

Controlled tautomerism – a switching caused by an “underground” anionic effect

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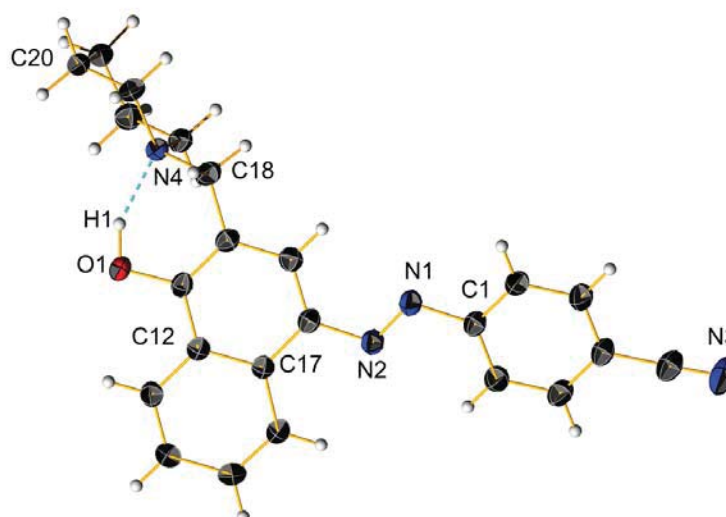


Figure S1. View of the molecular structure of the enol form of compound **3**, ellipsoids are drawn with 50% probability. N atoms are in blue, O in red, C in black and H in white.

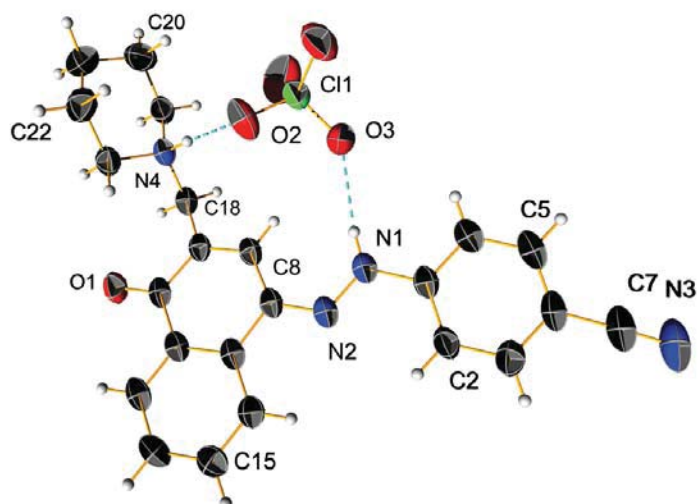


Figure S2. View of the molecular structure of the keto form of compound **3** with perchloric acid, ellipsoids are drawn with 50% probability. N atoms are in blue, O in red, C in black, H in white and Cl in green.

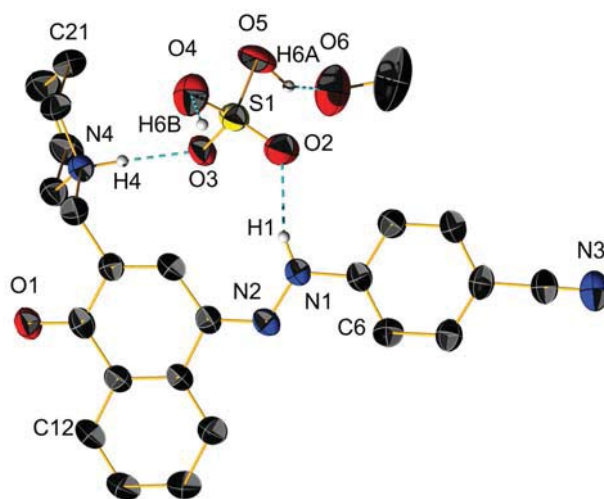


Figure S3. View of the molecular structure of the keto form of compound **3** with sulfuric acid. Ellipsoids are drawn with 50% probability, some hydrogen atoms are omitted for clarity. N atoms are in blue, O in red, C in black, H in white and S in yellow.

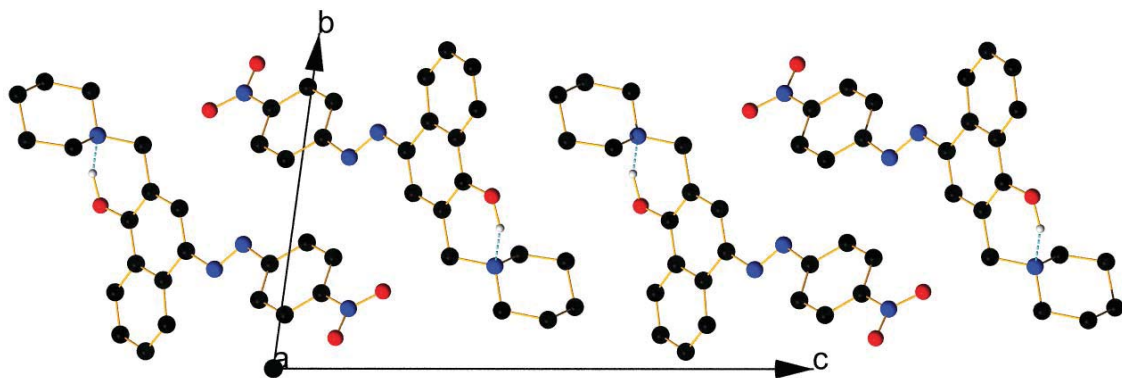


Figure S4. View of the packing along a axis in the enol form of compound 4.

