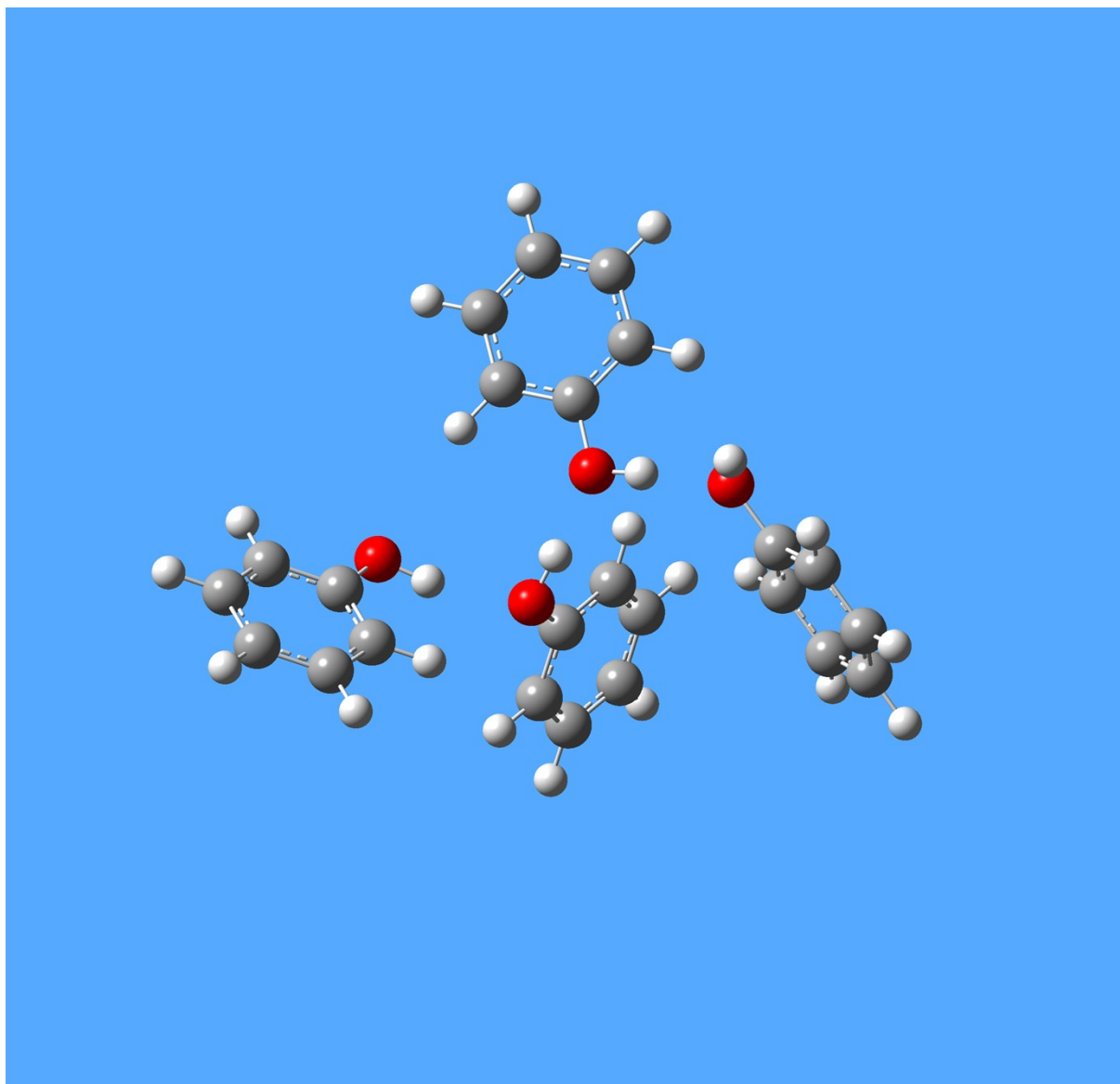


Figure S8. Optimized (B3LYP/6-311++G(2df,2pd)) structure of linear tetramer of phenol.

