Seventy-six diamonds with detectable C centers were selected based on the presence of a 1344 and/or 2688 cm\(^{-1}\) absorption in their infrared (IR) spectra. Such diamonds are always distinctly colored, often in yellow to orange with various modifications of colors such as brown and green. Fifty-seven of them had an IR spectrum exhibiting the well-known C center-related 1344.4 cm\(^{-1}\) (hereinafter 1344 cm\(^{-1}\)) IR absorption peak with an absorption coefficient of more than 0.1. The IR spectra of 15 diamonds had a 1344 cm\(^{-1}\) peak with an absorption coefficient below 0.1 cm\(^{-1}\). Finally, in the spectra of 4 samples the 1344 cm\(^{-1}\) peak was undetectable because of strong aggregated nitrogen absorption but the 2688 cm\(^{-1}\) line was present. When the 1344 cm\(^{-1}\) absorption is superior to 0.1 cm\(^{-1}\), this fairly sharp line (FWHM = 3.3–4.2 cm\(^{-1}\)) at 2688 cm\(^{-1}\) is detected, which correlates in intensity with the 1344 cm\(^{-1}\) feature.

**Keywords:** C center, infrared spectroscopy, overtone absorption, nitrogen concentration.

**Introduction.** Diamonds are roughly classified as "types" based on the presence and aggregation state of nitrogen combined with the presence of boron, and finally the absence of detectable nitrogen [1]. Table 1 gives an overview of the different types and their mixtures in natural and synthetic diamonds, as determined with infrared absorption spectroscopy and often used in gemmological literature. Type Ib diamonds are defined as those containing mainly C centers [2]; such diamonds are rare in nature, especially above approximately 0.20 ct, but very common for high-pressure high-temperature (HPHT) grown synthetic diamonds, with record sizes above 30 ct. The latter grow as type Ib, unless a nitrogen getter such as Al, Ti, or Zr is used [3], which results in type IIa.

Synthetic type Ib diamonds are yellow with the color deepened with the C center content, provided that they are low in other defects such as nickel. Natural type Ib diamonds are very rarely pure yellow; usually they exhibit mixed orange/yellow colors, often with a brownish or a greenish component. The most common color of type Ib diamonds is "olive" (sometimes referred to in the trade as "greenies," yet in reality being a mixture of yellow, brown, and green, even sometimes gray, in various proportions [4]); "pure" brown is very uncommon.

The C center defect causes absorption in the violet and blue portions of the visible spectrum due to its electron-donor properties and the resulting energy level in the band gap at about 1.7 eV [5]. This results in a mostly yellow or orange color due to a featureless, fairly steep increase of the absorption between 560 and 400 nm, in the absence of further defects. The C center is responsible for a broad, complex absorption system with its principal peak at 1130 cm\(^{-1}\) and a very sharp absorption at 1344 cm\(^{-1}\). The peak at 1130 cm\(^{-1}\) has been attributed to a quasi-local vibration at substitutional nitrogen atoms [6]. The sharp 1344 cm\(^{-1}\) absorption is assigned to a vibration of the carbon atom at the C–N bond with the unpaired electron [7].

C center nitrogen content calculations are usually based on the absorption coefficient at 1130 cm\(^{-1}\) [8]; when this feature is hidden in the spectra of diamonds with a high content of aggregated nitrogen, then the intensity of the

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1344 cm\(^{-1}\) absorption peak can be used instead, since the two features correlate in intensity. In the spectra of diamonds with a very high A (and/or B) center nitrogen content, this peak is often only partially visible since it is superimposed on intense, steep absorptions assigned to aggregated nitrogen. Consequently weak 1344 cm\(^{-1}\) absorption is very difficult to detect in such nitrogen-rich diamonds. For example, when the standard resolution of 4 cm\(^{-1}\) is used due to time constraints, then even a distinct 1344 cm\(^{-1}\) peak may be undetectable or hardly visible as an indistinct shoulder. Therefore reliable measurements of the isolated N content based on the 1344 cm\(^{-1}\) absorption require a resolution of at least 1 cm\(^{-1}\).

**Materials and Methods.** Seventy-six diamonds weighing 0.01 to 1.34 ct with C centers detectable by infrared absorption spectroscopy were analyzed and selected for this study. The luminescence of the diamonds was observed by the use of 254 nm short-wavelength and 365 nm long-wavelength light from a UVP UVSL-26P 6 Watt UV lamp and by broad band UV (300 to 410 nm) emission of a suitably filtered 200 watt Suprasil Xenon lamp mounted in a home-made luminescence microscope.

IR spectra of all the samples were recorded with resolutions of 4 and 1 cm\(^{-1}\) on a Perkin-Elmer Spectrum 100S FTIR spectrometer equipped with a thermoelectrically cooled DTGS detector, using a diffuse reflectance accessory as a beam condenser [9]. The spectra were recorded over a range of 8500 to 400 cm\(^{-1}\) with 100 to 500 scans for each diamond.