Application Note: **Diamond classification – the diamond types**

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January 29, 2015

Understanding diamond type classification is essential, especially nowadays. New diamond treatments and synthetics are hitting the market always more frequently . FTIR spectroscopy is an invaluable tool providing for essential information helpful to face such related issues.

Diamond was originally classified by using classical gemological tools. The first distinction between two main groups was established by Robertson et al. (1934, 1936), depending on their transparency to UV and IR wavelengths. Nowadays we know that these features are strictly correlated with nitrogen content as impurity in the diamond lattice (Kaiser and Bond, 1959). Diamonds containing detectable amount of nitrogen belong to type I and nitrogen-free diamonds to type II. Depending on how nitrogen impurities are arranged in the diamond lattice, we have a further sub-classification in the type I group and, depending on the presence of boron as impurity in the type II diamonds, we have another splitting in this group too (Figure 1) .

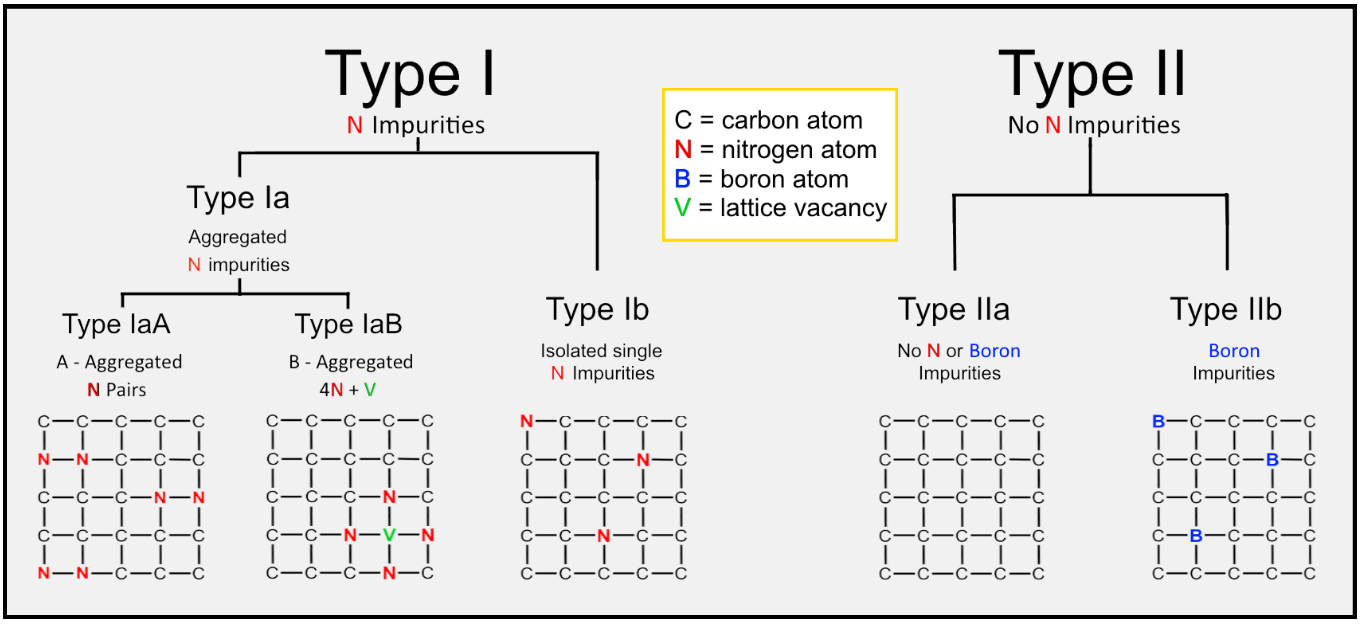

Fig 1. Diamond types

The most widely used technology to identify diamond type is FTIR-spectroscopy. This vibrational technique, in fact, is capable to identify absorption bands caused by the major nitrogen and boron impurity related defects. The IR region between 400 and 4000 cm^{-1} contains all the information we need to identify the diamond type. By observing the figure 2 we can subdivide the spectrum of diamonds in three main areas. The *one phonon* area (400-1332 cm^{-1}) features the major absorption bands related to nitrogen contents, so the presence or lack of peaks here tells us whether the diamond belongs to type I or II. The two *phonon area* (1332-2665- cm^{-1}) identifies the diamond as material and the three phonon area (2665-4000 cm^{-1}) still identifies the diamond and can contain hydrogen– and irradiation- related absorption bands.