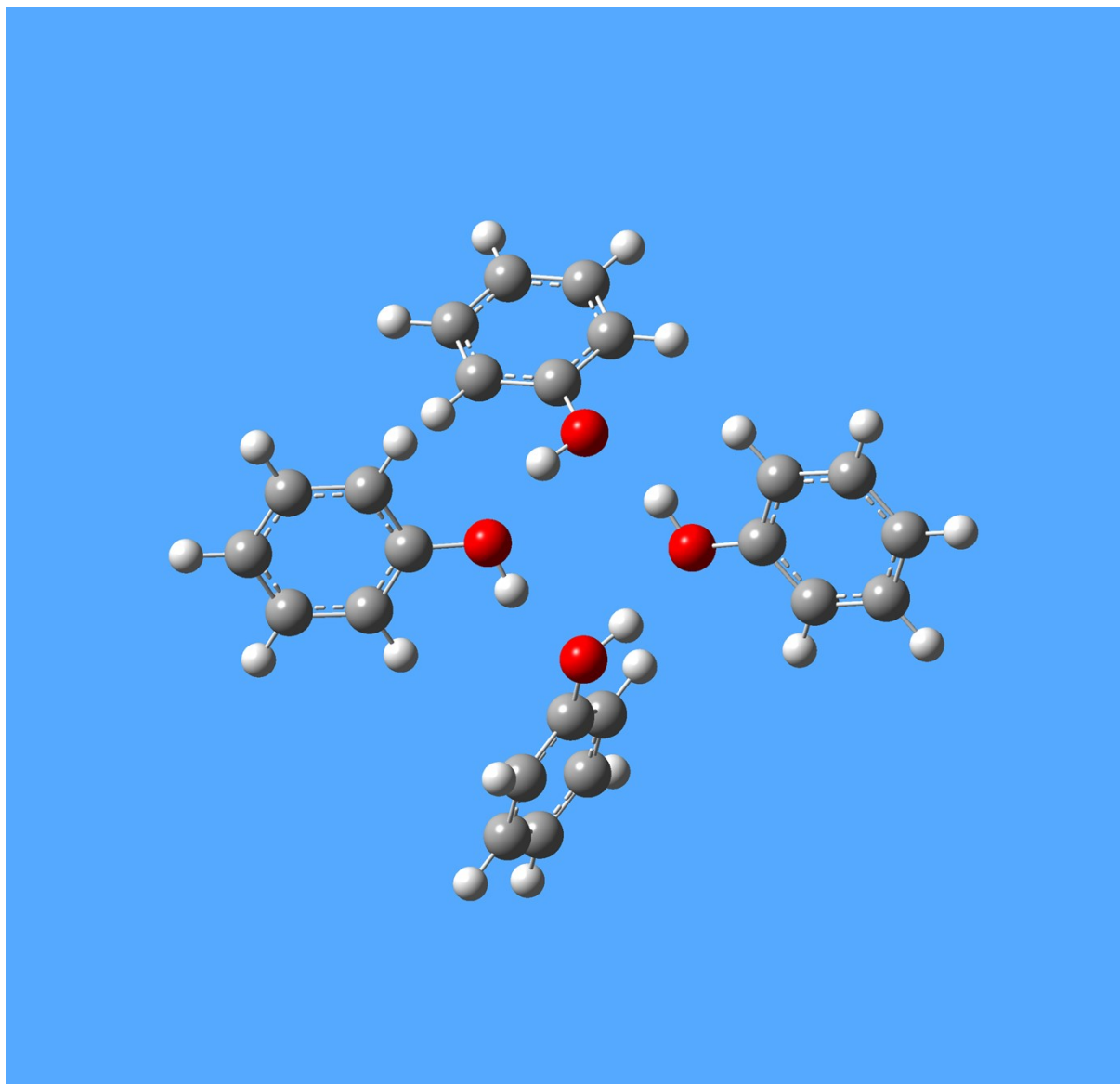


Figure S9. Optimized (B3LYP/6-311++G(2df,2pd)) structure of cyclic tetramer of phenol.