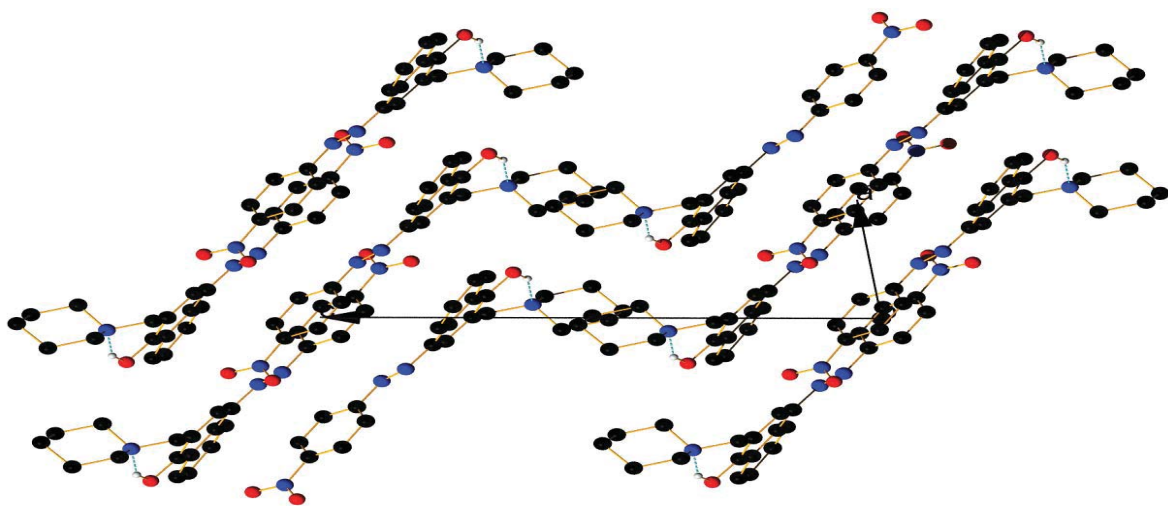


Figure S5. View of the packing along b axis in the enol form of compound 4.

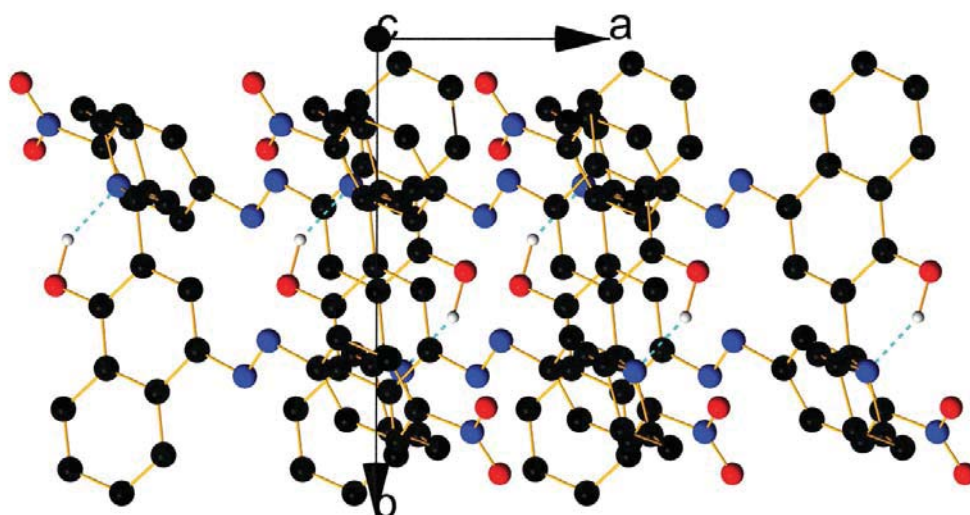


Figure S6. View of the packing along c axis in the enol form of compound 4.

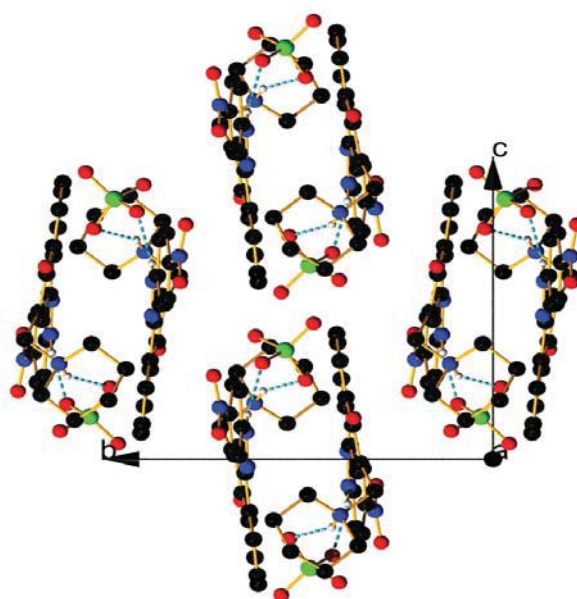


Figure S7. View of the packing along a axis in the keto form of compound 4 with perchloric acid.