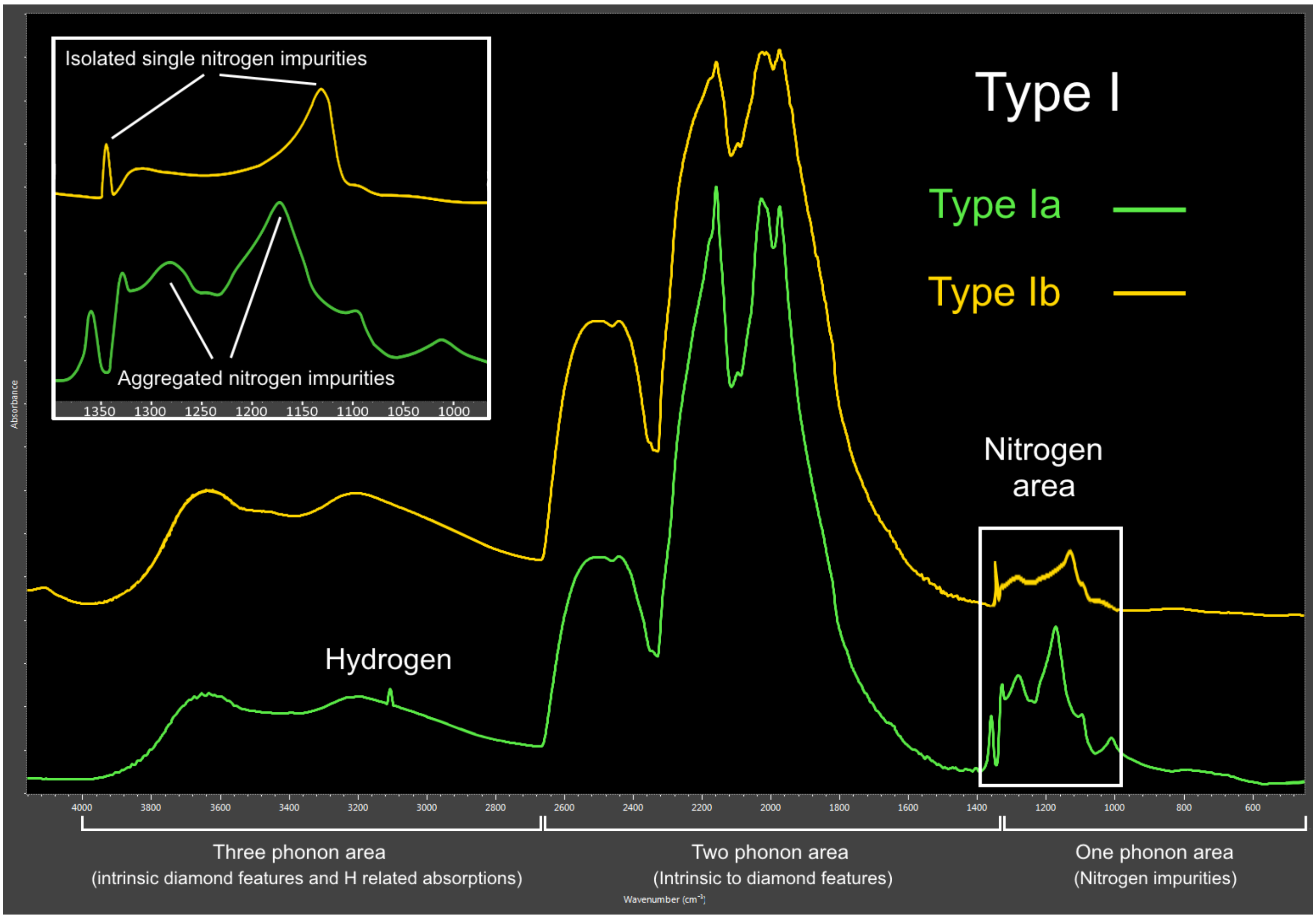

Fig 2. FTIR spectra of Type I diamonds and zoomed section of the one phonon area with nitrogen impurities.

The same spectrum areas for type II diamonds must be read differently since boron as impurity in type IIb causes bands at two– and three phonon areas and the type IIa can be readily identified as such by its lack of any impurity-related features (Figure 3).

