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Het Colloquium Spectroscopicum Internationale XXIV omvatte 61 voordrachten op uitnodiging in 3 parallelseries en ongeveer 340 posters, gegroepeerd in 40 onderwerpen. Er waren 891 deelnemers uit 42 landen. Aan de instrumentententoonstelling namen 43 firma's deel.

In het navolgende wordt verslag gedaan over een aantal voordrachten en posters. De titels van alle voordrachten en posters zijn in de bijlage vermeld.

Isotoopeffecten van door enzymen gekatalyseerde reacties veroorzaken verschuivingen in de isotopenverdeling van H, C, N en S in organische moleculen. Uit deze verschuivingen uitgedrukt in " δ -waarden", bepaald met MS of NMR, kunnen conclusies getrokken worden omtrent aard en herkomst van voedingsmiddelen. Er kan op deze wijze o.a. onderscheid gedetecteerd worden in klimatologische omstandigheden. Andere toepassingen van deze "natuurlijke labelling" zijn: aantonen van vervalsingen van wijn, vruchtesappen, honing, toevoegingen van water aan dranken, onderscheid tussen biogene of synthetische vanilline, menthol of azijnzuur, onderscheid tussen riet- en bietsuiker (Schmidt).

Na een eenvoudige monstervoorbereiding (alleen malen en tabletteren) is röntgenfluorescentie een handige techniek voor het bepalen van een reeks elementen in tal van matrices: bodem, stof, meststoffen, zuiveringsslib, afvalwater, voedingsmiddelen en veevoeders, vruchten (Rethfield).

Demtröder besprak high-resolution moleculaire UV en IR spectroscopie met behulp van lasers van moleculen in de gasfase. Hiermee kunnen ondubbelzinnige UV spectra verkregen worden met de fijnstructuur van de electronenovergangen. Ten opzichte van "normale" UV detectie zou de gevoeligheidswinst bovendien een factor 10^6 bedragen; in het IR gebied, met gebruikmaking van een IR laser en een bolometer, gekoeld met vloeibare He, een factor 10^3 . Apparatuur voor een en ander is voorlopig nog niet commercieel verkrijgbaar.

Er zijn recente ontwikkelingen in de bestudering van polymorfie van farmaceutische preparaten met spectroscopische technieken (Röntgen-diffractie en IR spectroscopie). Dit is van grote praktische betekenis in verband met verschillen in eigenschappen van de verschillende modificaties. Een en ander werd door Hegedüs gedemonstreerd aan de hand van prednisolon (3 modificaties met verschillende oplosselheden), mebendazol (verschillende bioactiviteit) en cimetidine (verschillende technologische parameters bij de bereiding).

Grasselli besprak toepassingen van FTIR en Raman in industriële laboratoria, onder andere onderzoek van ongerechtigheden op het oppervlak van plastic flessen, het opnemen van alkanen onder druk en onderzoek aan krukassen met diffuse reflectie. Ze was erg trots op een fraai spectrum van 500 ng polystyreen en zag grote mogelijkheden voor Raman, o.a. bij de analyse van micromonsters drugs (heroïne).

Een on-line combinatie GC-FTIR-FTMS geeft informatie over functionele groepen (IR), fragmentatie (EI-MS) en moleculair gewicht (CI-MS). Nodig: μg hoeveelheden (Wilkins).

Met time-resolved FTIR na matrix isolatie kunnen spectra van onstabiele moleculen worden opgenomen (Turnec). Hoewel de theoretische detectiegrens van IR in de orde van 1 ng ligt, wordt IR spectroscopie zelden toegepast voor hoeveelheden beneden 10 μg . Matrix isolatie van b.v. HPLC fracties biedt de mogelijkheid de praktisch toegankelijke detectiegrens omlaag te brengen (Bode).

Interessant vond ik de poster van Mrs Zięba over forensisch onderzoek van smeerolies m.b.v. infraroodspectroscopie, nl. voor het identificeren van verdachten bij auto-ongevallen, waarbij een betrouwbaarheid van 1% veelal voldoende geacht werd.

Met behulp van informatietheorie werd door Flórián inzicht verkregen in de betrouwbaarheid van spectrochemische meercomponent-methoden, terwijl Doerffel met behulp van correlatiefuncties de signaal-ruis verhouding wist te verhogen.

Mantsch besprak biologische toepassingen van infraroodspectroscopie. Met FTIR is het thans mogelijk biologische monsters in water te bestuderen: identificatie en differentiatie van pathogene bacteria, *in situ* onderzoek van bloed, bacteriën behandeld met alkohol, enz.

Recente ontwikkelingen hebben de toepassing van NMR bij onderzoek van enzymen mogelijk gemaakt, zowel *in vitro* als *in vivo*. Volledige structuurheldering is thans mogelijk. Het NMR onderzoek van intacte systemen is een multimiljoen dollar bussiness (Campbell).

Wat de atoomspectroscopie betreft, werd er uiteraard veel aandacht besteed aan ICP, maar ook aan grafietoventechnieken. Sturgeon wees er op dat deze laatste techniek nog moeilijk theoretisch te onderbouwen is, vooral omdat er geen evenwichtstoestand optreedt, Chakrabarti daarentegen presenteerde een thermodynamisch evenwichtsmodel. Bij de posters waren er talrijke toepassingen.

Er was relatief weinig op het gebied van massaspectrometrie, vermoedelijk vanwege het vrijwel gelijktijdige gespecialiseerde massaspectrometercongres in Swansea.



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