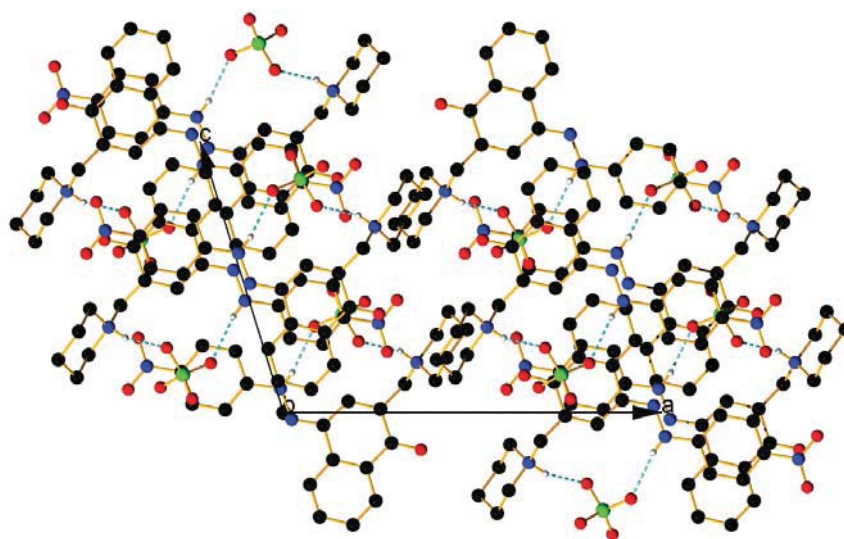


Figure S8. View of the packing along b axis in the keto form of compound **4** with perchloric acid.

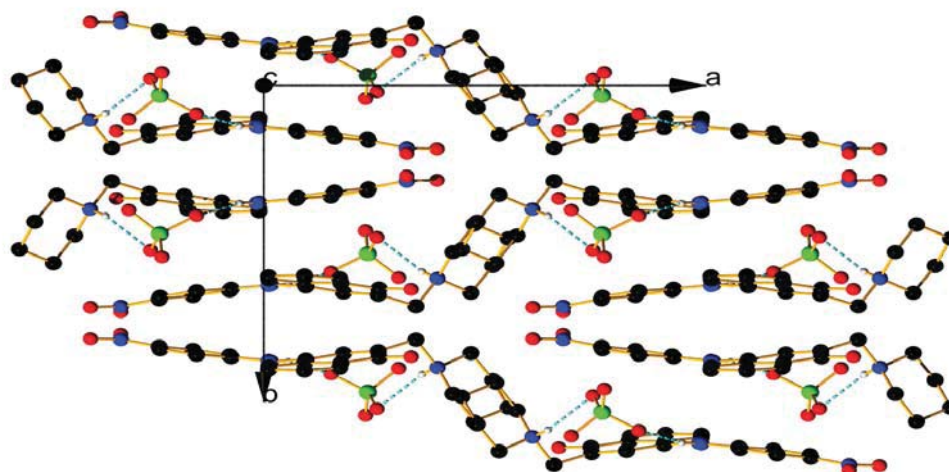


Figure S9. View of the packing along c axis in the keto form of compound **4** with perchloric acid.

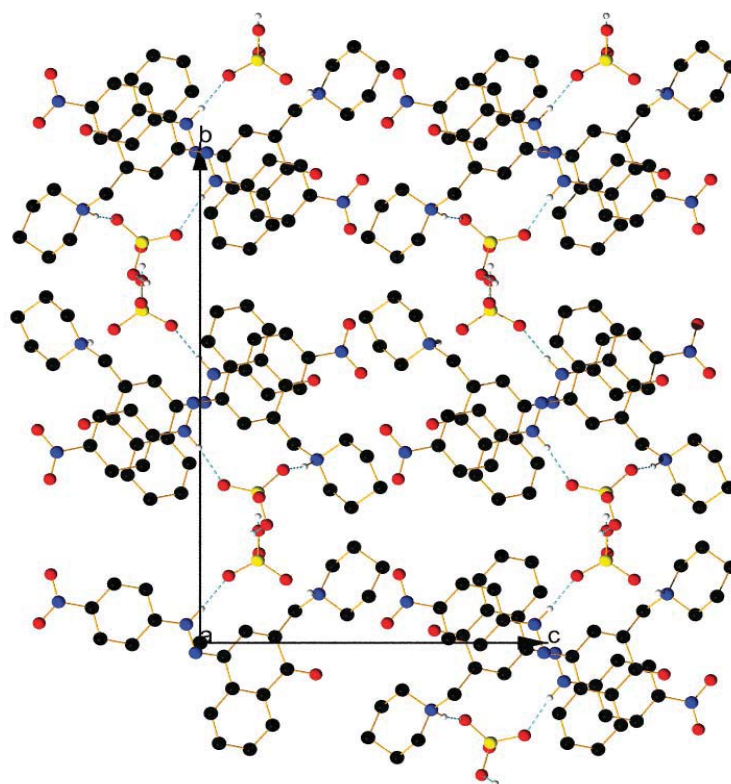


Figure S10. View of the packing along a axis in the keto form of compound **4** with sulfuric acid.

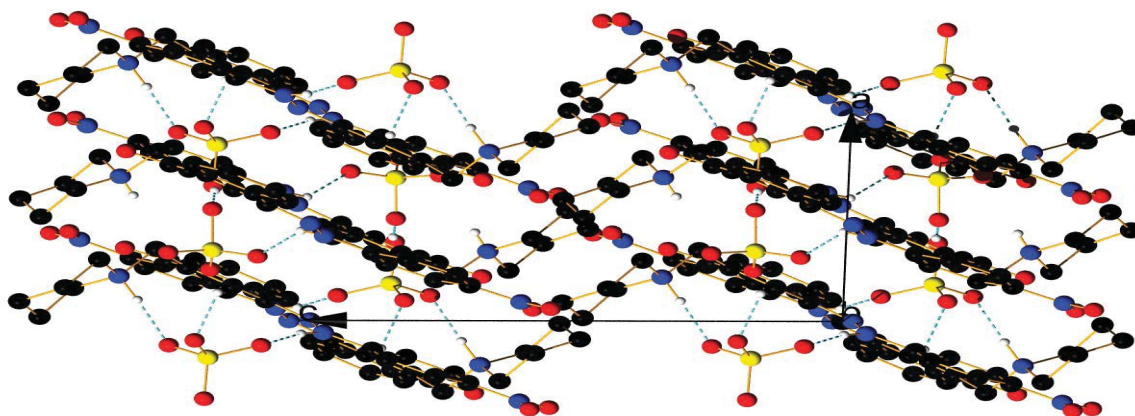


Figure S11. View of the packing along b axis in the keto form of compound **4** with sulfuric acid.