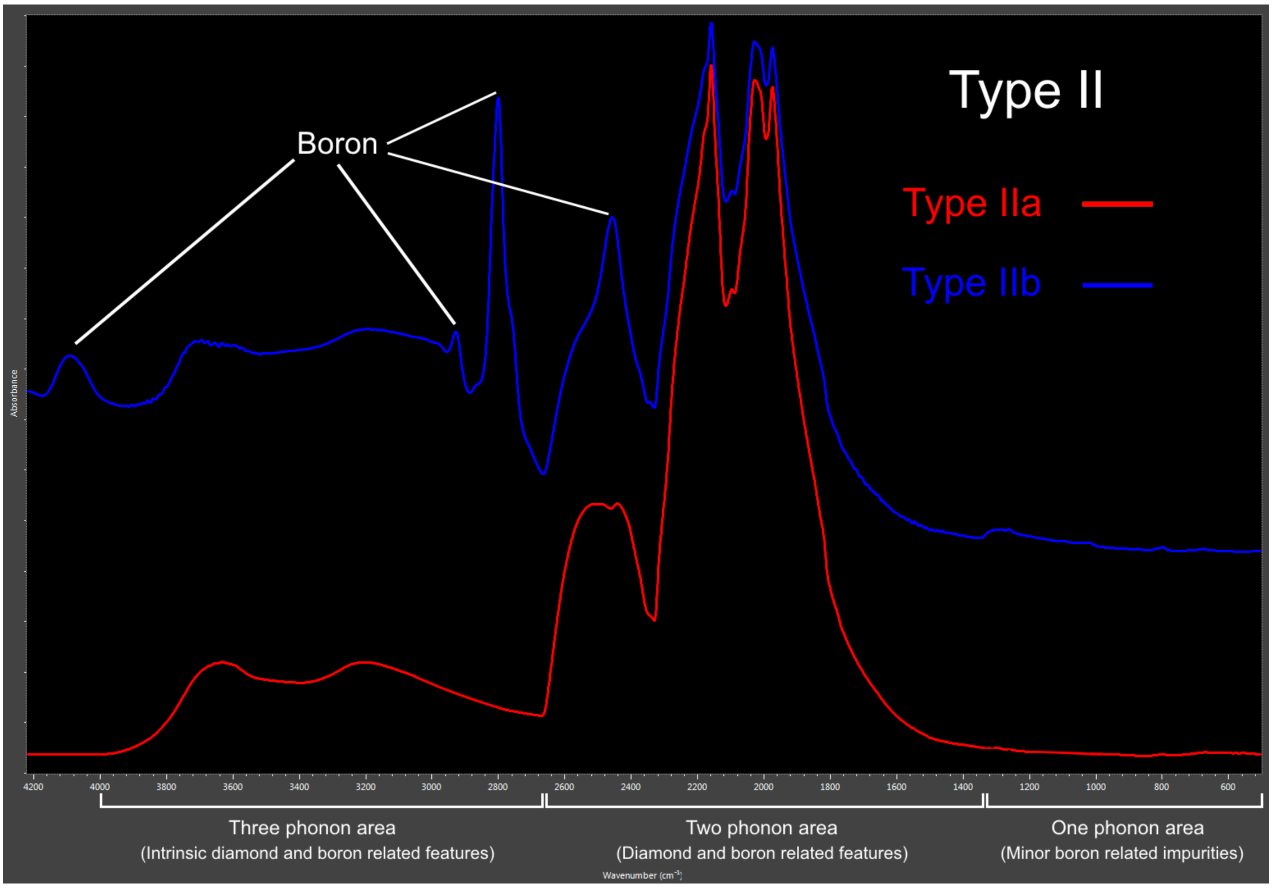

Fig 3. FTIR spectra of type II diamonds with major peaks related to boron impurities in type IIb.

Nitrogen is commonly trapped in diamond lattice in all its various aggregate forms or as free single atoms. Approximately 98% of all natural diamonds, in fact, belongs to type I. It is important to consider that both nitrogen A and B aggregates are very often present at the same time in diamond lattice; hence, "pure" diamond types, although existing, should be considered a very rare occurrence (Figure 4).

