



PRECISION YOU CAN CONTROL: WDXRF PERFORMANCE FOR PETROCHEMICAL QUALITY AND PROCESS CONTROL

Reliable elemental analysis for sulphur, additives, and trace metals – ensuring specification compliance and stable processes for upstream, refining, and blending – delivering fast, accurate results at every production stage.

Bruker's S8 TIGER Series 3 is a wavelength dispersive X ray fluorescence (WDXRF) spectrometer designed to deliver high precision elemental analysis across the entire petrochemical value chain. It supports upstream crude characterisation, midstream quality monitoring, and downstream refining, blending, and lubricant production. Its analytical performance, method compliance, smart sample handling, and low total cost of ownership make it a versatile tool for laboratories that must meet strict regulatory, operational, and economic demands.

Role of XRF in the Petrochemical Industry

Elemental analysis is critical in petrochemical operations because sulphur, chlorine, and trace metals directly affect product quality, environmental compliance, catalyst lifetime, and overall plant reliability. Sulphur content is tightly regulated in fuels, making accurate and repeatable determination essential for gasoline, diesel, jet fuel, and biodiesel. ASTM D2622—the globally recognised WDXRF method for total sulphur—applies to materials from crude oils to diesel, jet fuels and lubricant products. Its scope covers sulphur concentrations from 3 mg/kg upward to 4.6 wt%. In lubricants, elemental verification ensures additive packages meet formulation specifications. ASTM D6443 defines WDXRF procedures for determining Ca, Cl, Cu, Mg, P, S, and Zn in unused lubricating oils and additives, allowing manufacturers to check detergent, anti wear, and antioxidant components. Thus, XRF analysis enables compliance, quality consistency, catalyst protection, contamination screening, and operational efficiency across the sector.

System Architecture and Petrochemical Design

The S8 TIGER Series 3 is engineered to provide high sensitivity, excellent spectral resolution, and long term stability. It uses a high power X ray tube with up to 4 kW excitation power and a sequential goniometer equipped with optimised analysing

crystals and detectors that allow precise quantification for liquids - from Na to heavy elements – and even in challenging hydrocarbon matrices from Be upwards for solids. For petrochemical liquids, Bruker integrates features that ensure safe and reliable operation:

- EasyLoad™ with Camera AI automatically checks sample cup integrity and alignment, preventing mix ups and reducing rework.
- Spill and leak protection safeguards internal components and the tube window, which is essential when handling volatile gasoline, kerosene, or aromatic materials.
- Flexible vacuum/helium operation allows laboratories to use vacuum for less volatile samples and helium for volatile ones, reducing operating costs compared to always helium systems. Additionally, Bruker's SPECTRA.ELEMENTS and PETRO-QUANT software packages provide petrochemical specific method templates, quantitative algorithms, drift correction, QC charting, and LIMS ready data structures. Bruker documentation also lists applicable petrochemical standards such as ASTM D2622, ISO 14596, and ASTM D6443. Additionally, Bruker's SPECTRA.ELEMENTS and PETRO-QUANT software packages provide petrochemical-specific method templates, quantitative algorithms, drift correction, QC charting, and LIMS-ready data structures. Bruker documentation also lists applicable petrochemical standards such as ASTM D2622, ISO 14596, and ASTM D6443.

Analytical capabilities across upstream, midstream and downstream operations:

1. Upstream Exploration & Production In crude oils, condensates, and heavy residues, sulphur varies widely—from mg/kg traces to percent level concentrations. ASTM D2622 explicitly



Figure 1: S8 TIGER Series 3

supports crude oil measurement within its scope of 3 mg/kg to 4.6 wt% sulphur. In addition to sulphur, metals such as Ni, V, and Fe adversely affect downstream catalysts and equipment. The S8 TIGER Series 3 quantifies these elements reliably, helping producers classify feedstocks, predict processing behaviour, and reduce corrosion risks.

2. Midstream Transport & Storage Pipelines, terminals, and tank farms require rapid, non destructive quality checks. Sulphur remains the primary regulated parameter, while chlorine serves as a contamination indicator. The S8 TIGER Series 3 offers short analysis times—ASTM D2622 cites typical runtimes of 1–2 minutes per sample—making it suitable for custody transfer and batch release. Its calibration stability and automation functions benefit midstream labs that often operate with limited staff.