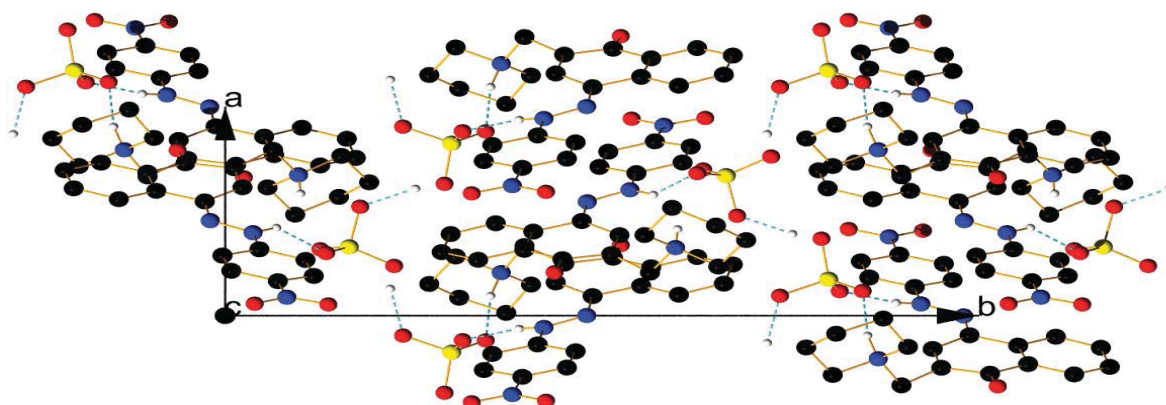


Figure S12. View of the packing along *c* axis in the keto form of compound **4** with sulfuric acid.

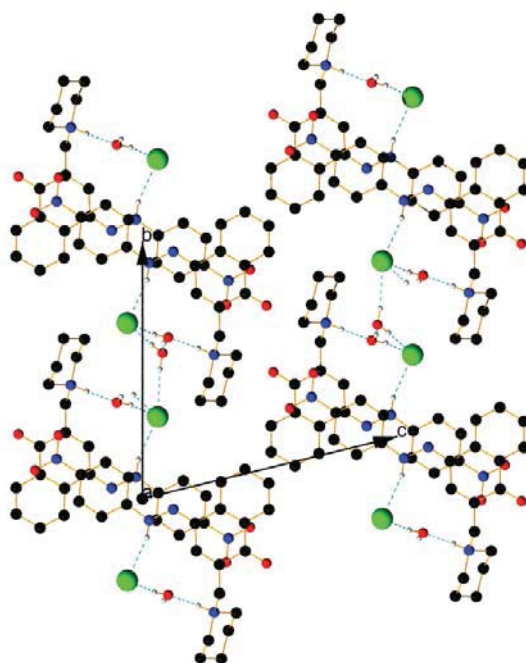


Figure S13. View of the packing along *a* axis in the keto form of compound **4** with hydrochloric acid.

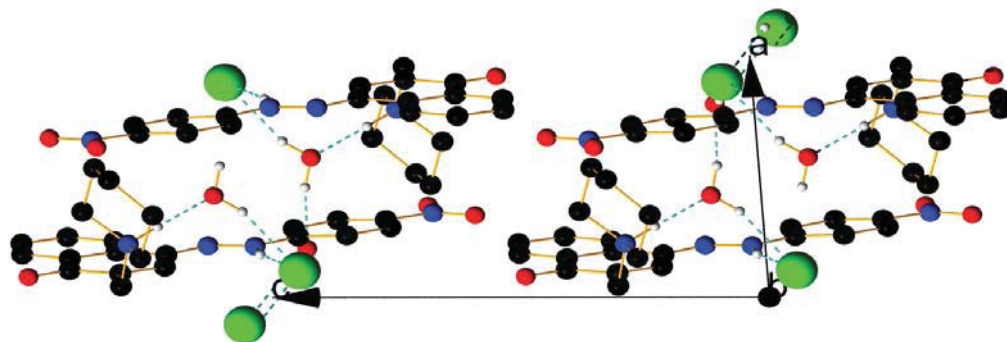


Figure S14. View of the packing along b axis in the keto form of compound **4** with hydrochloric acid.

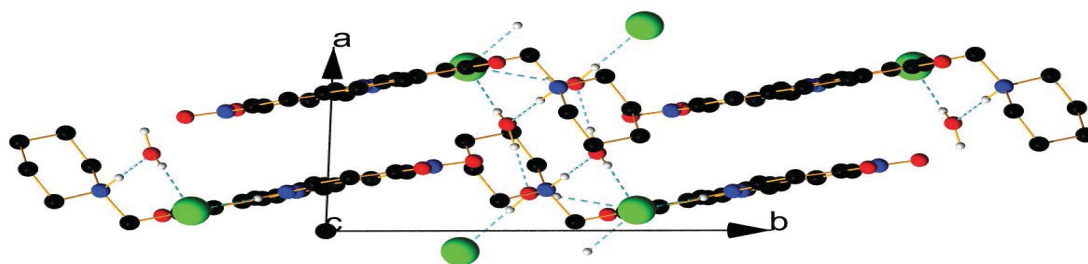


Figure S15. View of the packing along c axis in the keto form of compound **4** with hydrochloric acid.

