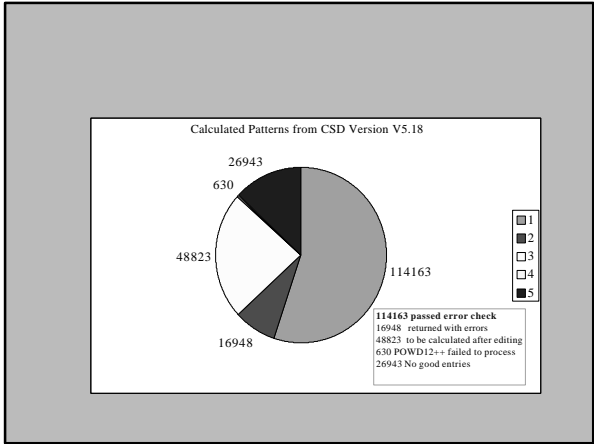


# Calculated Patterns



Calculated Patterns from ICSD

Handling the updates  
Completed ICSD update 9801U

Checking the pattern cross-referencing (Additional Pattern)

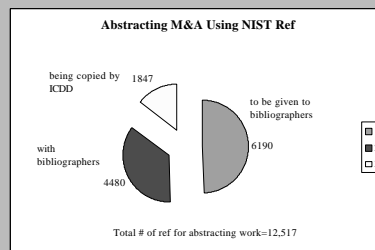
Identifying and correcting the existing problematic patterns

- Problematic TF
1. Beta (i,j) + U(i,j)
  2. B(i,j) + Beta(i,j)
  3. U(i,j) + B
  4. Beta (i,j) +U(i,j) + B
  5. B(i,j) +U
  6. Beta (i,j)+U
  7. Beta (i,j)+U(i,j) + U
  8. B + U
  9. U(i,j) +B + U
  10. U(i,j)+missing TF
  11. U(i,j) + B + missing TF
  12. U+ missing TF
  13. Beta(i,j)+U+ missing TF
  14. U(i,j)+U+missing TF
  15. B+U+missing TF

1251 patterns were recalculated to fix error due to mixed TF

Modified the program ICSD\_TO\_PWD to handle mixed TF

### ICDD-NIST Joint Project on M&A



Developing the program to write NIST data in \*.pwd format