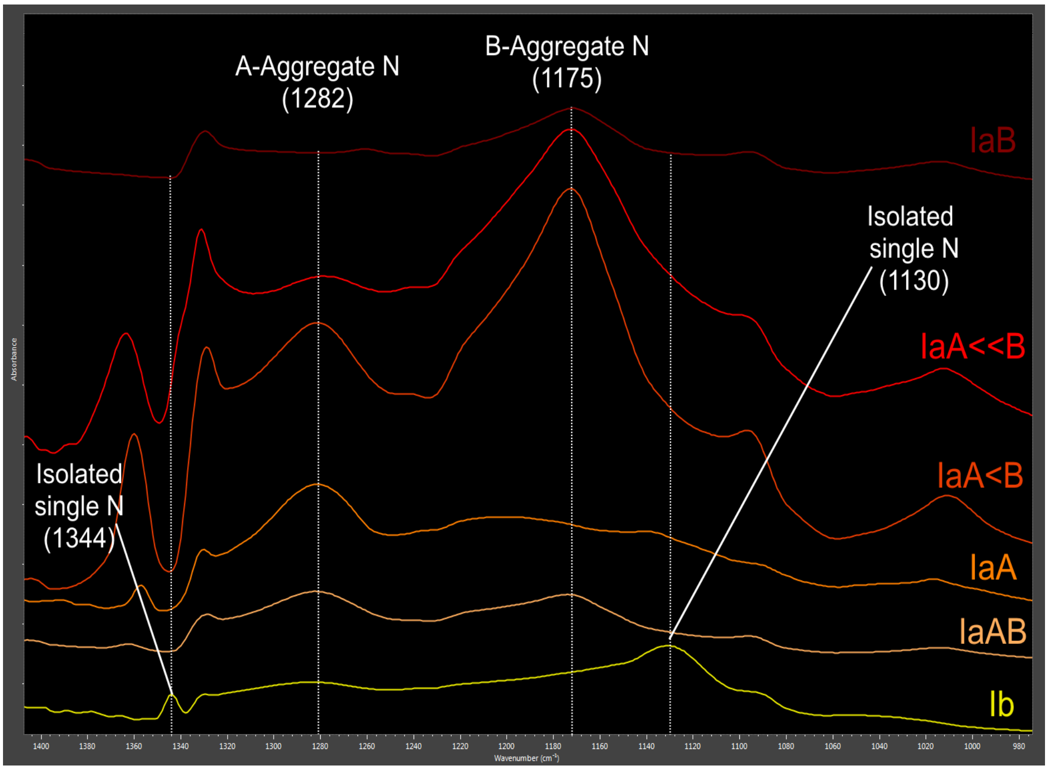

Fig 4. One phonon area with nitrogen impurities from different diamond types

The reason why it is so critical today to be able to correctly identify the type of a diamond is connected to the recent development of enhancement methods and synthetics. One of the most important case is the HPHT color enhancement. By this method it is possible to turn a brown or brownish color diamond into a colorless one.