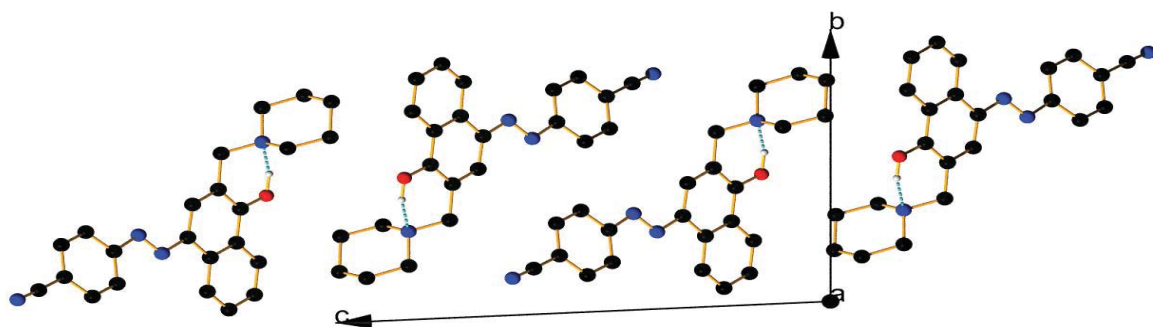


Figure S16. View of the packing along a axis in the enol form of compound 3.

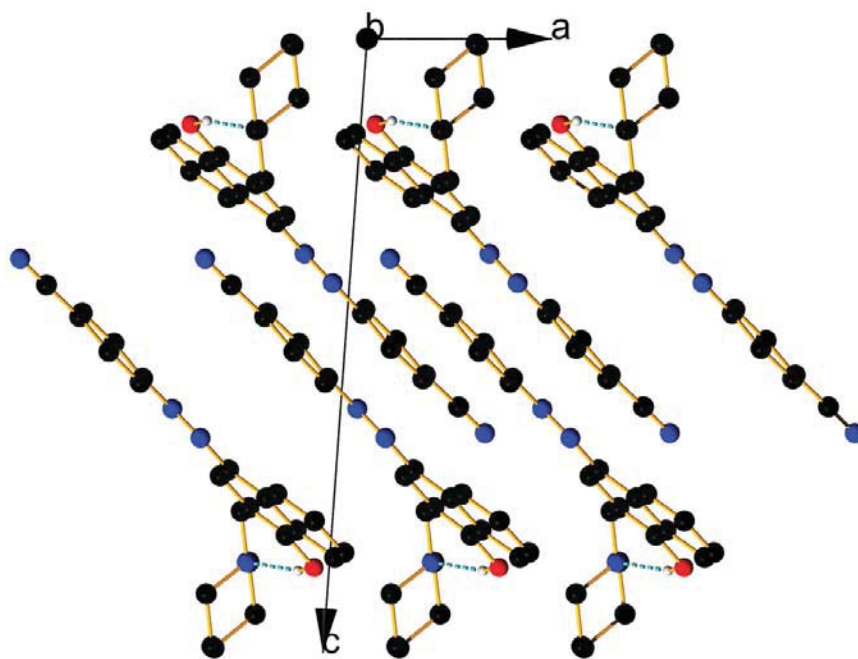


Figure S17. View of the packing along b axis in the enol form of compound 3.

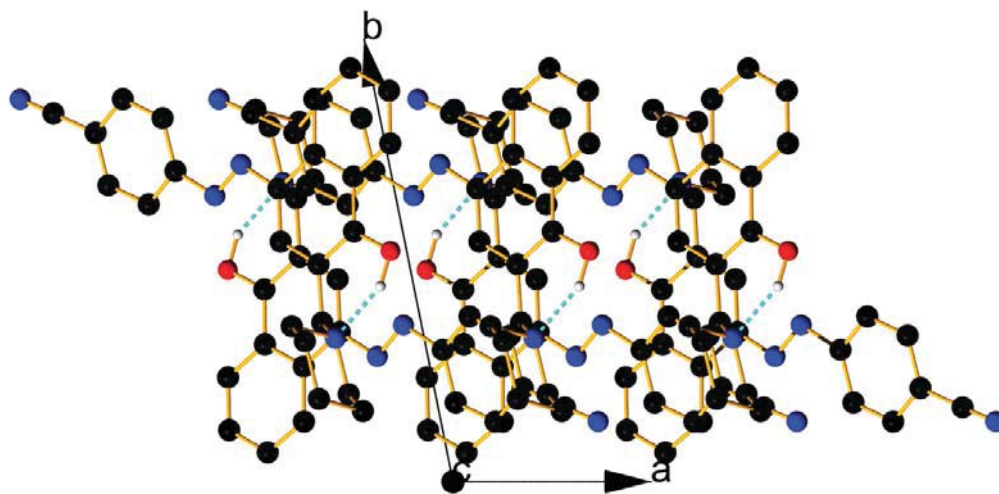


Figure S18. View of the packing along c axis in the enol form of compound **3**.