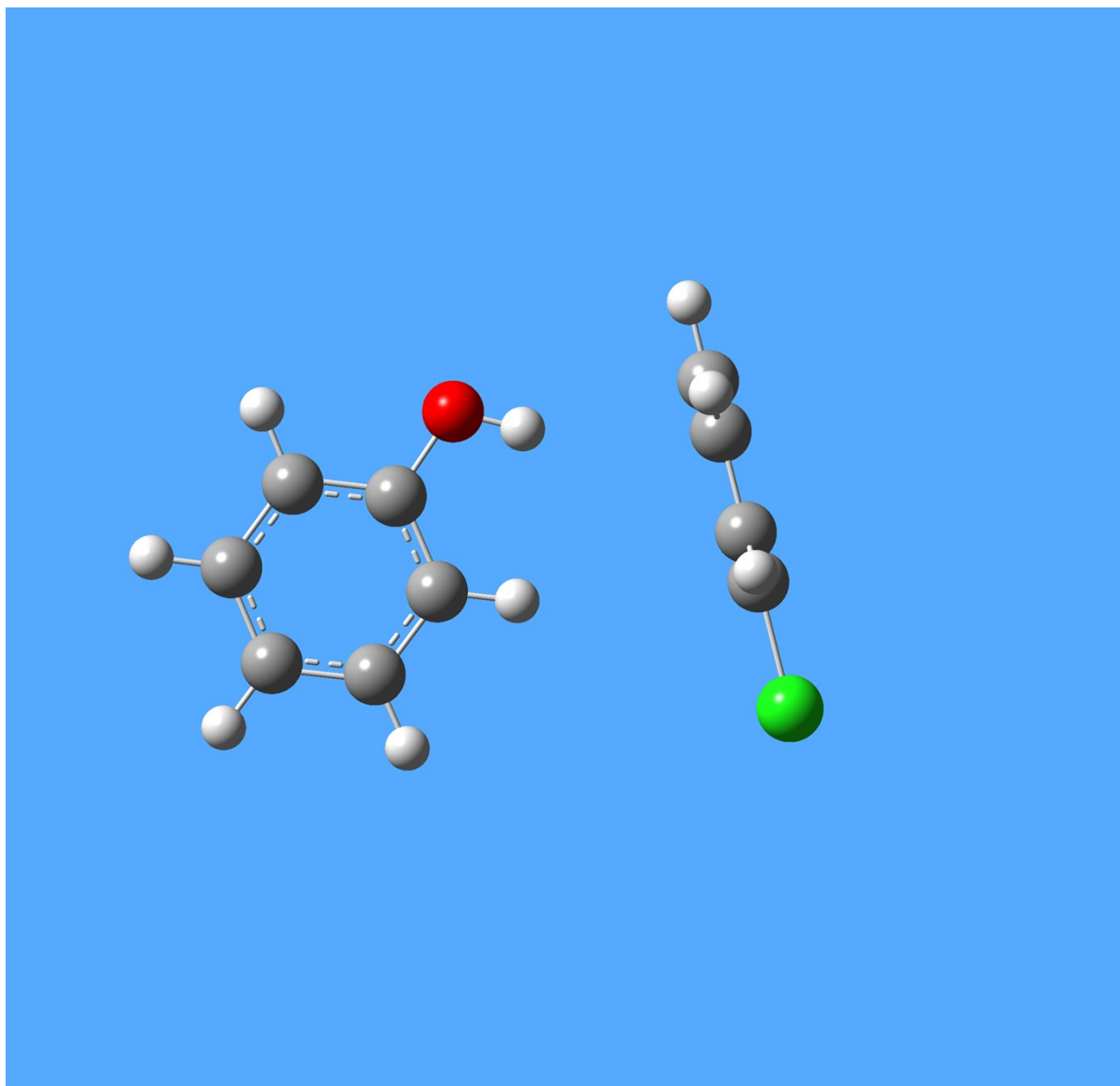


Figure S10. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-chlorobenzene complex.