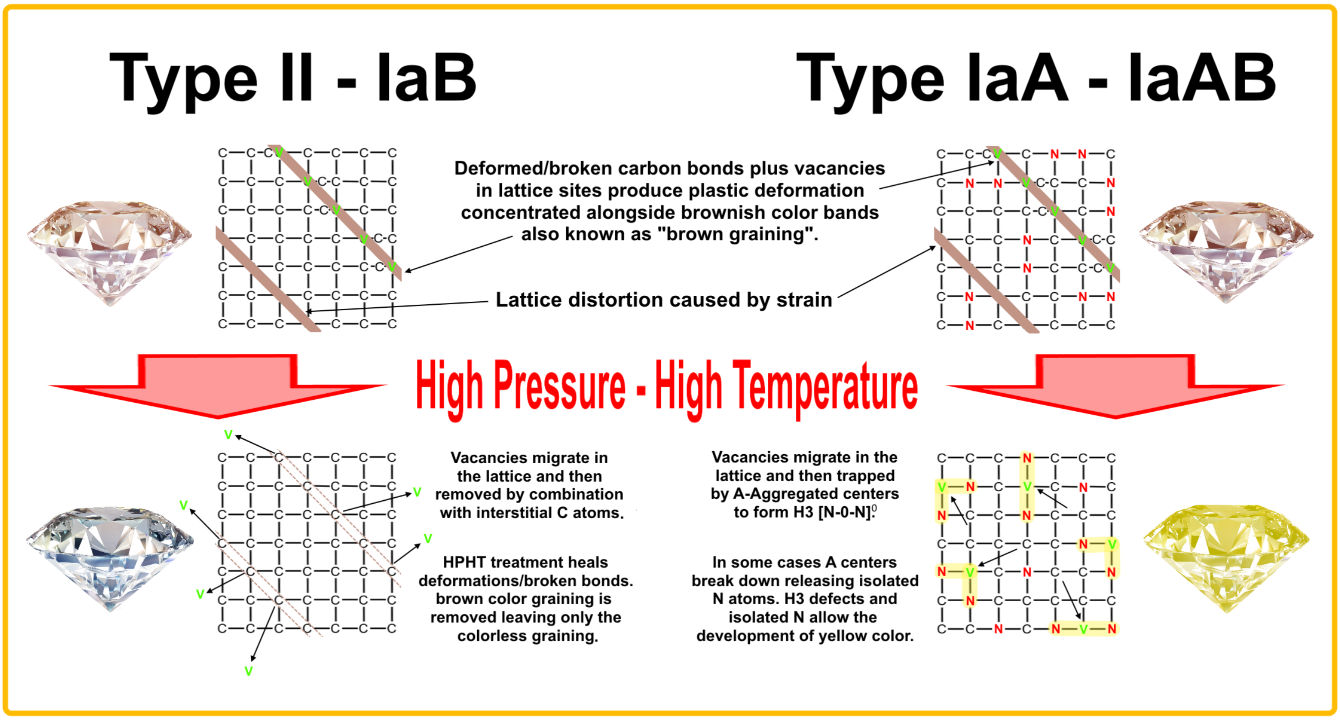

Fig 5. HPHT process on different diamond types.

In some cases, type IIa diamonds displaying unattractive color due to crystal lattice deformation caused by internal strain, and extremely rare low nitrogen IaB diamonds, can be enhanced to virtually colorless stones. It is even widely known that to date, HPHT or CVD grown synthetic colorless diamonds belong to type IIa. Being able to positively identify a colorless/near-to-colorless diamond as type Ia will lead to exclude synthetics and HPHT treatment.

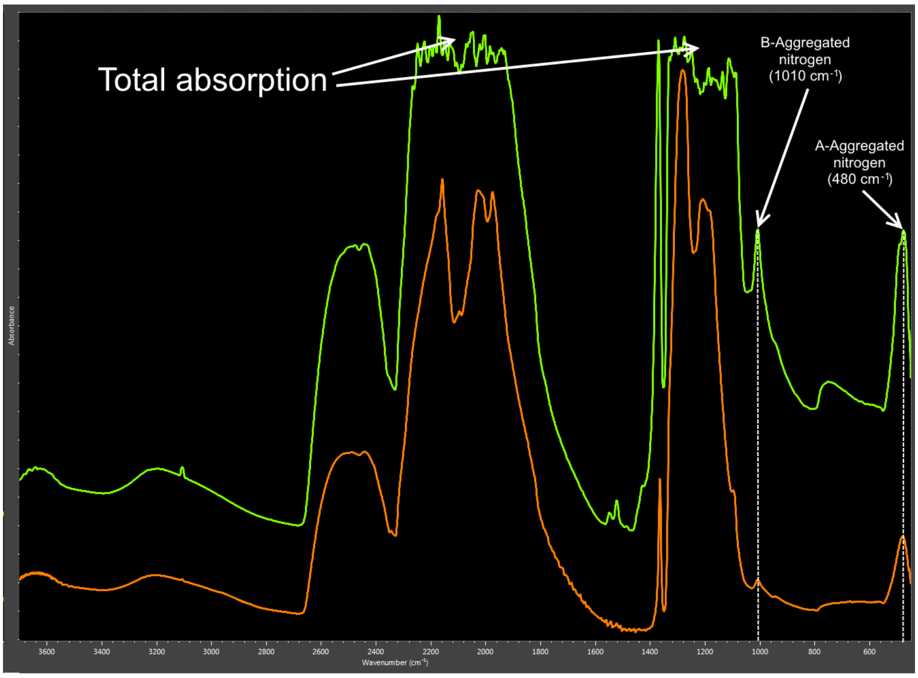

Fig 6. Sometimes a total absorption occurs in some parts of the spectrum. It may happen due the size of the diamond, as IR beam is completely absorbed. In the case displayed here (green line) the diamond type can still be identified by checking the peaks , usually minor features..

Not only type II and IaB diamonds are suitable for HPHT treatment but, as featured in the Figure 5, by treating a type IaA or IaAB, the outcome will never be a colorless/near-to-colorless stone.

The GemmoFTIR™ software includes a dedicated tool for identifying the diamond type (Figure 7). Thanks to the development of specific algorithms, it is able to effectively normalize the spectrum and to calculate the relative nitrogen content.

Fig 7. The top left window features the *one phonon* area zoomed with labels on the relative nitrogen impurities peaks. Those features are detailed in the top right window. In this window are even included the H1a, H1b and H1c centers, typical of the irradiated diamonds. The bottom left window displays the nitrogen level by showing the One phonon area in red color and the full spectrum in the 1000-2950 cm^{-1} range. The bottom right window features the result of the analysis, in this case a IaAB diamond with low-moderate nitrogen content.