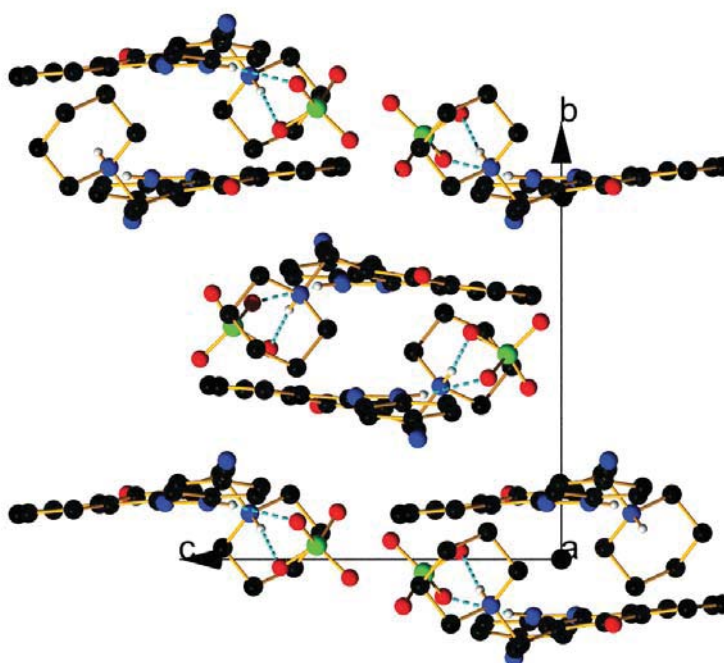


Figure S19. View of the packing along a axis in the keto form of compound **3** with perchloric acid.

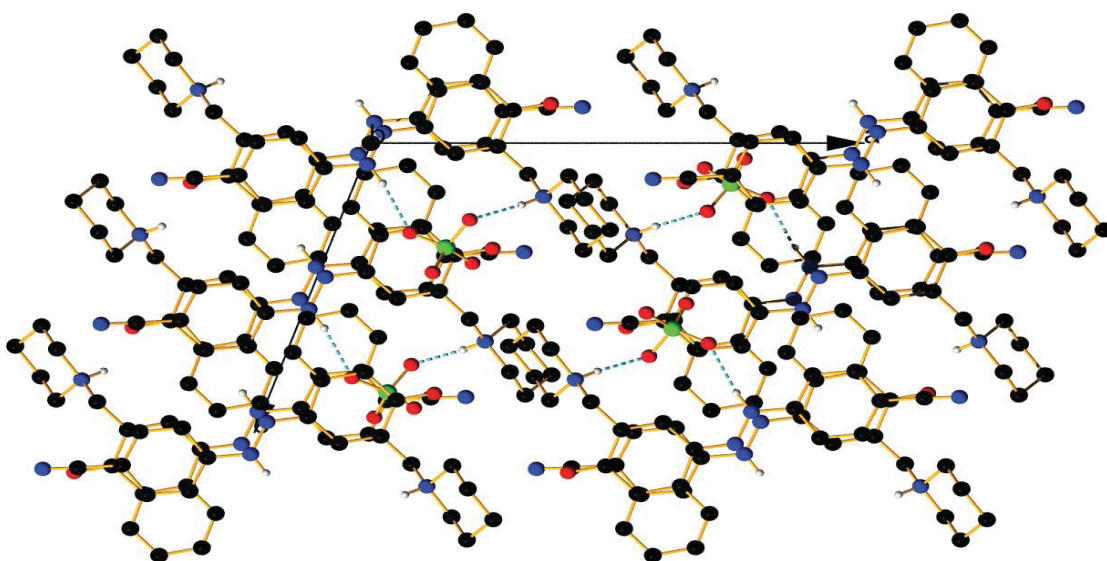


Figure S20. View of the packing along *b* axis in the keto form of compound **3** with perchloric acid.

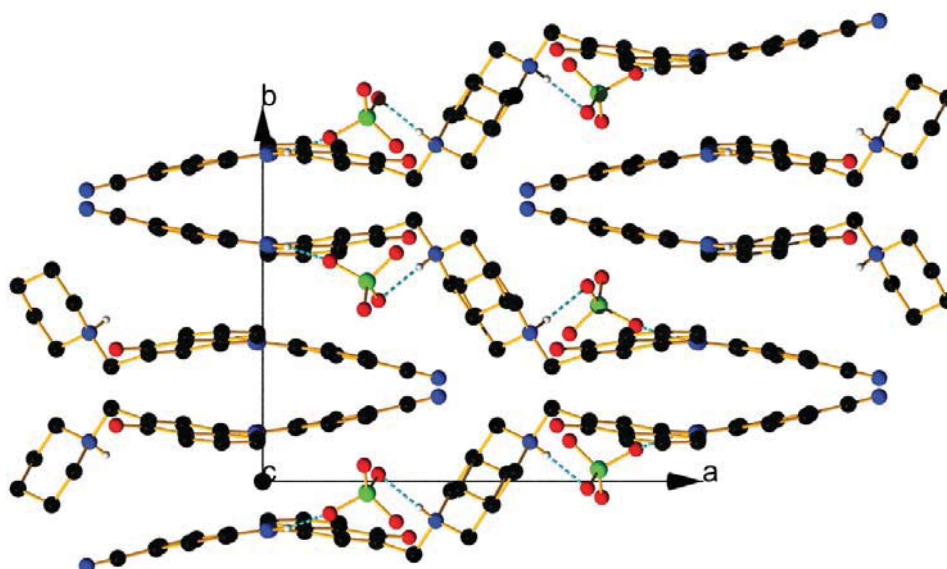


Figure S21. View of the packing along *c* axis in the keto form of compound **3** with perchloric acid.