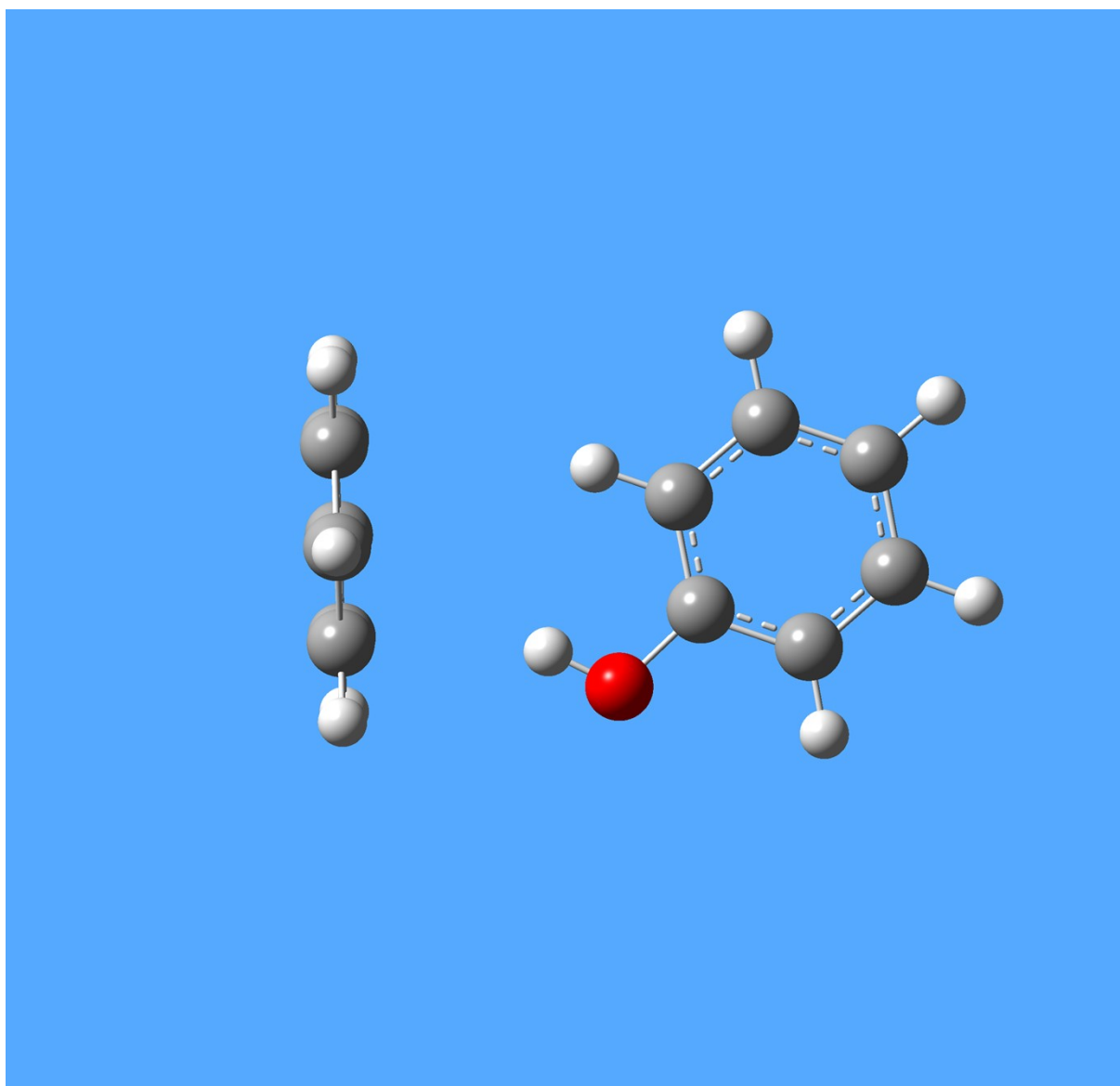


Figure S11. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-benzene complex.

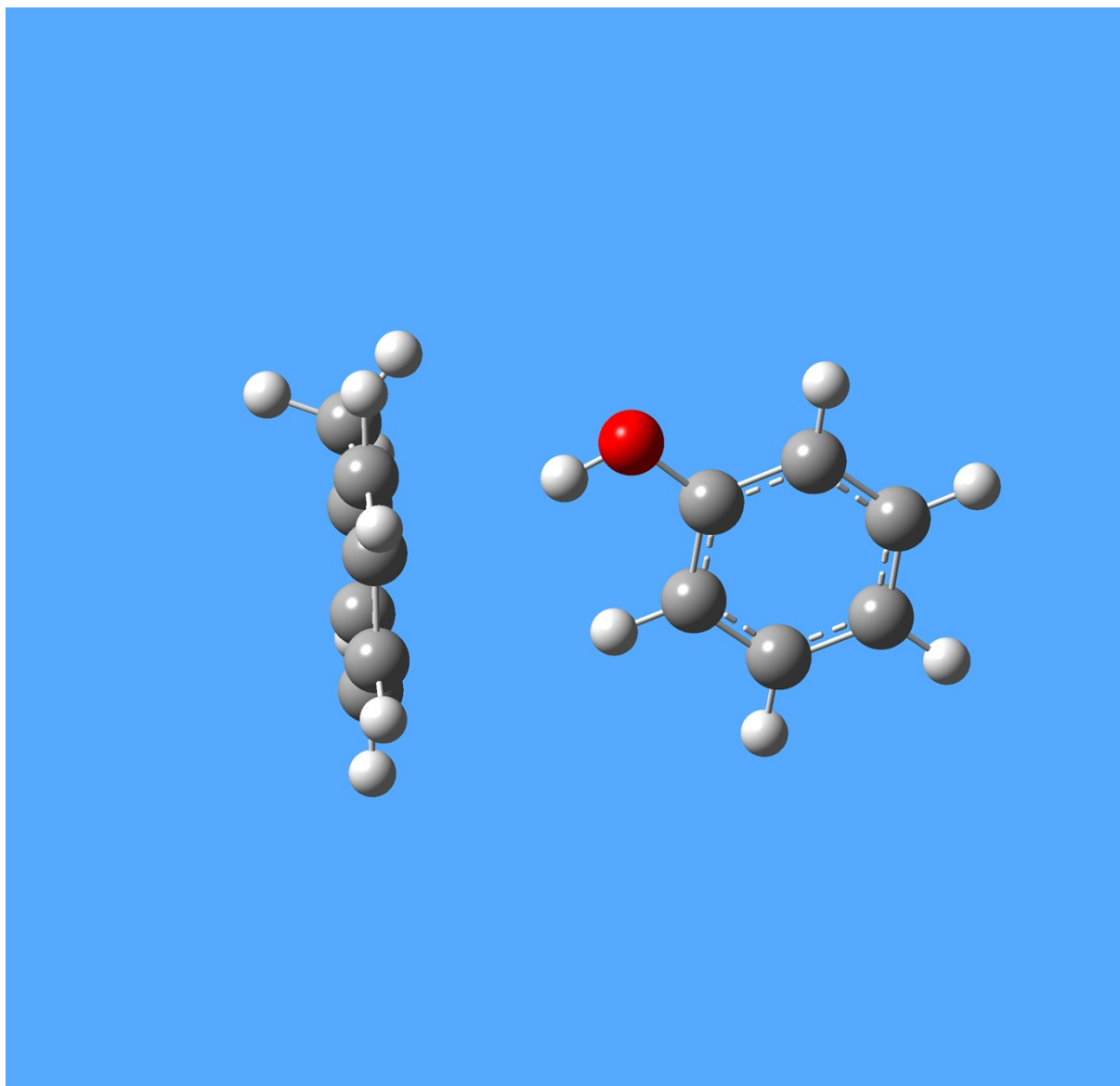


Figure S12. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-toluene complex.