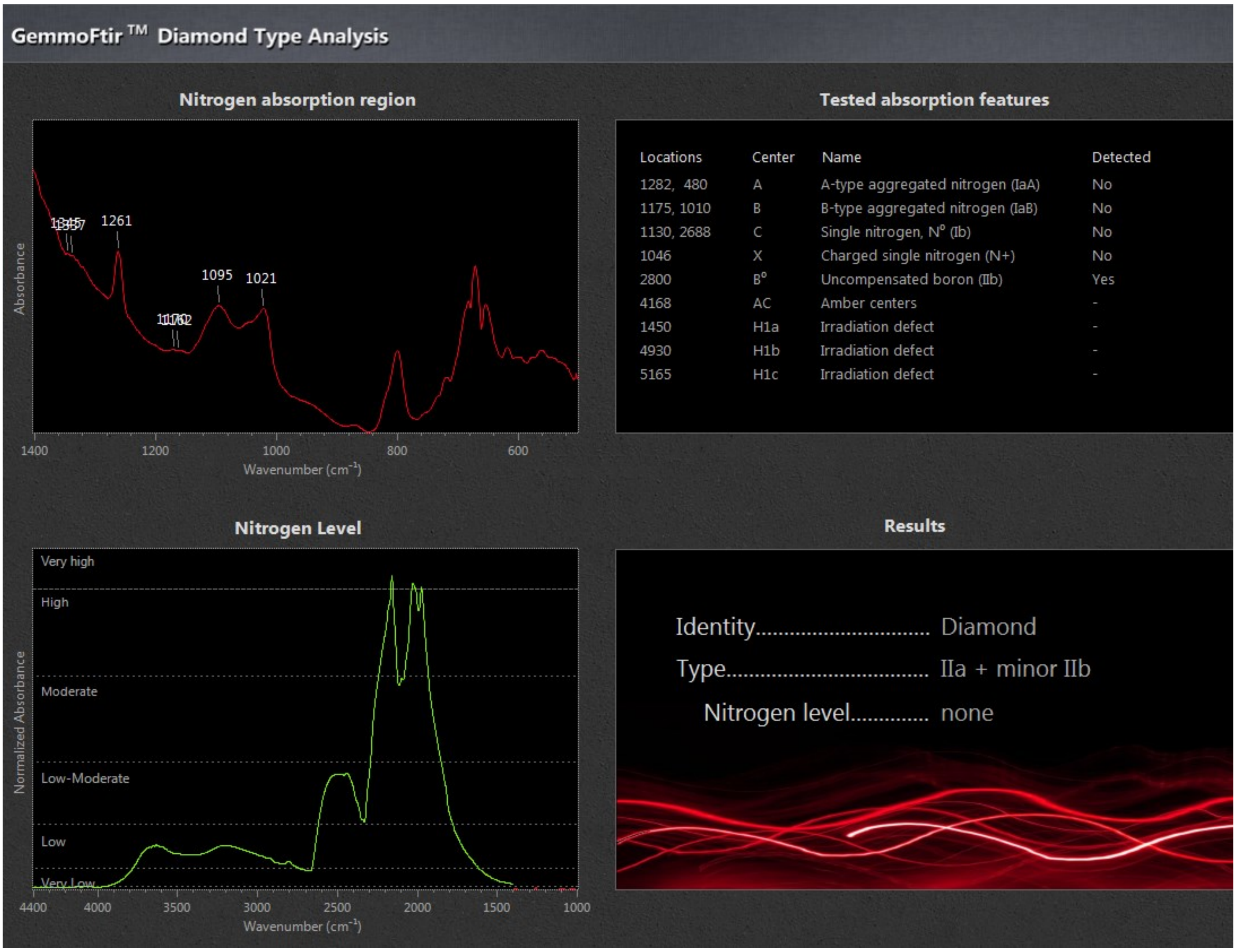

Fig 8. In this case the one phonon area contains almost non distinguishable features and the software was not able to identify any nitrogen related peaks. As it can be seen from the bottom left window, the One phonon area is almost non existent, so the diamond should be labeled as a type IIa. The system, though, has found an uncompensated boron defect (B^0 at 2800 cm^{-1}) so the diamond has been identified as IIa + minor IIb. This specific peak, if present along with another one, at 4092 cm^{-1} seems to be typical of bulk presence of boron in the vast majority of HPHT synthetic colorless/near-to-colorless produced by BARS method by AOTC and other manufacturers. Being nitrogen related, the presence of H1a and H1b centers are not even checked in this case, hence the dash symbol instead of the “No” labels as seen in the Fig 7.

