MERCK
Research Laboratories

Industrial NMR Facility Design 101

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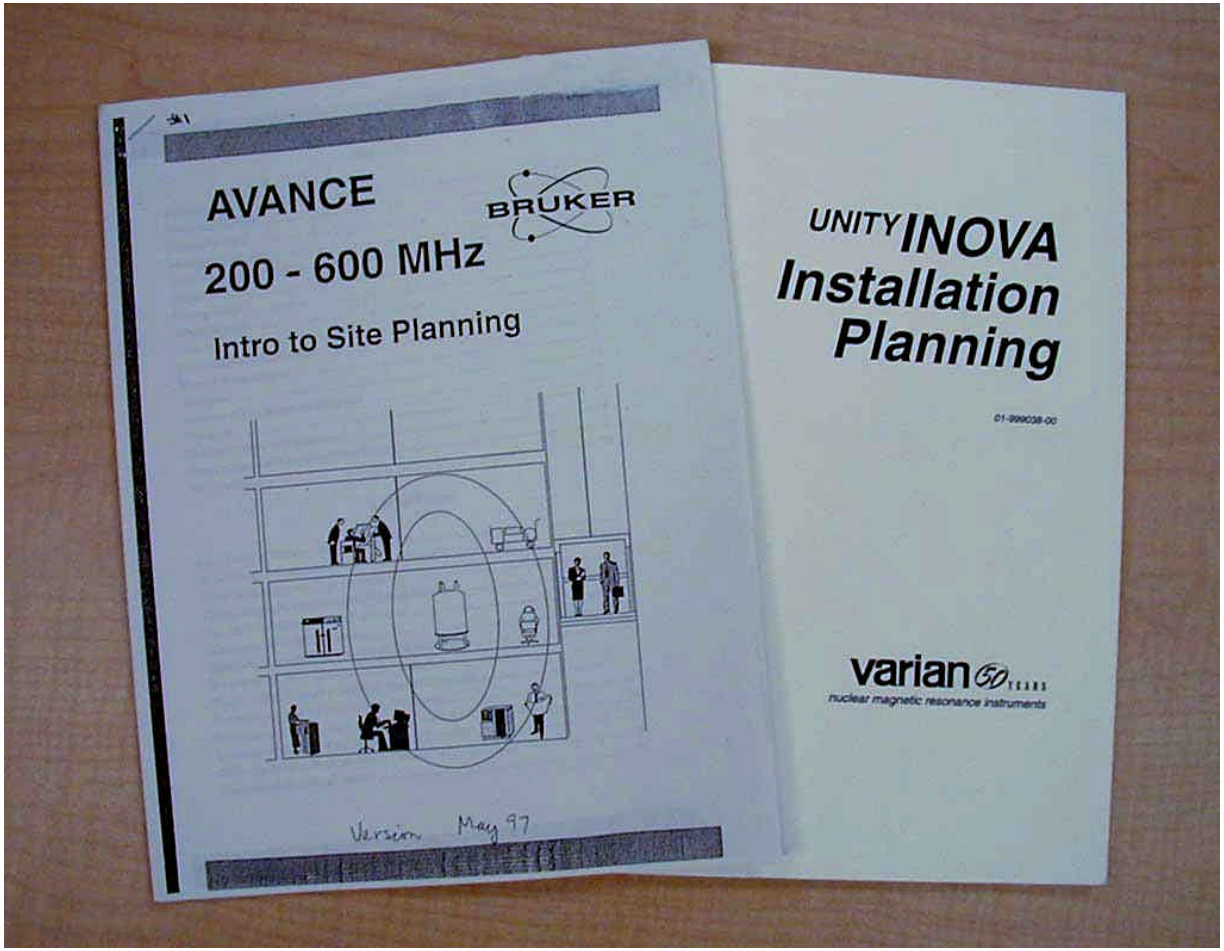
Process

Guiding Principles

- Optimize accessibility
  - Location, workflow, ergonomics, e-access, cryo-maintenance
- Optimize instrument environment
  - Environmental room, 5 G line, RFI, metal, power
- Consider safety
  - 5 G line, monitor oxygen, air exchanges
- Consider intended use
  - Open-access, research, automation
- Anticipate the future
  - Higher fields / larger magnets, accessories

Required Reading



Our Objectives

- "Open-access"

  Used by bench chemists in their daily operations to assess structure and purity of synthesized samples. They need quick access.

