



Application Note AN-NIR-094

Bromine number in pyrolysis gasoline

Fast determination of bromine number without chemicals

Pyrolysis gasoline (pygas) and its distillate fractions often contain high levels of reactive unsaturated compounds, making it unusable as a motor fuel. In addition to the amount of diolefins (determined by the Diels-Alder method), the total amount of aliphatic olefinic components also need to be monitored. The standard method to quantify the degree of unsaturation (bromine number) in unsaturated hydrocarbons is titration.

This wet chemical method requires cooling of the sample below 5 ° C to minimize side reactions like oxidation or substitution. In contrast to the primary method, near-infrared spectroscopy (NIRS) needs no sample preparation and is able to determine the bromine number within one minute. NIRS technology fulfills ASTM norms D8321 and D6122.

EXPERIMENTAL EQUIPMENT

180 pygas samples were analyzed on a Metrohm DS2500 Liquid Analyzer equipped with disposable glass vials. All measurements were performed in transmission mode from 400 nm to 2500 nm. The temperature control was set to 40 ° C to provide a stable sample environment. For convenience reasons, disposable glass vials with a pathlength of 8 mm were used, which made a cleaning procedure unnecessary. Data acquisition and prediction model development were performed with the software package Vision Air complete.



Figure 1. DS2500 Liquid Analyzer.

Table 1. Hardware and software equipment overview.

Equipment	Metrohm number
DS2500 Liquid Analyzer	2.929.0010
Disposable vials, 8 mm diameter, transmission	6.7402.000
Vision Air 2.0 Complete	6.6072.208

RESULT

The obtained Vis-NIR spectra (**Figure 2**) were used to create a prediction model for bromine number determination in pygas. To verify the quality of the prediction model, correlation

diagrams were created which display the correlation between Vis-NIR prediction and primary method values. The respective figures of merit (FOM) are displayed in **Figure 3**.

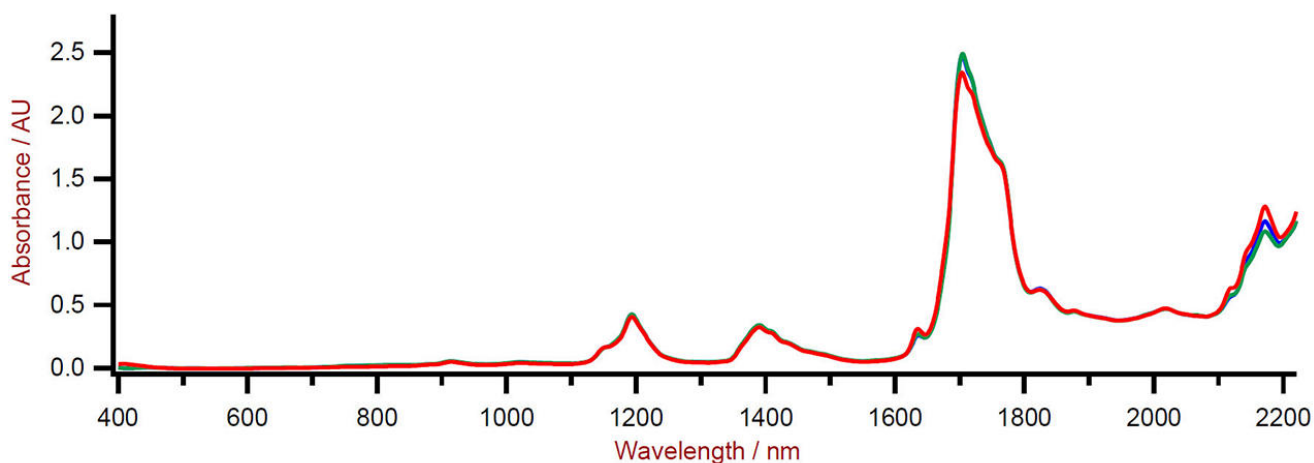


Figure 2. Selection of different pyrolysis gasoline Vis-NIR spectra obtained using a DS2500 Liquid Analyzer and 8 mm disposable vials.