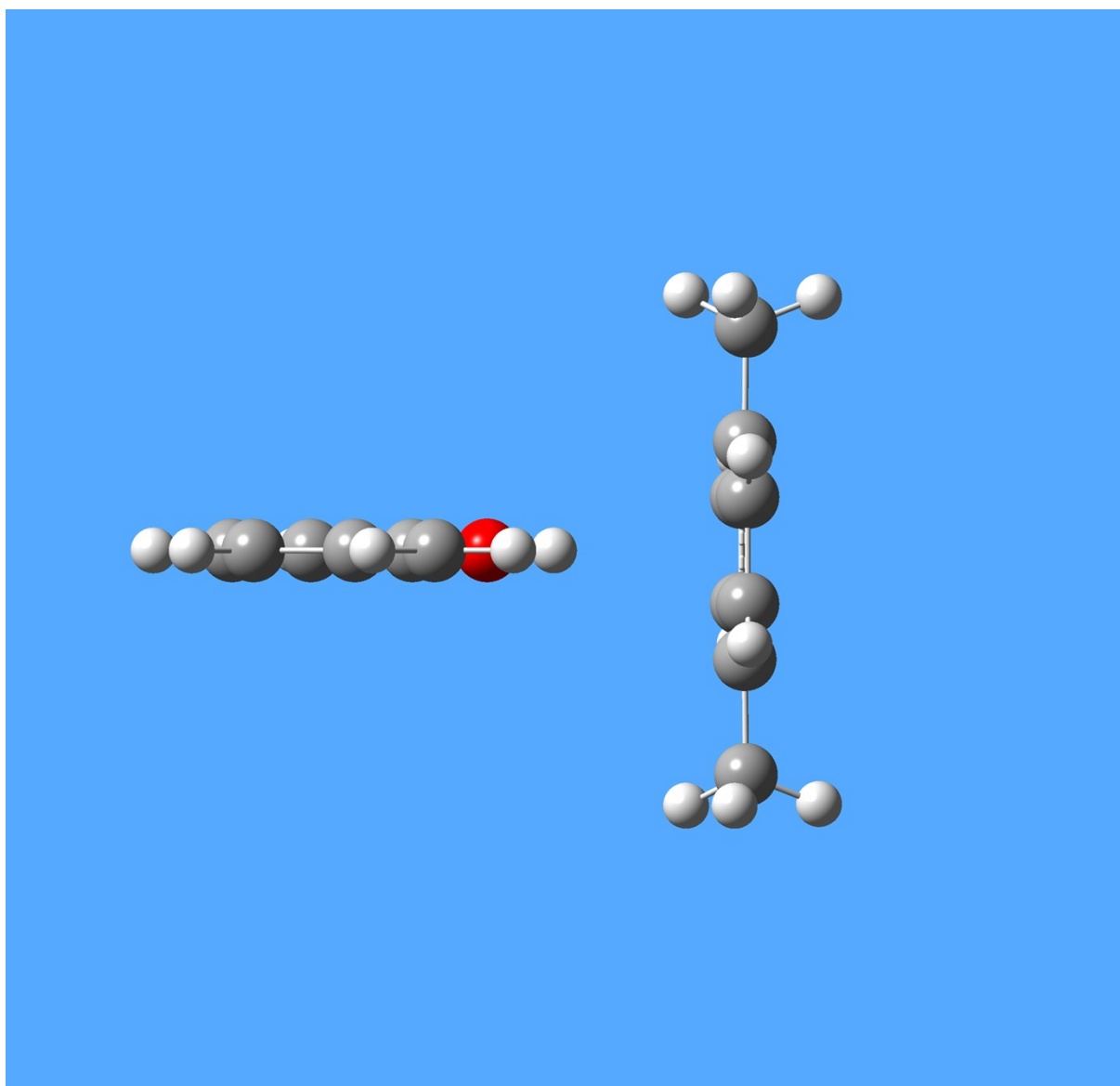


Figure S13. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-p-xylene complex.