  - Mostly proton 1D's at 25 C
  - Some instruments are automated
  - Mix of 300's, 400's, and 500's

- "Research"

  Used by NMR staff for all non-routine NMR studies:

  - Structure determination of unknowns
  - Conformational analyses
  - Ligand-receptor interaction studies
  - Analyses for purity and/or isomer composition

  - Wide variety of experiments and conditions
  - Greatest need for optimal stability
  - 600's

Location, Location, Location

- Where are the clients?
- Clear delivery path for instrument
  - Corridor and door dimensions vs.. crate sizes
    include allowances for turning
  - Elevator dimensions and capacity
- Floor loading

Location, Location, Location (cont.)

- Minimize magnetic perturbations from external sources
  - Include vertical dimension
    floor to floor spacing in older US labs 10-12'
    floor to floor spacing in many newer US labs is 16'
  - Absolutely no structural metal within 25 G shell
  - Ideally no structural metal in 5G
  - No ferromagnetic cabinets, desks, doors, refrigerators, carts, cylinders, piping, ductwork, magnetic stirrers, … in 5 G

    fully restrict ≥5 G space in designs
  - No pallet movers, large cylinders, delivery carts in 2G

    exclude material handling corridors from 2 G shell
  - No forklifts, autos, elevators, in 1 G
  - No trains, large trucks in 0.1 G
  - Sector mass spectrometers - 100'?

< frame >

Location, Location, Location (cont.)

Frame

Return

Location, Location, Location (cont.)

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Location, Location, Location (cont.)

- Minimize electromagnetic interference from external sources
  - Affects vary greatly

    one should avoid these sources when possible:
    - AC
      - Electric motors, transformers (some UPSs, line conditioners), power lines / feeds, electric trains, …
    - RFI
      - Broadcast transmitters, other NMR spectrometers at matching frequencies, ICP instruments (27, 40 MHz), welders, unshielded electronics (e.g. computers, bad ethernet connections), two-way radios, wireless ethernet

  - Mitigating circumstances
    - Large steel frame buildings
    - Below grade

Location, Location, Location (cont.)

- Consider perturbations that the NMR may cause externally
  - CRT's work best outside the 2G shell
  - Magnetic media (disks and tapes) should be kept outside the 10 G shell
  - Personal safety (pacemakers) - 5 G shell
  - Other NMR spectrometers
  - Alarm systems that use magnetic test switches
  - Any other sensitive magnetic or electronic instrumentation

Location, Location, Location (cont.)

- Minimize vibrations (vertical and horizontal)
  - Highest field instruments on grade
  - Floating slab?
  - Steel building design
    - Consult with structural engineer
  - Secure magnet legs and brace horizontally

- Accessibility for cryo-maintenance
  - Delivery path
    - Corridors and doors 40-48”
    - Not over cables
    - Does not perturb other spectrometers
  - Quick egress possible for service person

Magnet Room

- Research instruments
  - Greatest need for stability
    - Long-term experiments
    - S/N often limited
    - Prevent perturbations from unanticipated “guests”

    controlled environment for magnet and console is critical
    i.e. a fully enclosed environmental room

- Open-access instruments
  - High turnover
  - 24 x 7 access needed by users
  - Some long-term experiments

    Integrate operator environment into same space as magnet and console

Magnet Room (cont.)

