

A new type of the dinitrogen pentoxide–acid interaction

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Experimental

General Details

Dinitrogen pentoxide was prepared by the known procedure from HNO₃ and P₂O₅ and subjected to extra purification over P₂O₅ *in vacuo* (680 Torr)¹. The Raman spectra in the 100–2000 cm⁻¹ range were recorded using a Lab RAM Jobin-Yvon laser Raman spectrometer equipped with a cooled CCD detector. The excitation line was 632.8 nm of a He-Ne laser and the radiation power on the sample did not exceed 2 mW. The spectral resolution was 2 cm⁻¹. The spectra were recorded for the samples plugged in glass ampoules under argon atmosphere. The ¹⁴N NMR (21.69 MHz) spectra were recorded on a Bruker AM300 spectrometer with an external capillary with acetone-d₆ as a lock solvent when used with non-deuterated solvents. The ¹⁴N NMR spectra were recorded with MeNO₂ (10–15 mg) as the internal standard (the up-field chemical shifts have negative values). The quantum chemical calculations of the reaction equilibrium were performed using a programme package Gaussian 09 Revision D.01 DFT B3LYP/6-311++g(d,p)².

Experimental Details

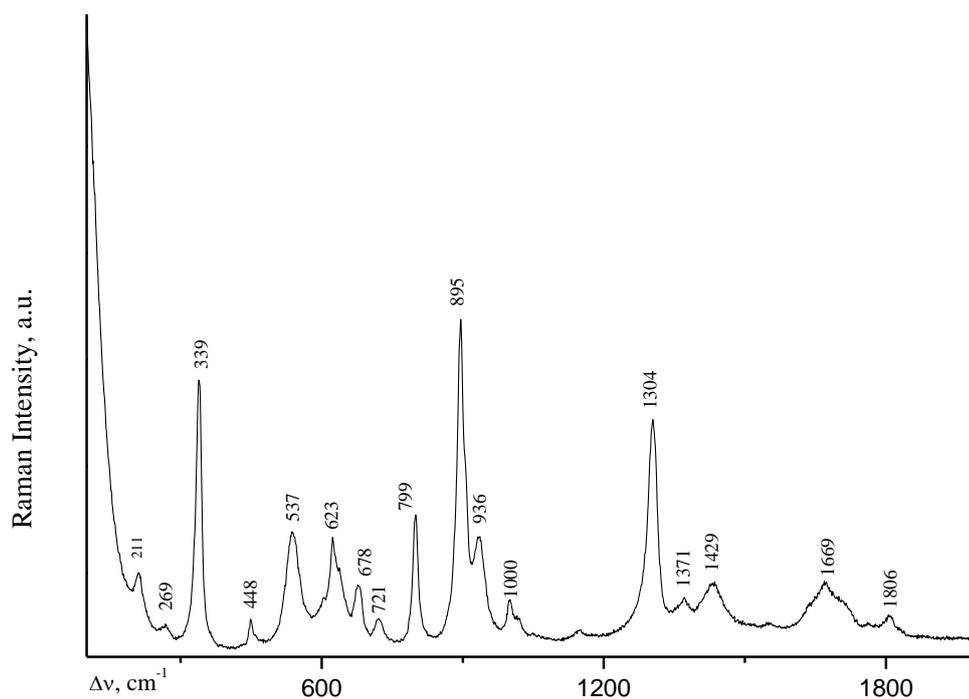


Figure S1 Raman spectrum of the $\text{AcONO}_2\text{—HNO}_3$ mixture in AcOH resulting from N_2O_5 dissolution in excess AcOH (1 : 4, mol).

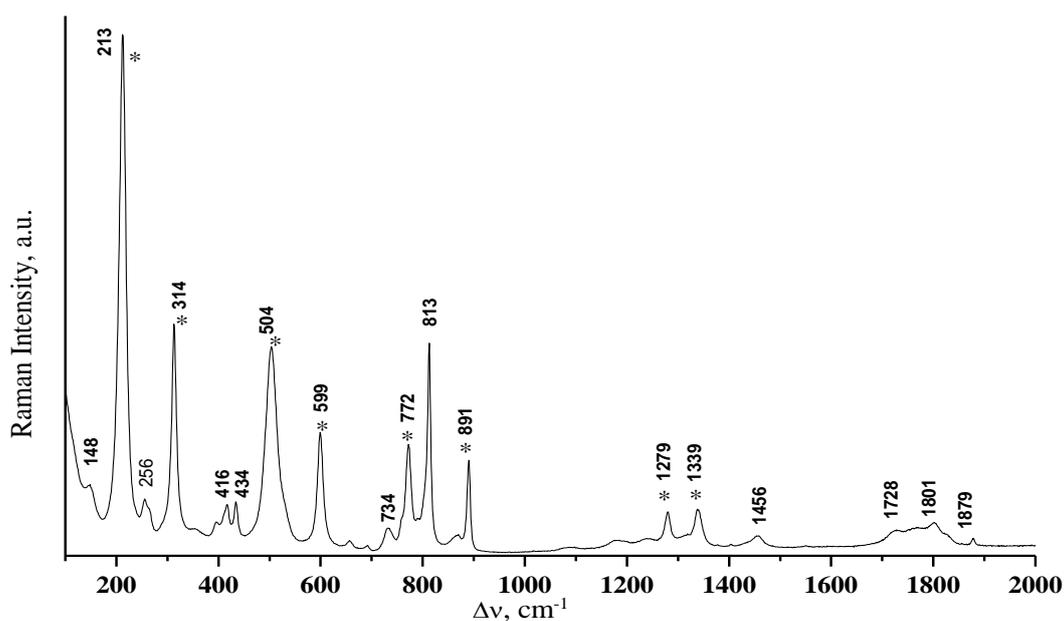


Figure S2 Raman spectrum of the freshly prepared TFAN solution in TFA resulted from the TFAA—HNO_3 mixture (1 : 1, mol, 0–5 °C, 0.5 h). The lines corresponding to the TFAN spectrum are marked with asterisks.