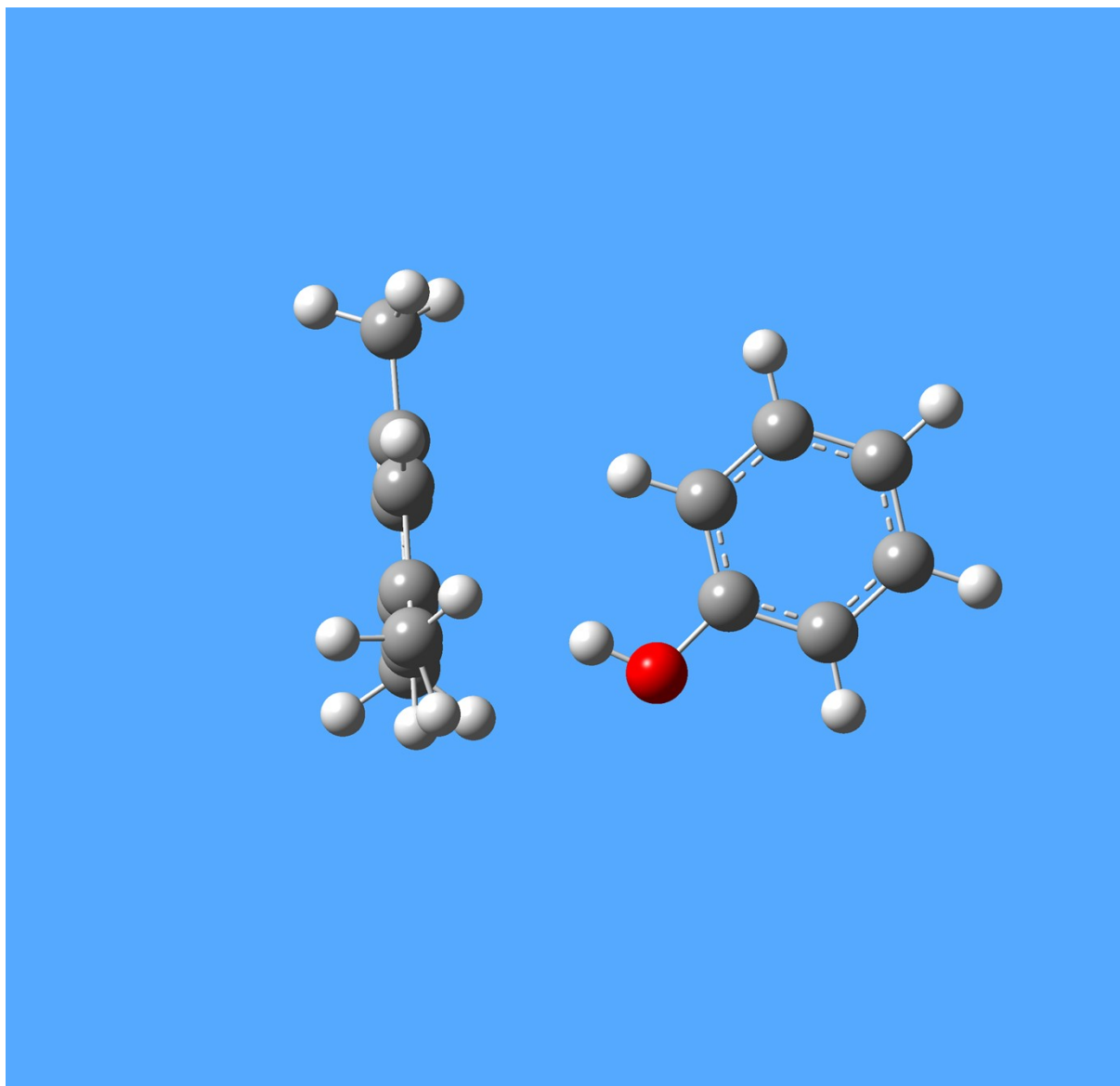


Figure S14. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-mesitylene complex.