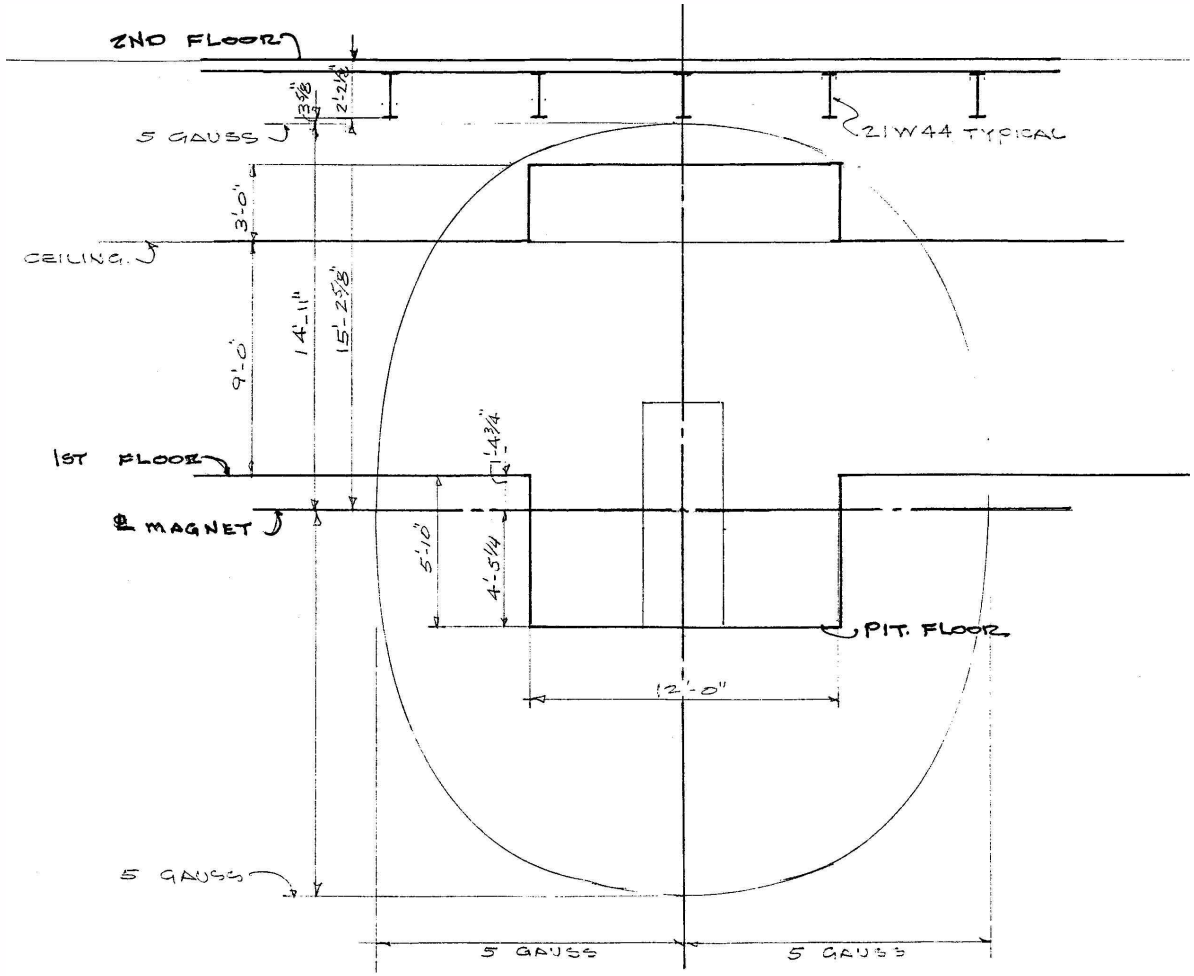
Magnet Room (cont.)

- Full containment of 5 G shell
  - Vertical as well as horizontal <600 5G>
  - Use pit to keep 5 G from upper floor <600 pit>
    - 12’ wide, 5’ 10” deep
    - Platform access to magnet
    - Safety railing
    - Lighting
    - Drain
- Workflow / ergonomics <600 draw>

Magnet Room (cont.)

600 5G

Return



Magnet Room (cont.)