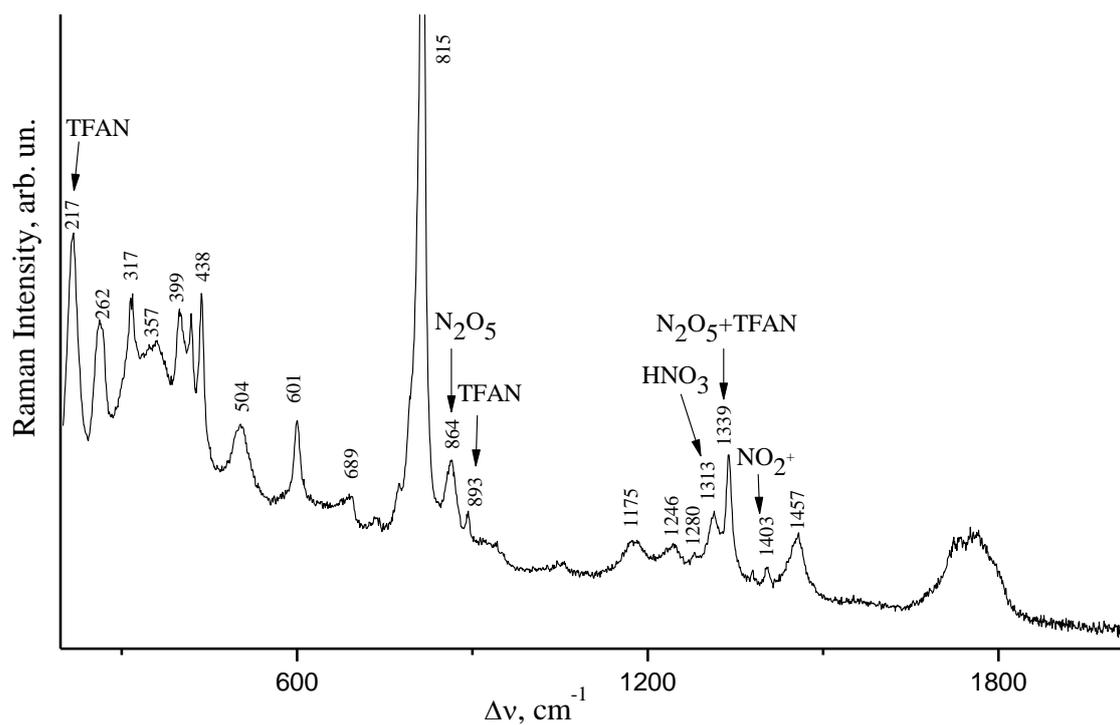


Figure S3 Raman spectrum of N_2O_5 solution in TFA (4 : 1, mol) at 0.5 h after dissolution, 0–5 °C.

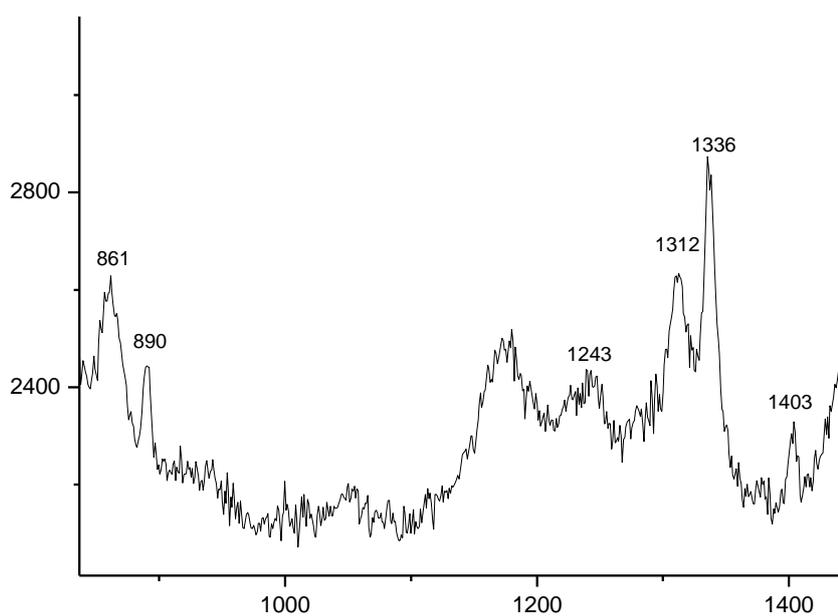


Figure S4 Raman spectrum of the N_2O_5 solution in TFA (8 : 1, mol) at 0.5 h, 0–5 °C.

References

- 1 V. P. Zelenov, S. S. Bukalov, L. A. Leites, R. R. Aysin, A. N. Subbotin, M. I. Struchkova and I. V. Fedyanin, *Mendeleev Commun.*, 2017, **27**, 31.
- 2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.