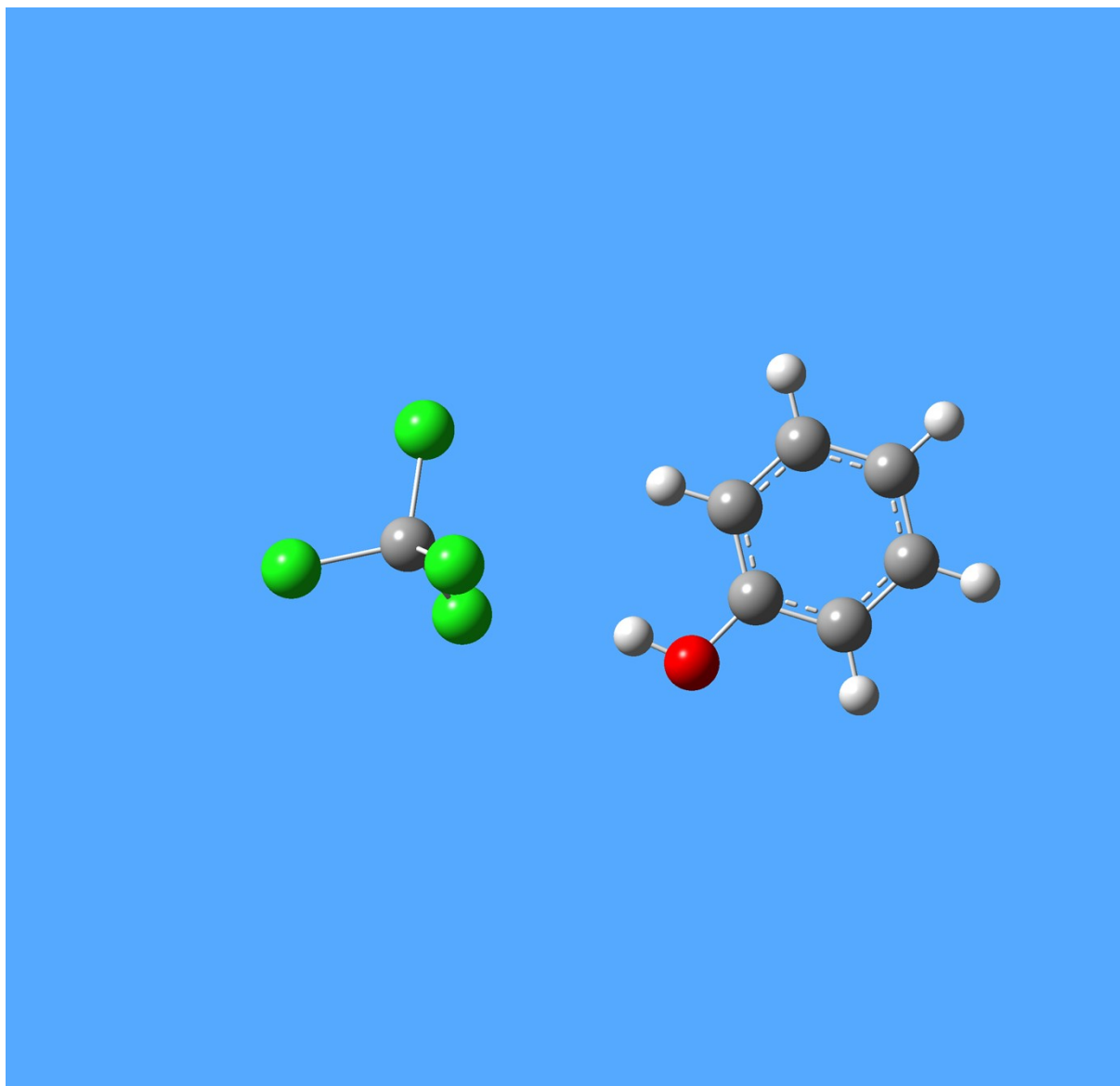


Figure S15. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-CCl₄ complex.