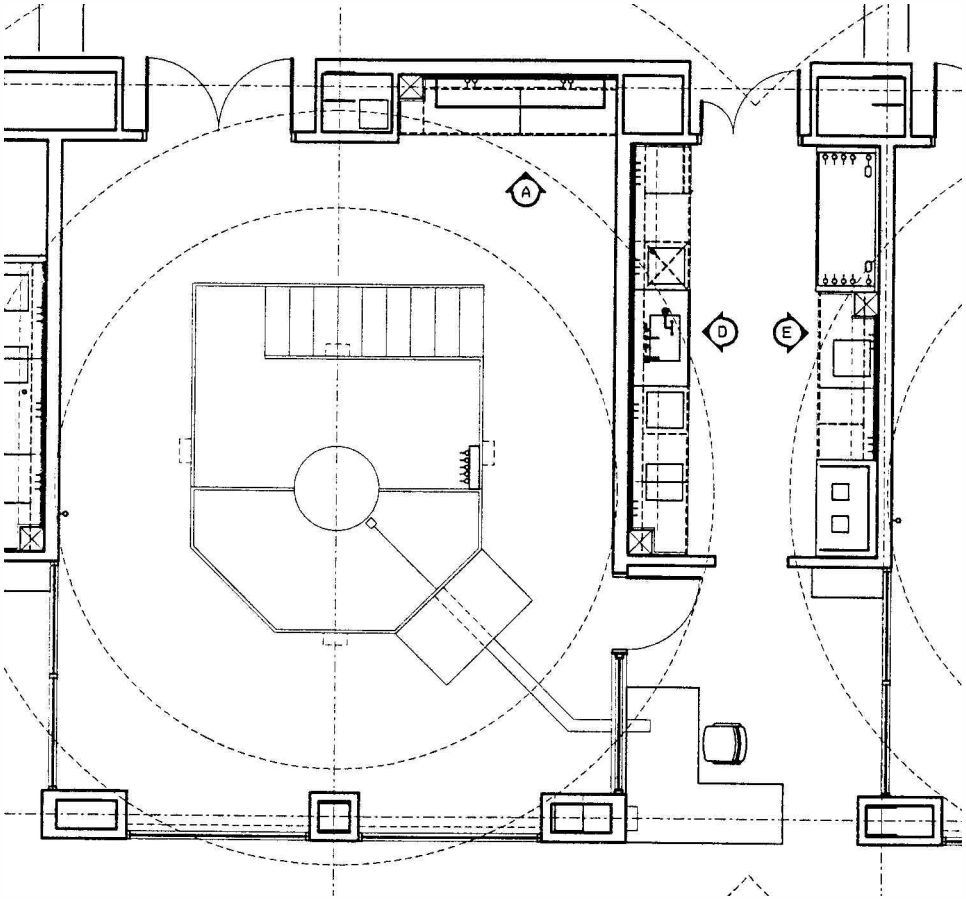
600 pit

Return

Magnet Room (cont.)

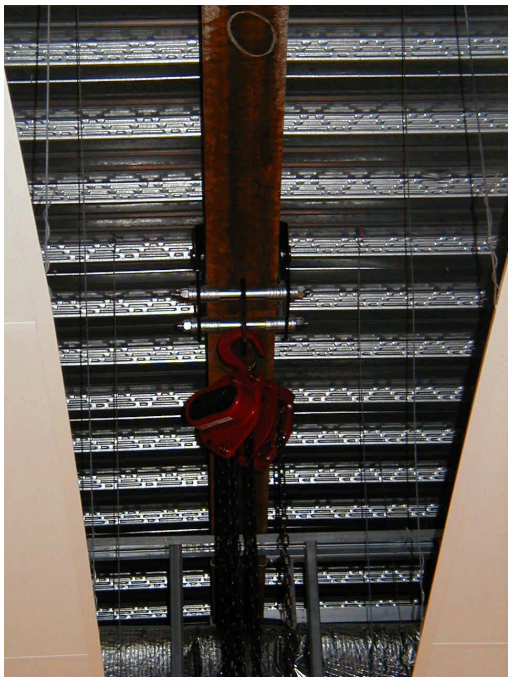
600j

Return



Magnet Room (cont.)

- Installation considerations
  - Magnet
    - Path for magnet
    - Hoist



Magnet Room (cont.)