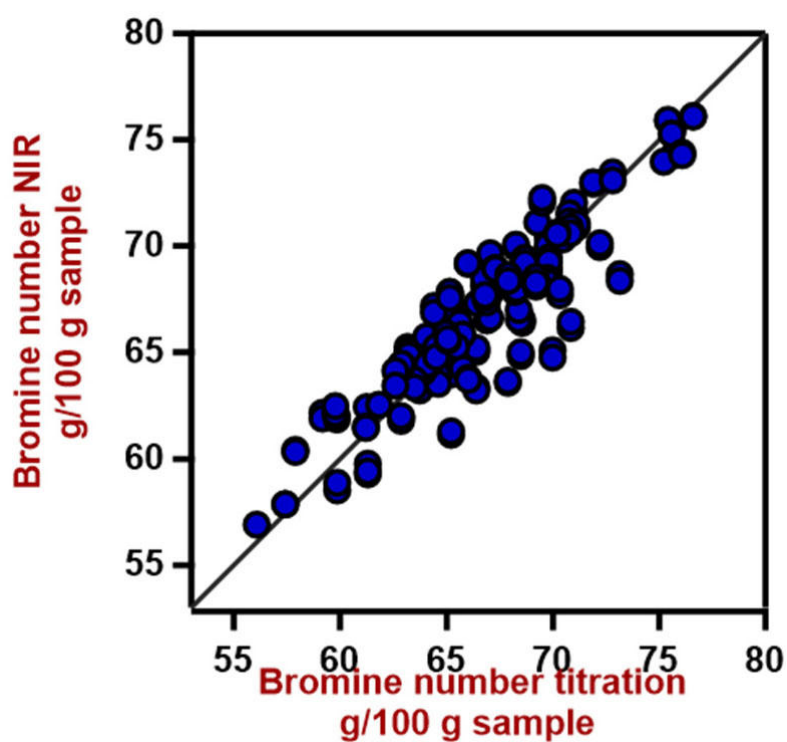


Figure 3. Correlation diagram for the prediction of the bromine number using a DS2500 Liquid Analyzer.

Table 2. Figures of merit for the prediction of the bromine number using a DS2500 Liquid Analyzer.

Figures of Merit	Value
R^2	0.836
Standard Error of Calibration	1.84
Standard Error of Cross-Validation	1.89

CONCLUSION

This application note shows the feasibility of NIR spectroscopy for the analysis of bromine number in pyrolysis gasoline. In contrast to the wet chemical method used in ASTM D1159 (Figure 4 and Table 3), no sample preparation or

chemicals are required with NIR spectroscopy. Aside from the bromine number, additional quality parameters like diene value can be determined in the same sample with NIR spectroscopy.

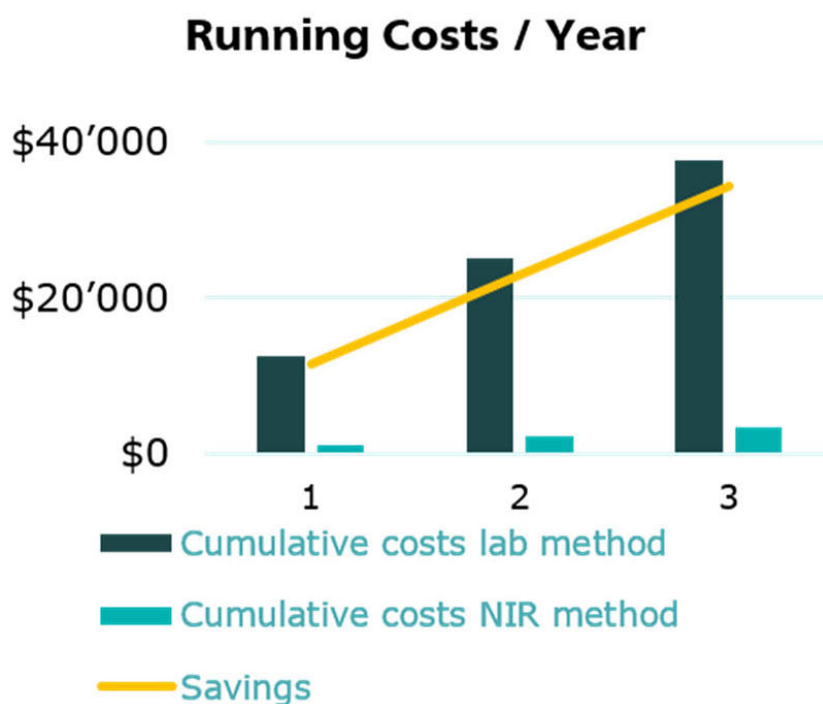


Figure 4. Comparison of running costs per year with the conventional wet chemistry lab method and NIRS.

Table 3. Comparison of costs and time to result (one-fold determination) with the conventional wet chemistry lab method and NIRS.

	Lab method	NIR method
Number of analyses (per day)	10	10
Costs of consumables and chemicals/measurement	\$6	\$0.50
Time spent per measurement	30 min	1 min
Total running costs / year	\$12,533	\$1,125

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DS2500 Liquid Analyzer

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 Liquid Analyzer 是一种成熟且灵活的解决方案,其用于在整个生产链中进行液体常规分析。其坚固结实的设计使 DS2500 Liquid Analyzer 不受灰尘、潮湿、振动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光谱范围,将样品加热至 80° C 高温,并与各种不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可适应您的个性化样品要求,帮助您在几分钟内获得精确和具有可重现性的结果。借助集成的样品架识别装置和自带的 Vision Air 软件,还保证了用户能轻松和安全地进行操作。

如果是较大的样品量,则可通过将流通池与一个 Metrohm 机器人自动进样器搭配使用的方法显著提高生产率。



Vision Air 2.0 Complete

Vision Air – 通用的光谱分析软件。

Vision Air Complete 是用于监管规范环境的先进易用的软件解决方案。

Vision Air 优点一览:

- 便捷的软件应用和经过适配的用户界面保证了直观简单的操作方式
- 操作过程的创建与维护方式简单
- SQL 数据库,可安全且简单地管理数据

Vision Air Complete (66072208) 版本包含所有用于可见近红外光谱分析质量保证过程的应用:

- 仪器和数据管理应用
- 方法开发应用
- 常规分析应用

其它 Vision Air Complete 解决方案:

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)



DS2500 8 mm

直径为 8 mm 且更加智能的一次性玻璃小瓶支架