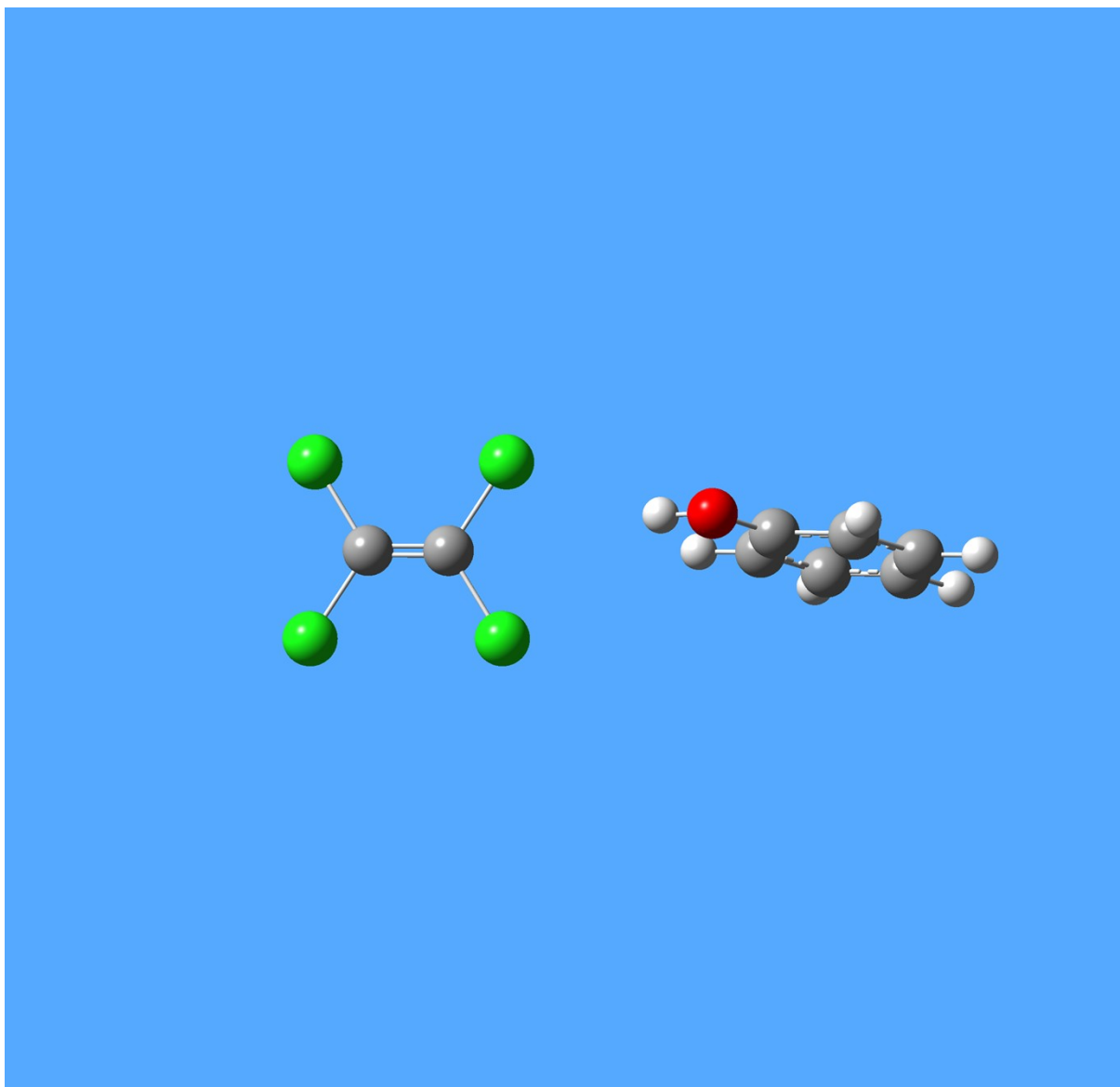


Figure S16. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-tetrachloroethylene complex.

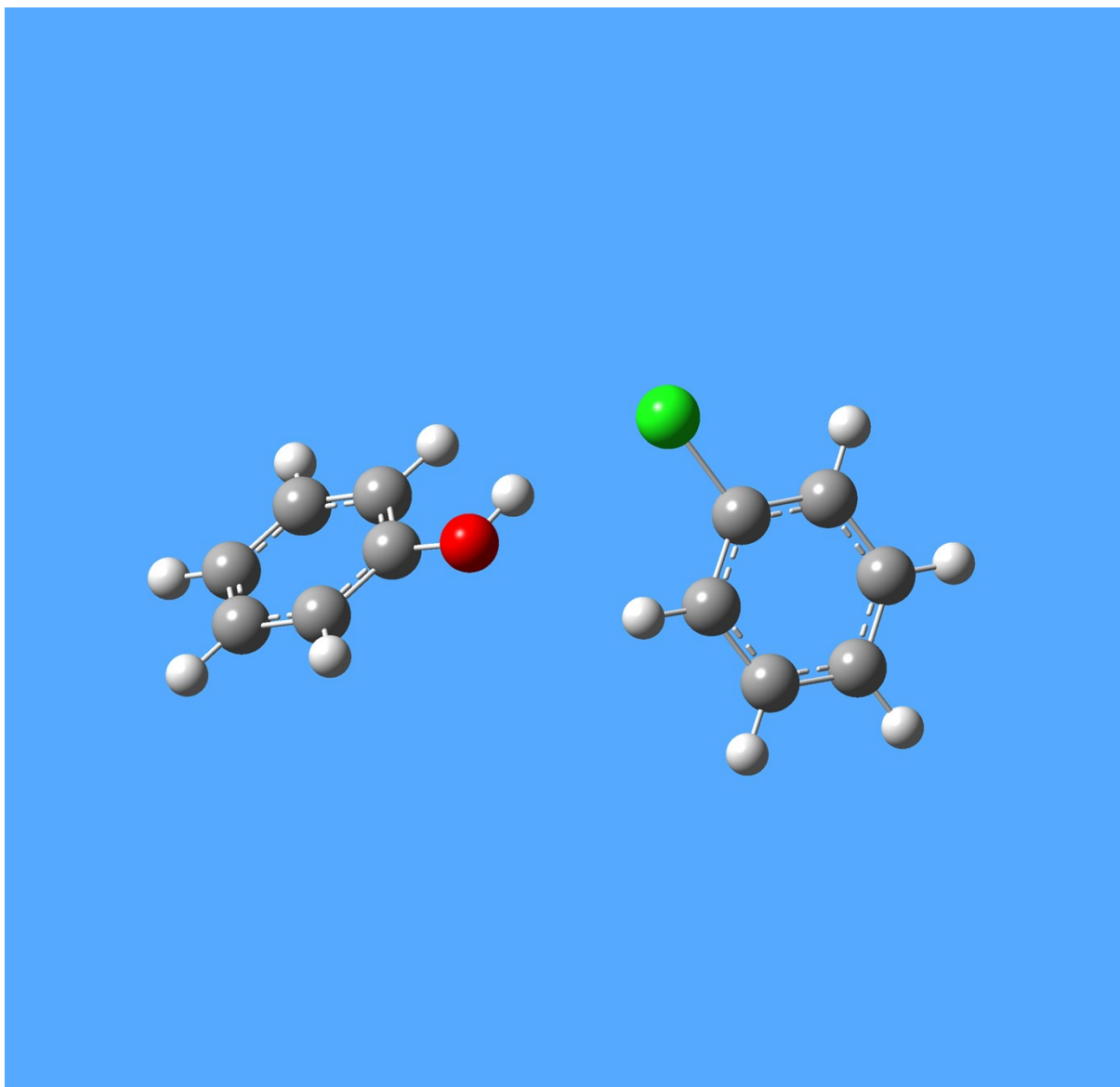


Figure S17. Optimized (B3LYP/6-311++G(2df,2pd)) structure of phenol-chlorobenzene complex.