Figure 2: Innovative EasyLoad™ magazine accommodates various sample types in a single design.

3. Downstream Refining, Blending & Distribution Refineries must maintain strict sulphur limits in road fuels, aviation kerosene, and marine fuels. ASTM D2622 coverage of diesel, jet fuel, kerosene, naphtha, gasolines (including ethanol blends), and biodiesel ensures comprehensive applicability. Similarly, lubricant production depends on accurate measurement of additive related elements defined in ASTM D6443—including detergents (Ca, Mg), anti wear packages (Zn, P), antioxidants (various metals), and chlorine contamination. Risk Reduction and Compliance Assurance Using standards compliant methods like ASTM D2622 and ASTM D6443 reduces the risk of regulatory violations, off spec batches, and customer disputes. Reliable measurement of sulphur ensures legal compliance for fuels, while accurate additive element measurement protects lubricant performance claims. Early detection of sulphur, chlorine, nickel, vanadium, and other contaminants protects expensive refinery catalysts and minimises corrosion, lowering operational risks and avoiding unplanned shutdowns. The S8 TIGER Series 3 therefore supports both fuel compliance and high value lubricant/additive formulation.

Method Compliance

ASTM D2622 and ASTM D6443 ASTM D2622 – Sulfur in Petroleum Products (WDXRF) ASTM D2622 is the central regulatory method for sulphur. It applies to single phase liquids that are liquid at ambient temperature, liquefiable with moderate heat, or soluble in hydrocarbon solvents. Examples include diesel, jet fuel, kerosene, naphtha, residual oil, lubricating base oils, hydraulic oils, crude oil, gasoline, gasoline ethanol blends, and biodiesel. The standard’s analytical range extends from 3 mg/kg up to 4.6 wt% S, with precision and LOQ depending on instrument power, matrix, and laboratory practices. It warns

Table 1: ASTM D2622 performance check for ultra-low sulfur

Sample ID	S (PPM) 10 7.3-12.7 PPM	Difference up to 0.9 PPM
ASTM-D2622 L_QC 1	10.38	
ASTM-D2622 L_QC 2	10.89	0.51
ASTM-D2622 L_QC 3	10.91	0.02
ASTM-D2622 L_QC 4	10.53	-0.38
ASTM-D2622 L_QC 5	10.54	0.01
ASTM-D2622 L_QC 6	10.68	0.14
ASTM-D2622 L_QC 7	10.43	-0.25
ASTM-D2622 L_QC 8	10.56	0.13
ASTM-D2622 L_QC 9	11.05	0.49
ASTM-D2622 L_QC 10	10.75	-0.30
ASTM-D2622 L_QC 11	11.01	0.26
ASTM-D2622 L_QC 12	10.43	-0.58
ASTM-D2622 L_QC 13	10.44	0.01
Mean value (ppm)	10.67	
Abs Std. Dev. (ppm)	0.23	

Table 2: ASTM D6443 performance check for additives in lubricants

	Mg [%]	P [%]	S [%]	Cl [%]	Ca [%]	Cu [%]	Zn [%]
Average concentration [%]	0.0795	0.1007	0.2806	0.0251	0.1997	0.02	0.1096
Abs. standard deviation[%]	0.0008	0.0006	0.0016	0.0002	0.0011	0.0001	0.0005
Average difference between duplicates [%]	0.0011	0.0005	0.0018	0.0002	0.00123	0.0001	0.0005
Allowed difference between 2 duplicates, defined in ASTM D6443 [%]	0.007	0.0042	0.0074	0.0012	0.0031	0.0005	0.0026
QC sample concentration [%]	0.08	0.0999	0.2754	0.025	0.1999	0.02	0.1101
Allowed concentration range, defined in ASTM D6443 [%]	0.0565 - 0.1035	0.0808 - 0.1192	0.2232- 0.3268	0.0207 - 0.0293	0.1777 - 0.2223	0.0176 - 0.0224	0.0955 - 0.1245

that very volatile samples (e.g., high vapour pressure gasolines) may show increased variability due to selective loss of light components. The S8 TIGER Series 3 addresses these challenges through spectral resolution, optimised background correction, stable optics, and helium-mode operation for volatile fuels.