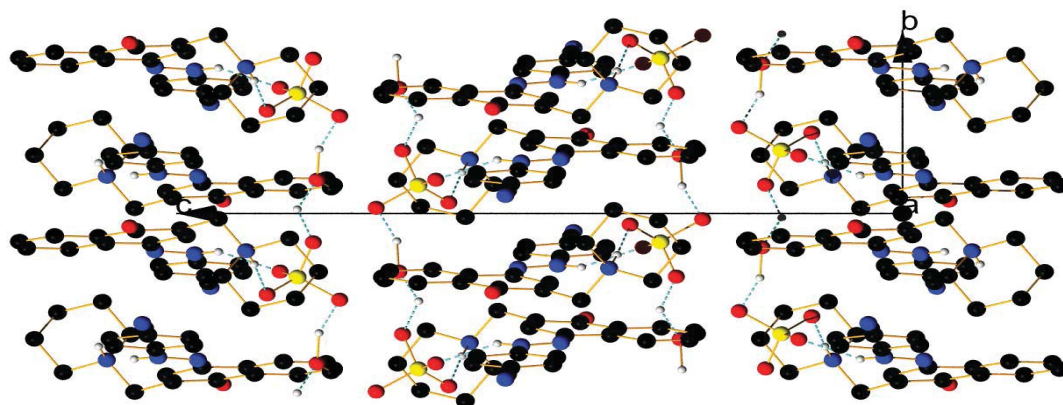


Figure S22. View of the packing along a axis in the keto form of compound **3** with sulfuric acid.

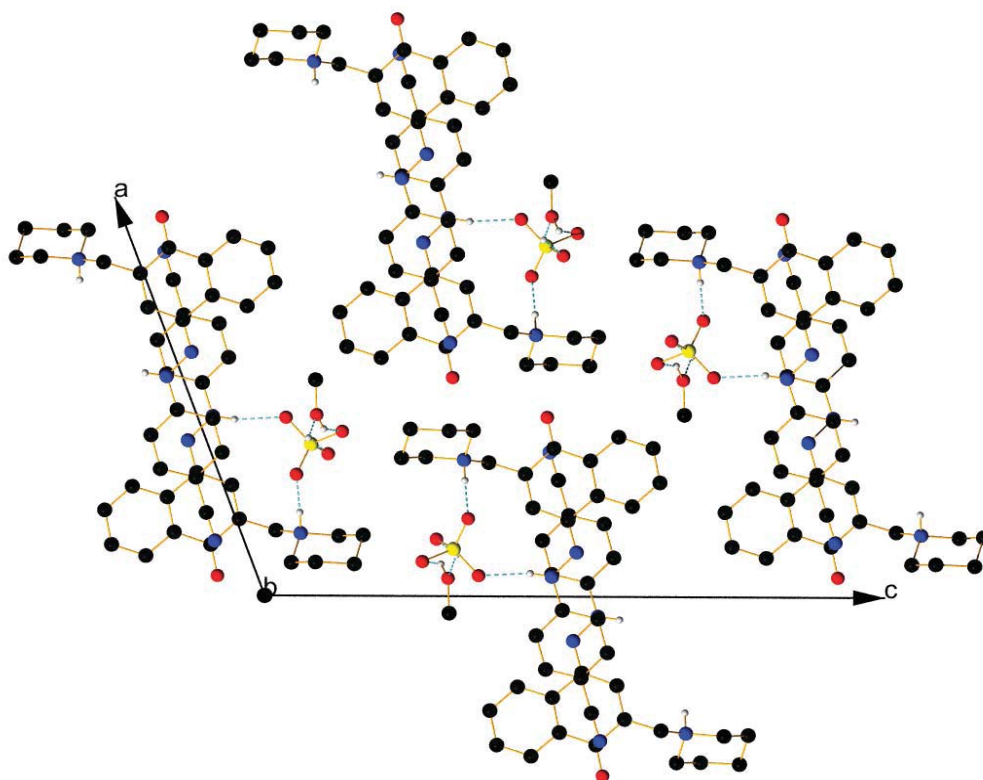


Figure S23. View of the packing along b axis in the keto form of compound **3** with sulfuric acid.

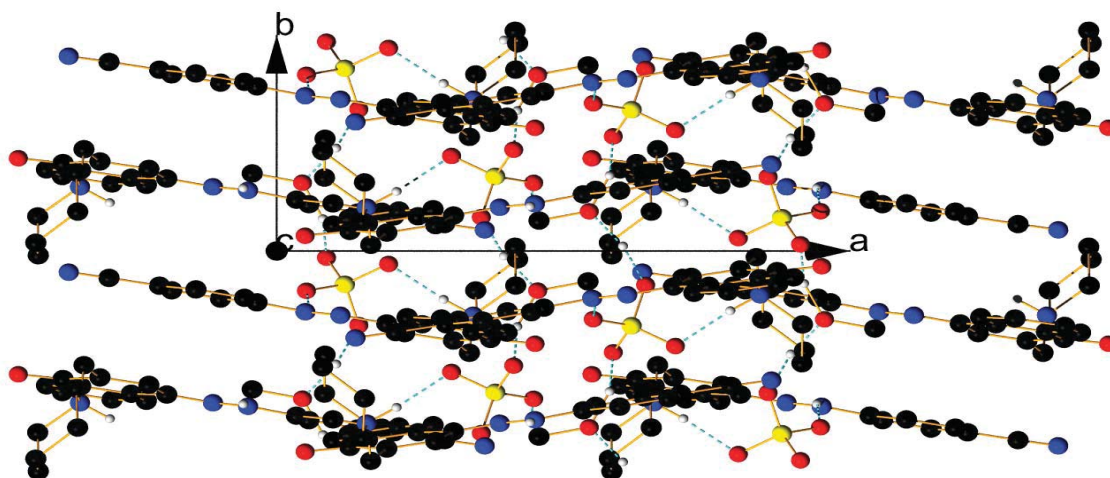


Figure S24. View of the packing along *c* axis in the keto form of compound **3** with sulfuric acid.