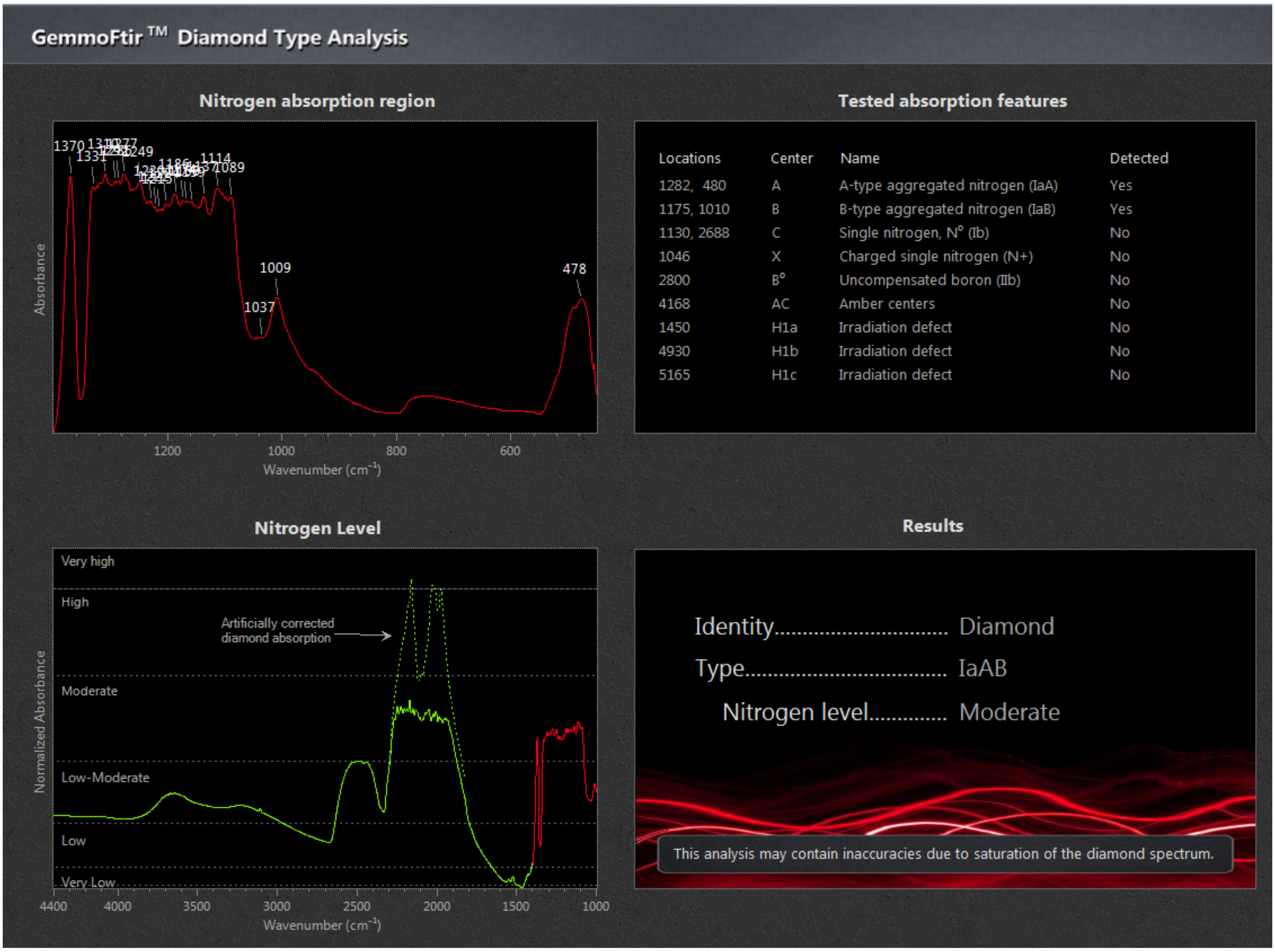

Fig 9. The image shows the analysis of the diamond featured in image 6 (green spectrum). In this case the main nitrogen aggregate peaks are not identified due to the saturated signal caused by the high nitrogen content. This can be visually evaluated by observing the bottom left window; The graph displays a lot of noisy peaks above the main part of the one –phonon area. Additionally, the two-phonon area containing the intrinsic absorption of diamond is saturated due to large sample size. As previously discussed, however, the software has been able to spot the minor peaks of A and B type aggregated nitrogen defects, so the diamond has been positively identified as type IaAB. The saturation at two-phonon area has been artificially corrected, and this correction causes underestimation of total nitrogen level. For this reason a small warning label is displayed at Results– area.

