New millimetre-wave study of the *para*-N_2–CO van der Waals complex

L. A. Surin[a,b], A. Potapov[a], V. A. Panfilov[b], and S. Schlemmer[a]

[a] I. Physikalisches Institut, University of Cologne, Germany, E-mail: surin@ph1.uni-koeln.de
[b] Institute of Spectroscopy RAS, 142190 Troitsk, Moscow, Russia

The spectra of the N_2–CO van der Waals complex have been measured in the past in the infrared, microwave and millimeter-wave regions (see [1] and references there). It was shown that the energy levels of N_2–CO could be labeled by j_{N2} and j_{CO}, referring to the free rotation of the N_2 and CO subunits, and they were divided into two distinct groups, corresponding to complexes involving *ortho*-N_2 or *para*-N_2 spin modifications. For *ortho*-N_2–CO, both expected $K = 1 - 0$ and $K = 0 - 0$ (K is the projection of the total angular momentum J on the intermolecular axis) subbands connecting the ground (j_{N2}, j_{CO}) = (0, 0) and the first excited (0, 1) free rotor states were observed and assigned [2, 3]. The *para*-N_2–CO modification displays a more complicated spectral pattern, and only two (of many possible) $K = 1 - 0$ and $K = 1 - 1$ subbands of rotational transitions from the lowest (j_{N2}, j_{CO}) = (1, 0) to the next excited (1, 1) state were detected [1]. For the latter state, representing simultaneous free rotation of both monomers, three $K = 0$, one more $K = 1$ and one $K = 2$ internal rotor states were expected to exist. In the present work three further $K = 0 - 0$, $K = 0 - 1$ and $K = 2 - 1$ subbands between the (j_{N2}, j_{CO}) = (1, 1) and (1, 0) states were measured and assigned. The assignments relied on the recently obtained new infrared data [4]. The origin energies and rotational constants of the newly detected $K = 0$ and 2 internal rotor states of *para*-N_2–CO were determined. The hyperfine quadrupole structure due to the presence of two equivalent ^{14}N nuclei was partly resolved for the most observed lines providing structural information about angular location of the N_2 within the complex.

L.A.S. acknowledges support from the Deutsche Forschungsgemeinschaft (Grants SU 579/1); L.A.S. and V.A.P. acknowledge support from Russian Foundation for Basic Research (Grant Nos. 12-03-00985, 12-02-91337).

[1] L. A. Surin, A. V. Potapov, H. S. P. Müller, V. A. Panfilov, B. S. Dumesh, T. F. Giesen, S. Schlemmer, *J. Mol. Struct*. **2006**, *795*, 198.
[2] Y. Xu, W. Jäger, L. A. Surin, I. Pak, V. A. Panfilov, G. Winnewisser, *J. Chem. Phys*. **1999**, *111*, 10476.
[3] L. A. Surin, H. S. P. Müller, E. V. Alieva, B. S. Dumesh, G. Winnewisser, I. Pak, *J. Mol. Struct*. **2002**, *612*, 207.
[4] A. R. W. McKellar, N. Moazzen-Ahmadi, **2013**, *private communication*.