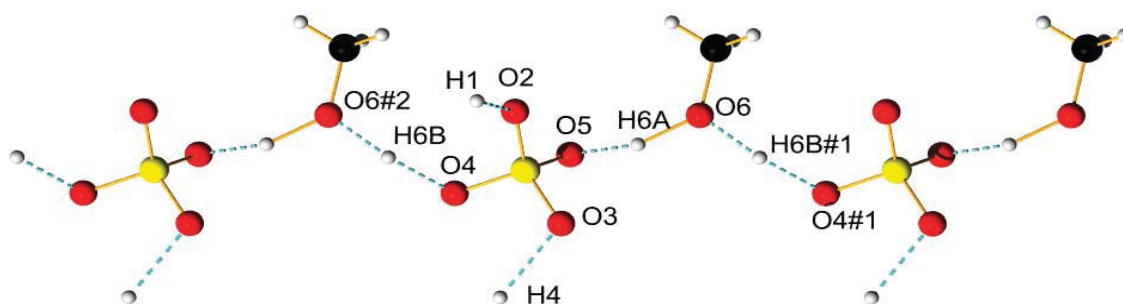


Figure S25. View of the counter anion chain in the packing of the keto form of compound **3** with sulfuric acid.

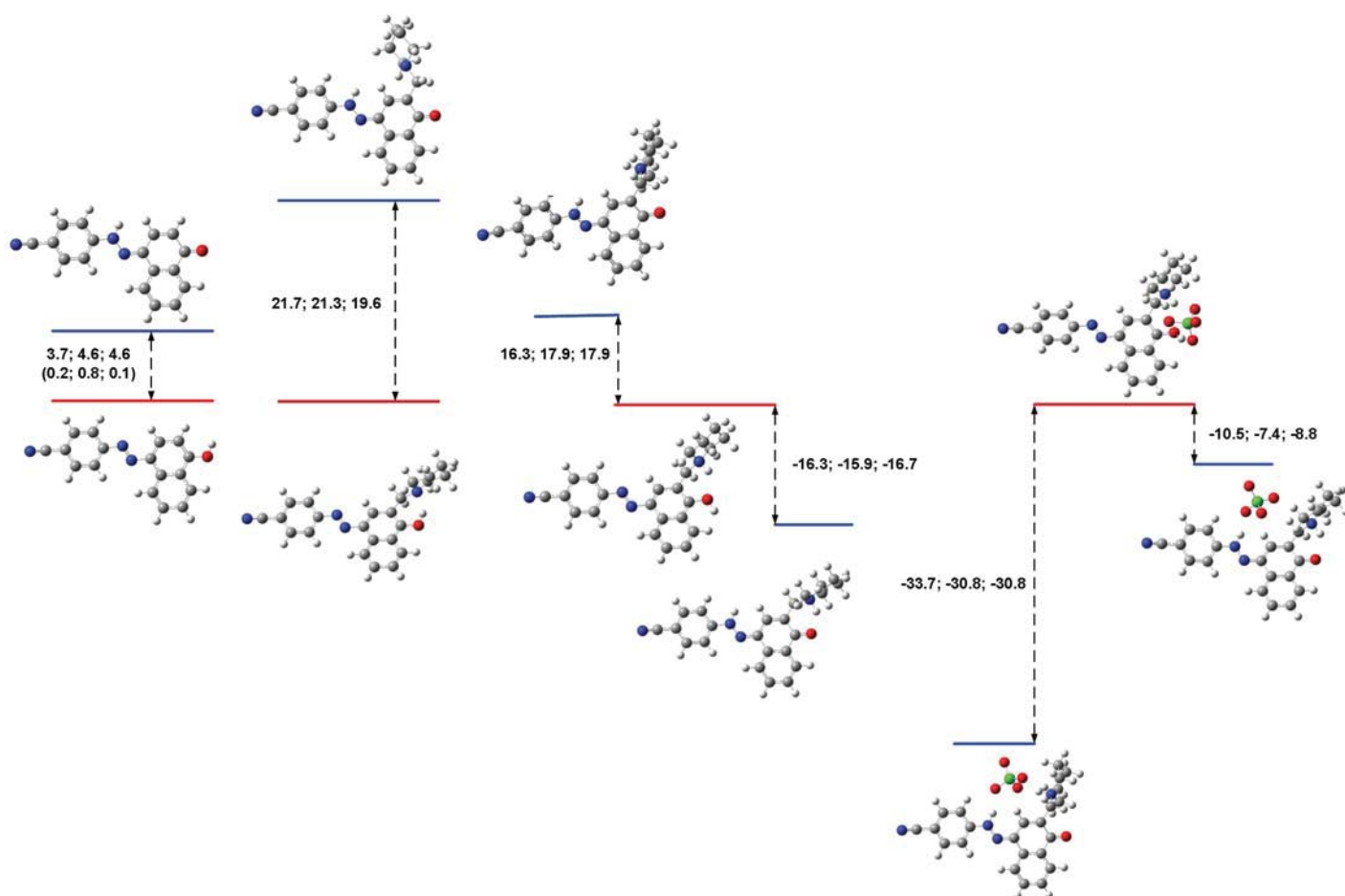


Figure S26. Change of the relative energy (M06-2X/def2TZVP) of the tautomers of the parent compound **1**, **3**, 3H^+ and $3\text{H}^+\text{ClO}_4^-$. The values of ΔE , $\Delta E + \text{ZPE}$ and $\Delta \Delta G$ are given in kJ/mol units.

Crystal data can be obtained on quoting the depository numbers CCDC- 928932 (**3**), 928933 ($3\text{H}^+\text{ClO}_4^-$), 928934 ($3\text{H}^+\text{HSO}_4^-$) (Fax: +44-1223-336-033; E-Mail: deposit@ccdc.cam.ac.uk).