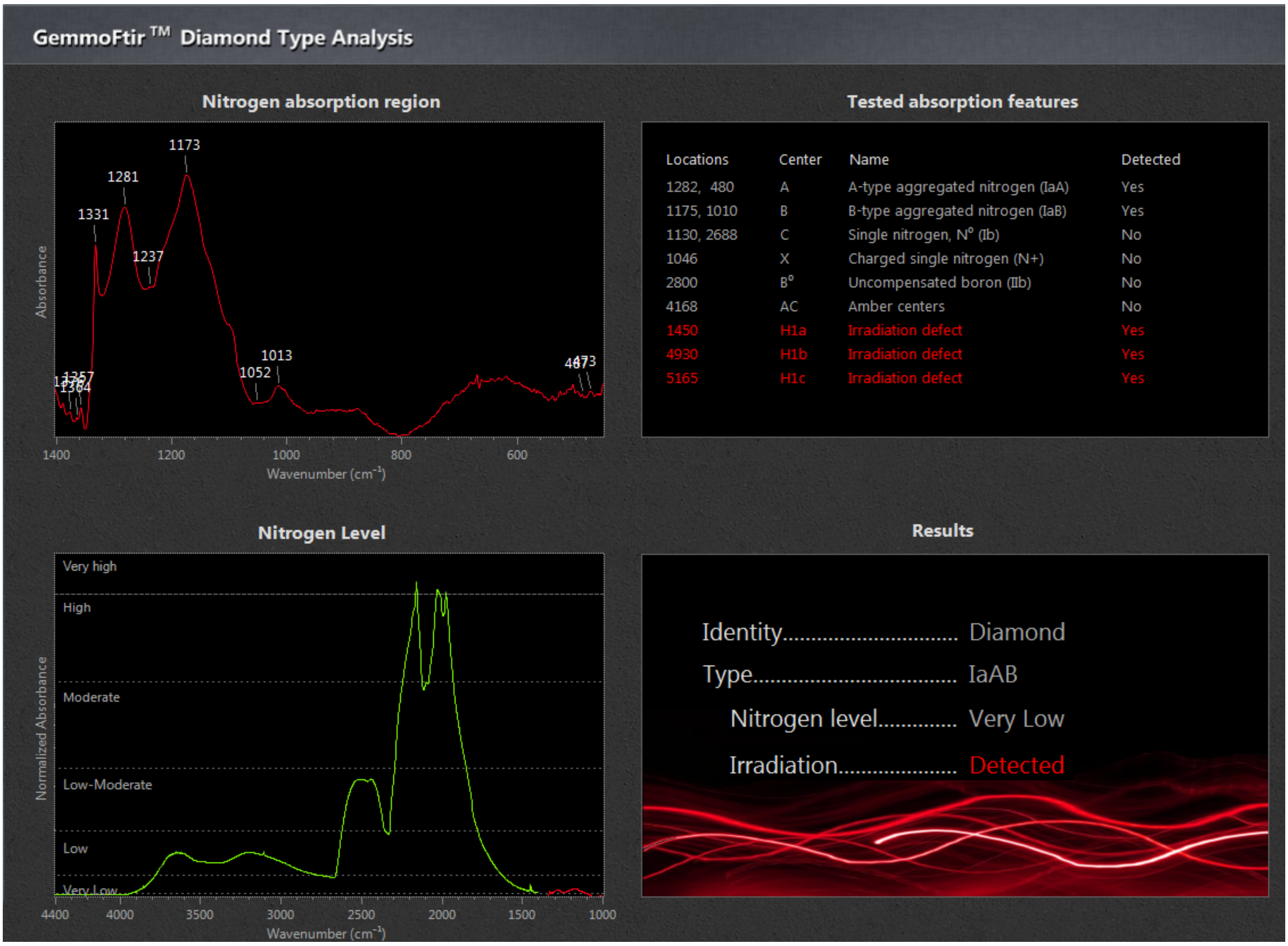

Fig 10. This spectrum belongs to a rare natural low-nitrogen 1aAB diamond treated by HPHT, irradiation and annealing in order to change its color to red. The software detected H1a, H1b and H1c– irradiation-related centers and thus warned the operator by displaying a blinking red alert.

References

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