Liquid petrochemical samples are easily prepared using disposable cups with polymer films. The S8 TIGER’s Camera AI verifies proper assembly and prevents problematic samples from entering the measurement chamber. ASTM D2622 requires careful matrix matching or rigorous mathematical corrections when sample and calibration matrices differ significantly (such as varying C/H ratios or oxygenated fuels). The standard also allows dilution for samples above 4.6 wt% sulphur.

ASTM D6443 – Elements in Unused Lubricating Oils & Additives (WDXRF) ASTM D6443 defines WDXRF analysis for Ca, Cl, Cu, Mg, P, S, and Zn in unused lubricating oils and additive packages. It accounts for matrix effects using mathematical correction procedures. Concentration ranges depend on the method’s tables, and samples exceeding these ranges may be diluted. LOD and LOQ vary by laboratory precision. This method is essential for verifying additive packages (detergents, anti wear agents, antioxidants), ensuring product integrity, and identifying contamination (e.g., chlorine).

ASTM D6443 likewise depends on matrix corrections to accommodate different lubricant base oils and additive chemistries.

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Throughput, Automation and Data Integrity

High throughput is achieved through short counting times, automated sample changers, and intelligent software. Because XRF is non destructive, no chemicals or digestion steps are needed, allowing rapid turnaround. Connectivity with LIMS ensures secure data transfer, while audit trails and electronic records support ISO certified laboratories. The system’s method lock down prevents unauthorised changes, and all metadata (sample ID, operator, method version, instrument status) is automatically logged.

Total Cost of Ownership (TCO)

Benefits The S8 TIGER Series 3 offers multiple economic advantages:

- Lower helium consumption because many samples can be measured under vacuum; helium is reserved for volatile fuels.

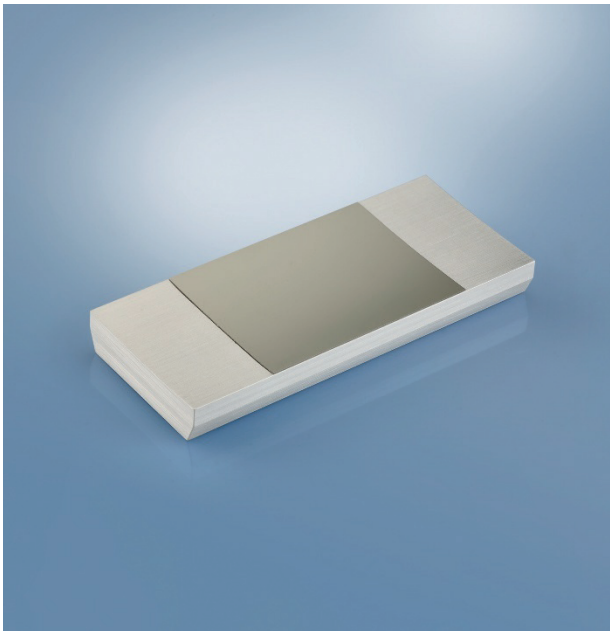


Figure 3: Curved XS-Ge-C crystal with focusing optics, ideal for traces in petrochemicals.

- No reagents, no waste disposal, and fewer consumables compared to wet chemistry methods.
- Long calibration intervals due to optical stability and drift correction.
- Reduced re runs thanks to precise sample checking and stable method performance.
- High uptime enabled by spill protection and durable components.

These benefits combine to produce a favourable long term cost profile and improved productivity for high volume petrochemical laboratories.

Conclusion

The S8 TIGER Series 3 is a versatile, high precision WDXRF spectrometer that satisfies the demanding analytical needs of petrochemical laboratories. It supports the full spectrum of upstream, midstream, and downstream samples while providing validated compliance with key methods such as ASTM D2622 for sulphur and ASTM D6443 for essential lubricant elements. Its rugged petrochemical design, automation features, software suite, and strong TCO advantages make it a reliable and cost effective cornerstone for quality control, process optimisation, and regulatory compliance.

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