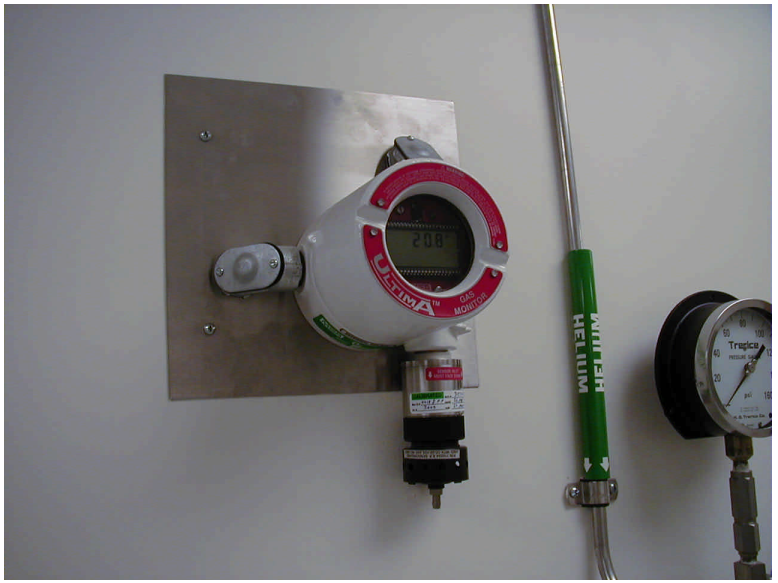
- HVAC
  - Objective is 70 +/- 1˚ F, 40 / 50 +/- 10% RH, neutral pressure, constant volume, laminar flow
  - Two operational modes - normal and purge
  - Exhaust is from low vents when in normal mode
  - Exhaust is from ceiling pocket when in purge mode
  - Mode is switched automatically by oxygen monitoring system
  - Manual mode switch is possible
  - 12 air changes per hour, 100% outside make-up air
  - Small return vent in ceiling pocket
  - Aluminum ductwork
  - No ducts directly above magnet
  - No occupancy temperature set-backs
  - No variable external heat sources (outside windows)

Magnet Room (cont.)

- Oxygen monitoring
  - Tied to HVAC
  - Switches for manual purge inside and outside of magnet room
  - Power supplied by UPS
  - Levels
    - 19.5 % - Warning:
      - sounds local alarm
      - warning signal sent to command center
    - 16.0 % - Danger:
      - automatic purge
      - danger signal sent to command center
    - 20.0 % - All clear:
      - purge is interlocked so that it cannot be shut off until oxygen level is at or above this point
  - Requires periodic calibration and sensor replacement
  - Subject to atmospheric pressure changes

Magnet Room (cont.)

Oxygen monitoring



Magnet Room (cont.)

- Electrical
  - Dedicated UPS for each instrument
  - Breaker panel in magnet room
  - UPSs put into a dedicated, air conditioned room
  - Monitored by remote status panel and web link
  - 240 / 120 v
  - Transformer for Varian console (240 -> 220 v)
  - Every device except laser printer powered by UPS
  - UPS sized to 50% load

Magnet Room (cont.)

Electrical

Magnet Room (cont.)

- Other
  - Ceiling pocket
  - Mylar faced acoustic ceiling tiles
  - Static dissipative, vinyl composite flooring
  - Bi-level lighting
  - Reflective lighting in pits
  - Emergency lighting
  - No lights directly above magnet
  - No sprinklers directly above magnet
  - Heat detectors instead of smoke detectors
  - Wood cabinets
  - Non-ferromagnetic doors
  - Safety railing around pits
  - Gravity drain with check valve in pit
  - 100 PSI nitrogen to manifold
  - Helium gas piped from an external tank

Ancillary Spaces

- Control Station
  - Outside magnet room for “research” instruments
  - Inside magnet room for “open-access” instruments
  - Power supplied by instrument UPS
  - Remote status panel for UPS
  - Network connection

Ancillary Spaces (cont.)

- Wet labs
  - Close proximity to “research” instruments
  - Not in “open-access” areas
  - Ventilate the same as a chemistry lab
- Computer room
  - Secure room for servers
    - Fiber hub
    - Data server
    - Reservation system server
    - Other servers
    - Space to configure workstations
- UPS room
  - Air conditioned
  - Ethernet connections

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