Calculated Patterns

Calculated Patterns from CSD Version V5.16

114163 passed error check
16948 returned with errors
48823 to be calculated after editing
630 POWD12++ failed to process
26943 No good entries

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. \text{Beta}(i,j) + \text{U}(i,j)
2. \text{U}(i,j) + \text{Beta}(i,j)
3. \text{U}(i,j)
4. \text{Beta}(i,j) + \text{B}(i,j)
5. \text{Beta}(i,j) + \text{U}(i,j)
6. \text{Beta}(i,j) + \text{B}
7. \text{Beta}(i,j) + \text{U}(i,j) + \text{B}
8. \text{B} + \text{U}
9. \text{U}(i,j) + \text{B} + \text{U}
10. \text{U}(i,j) + \text{missing TF}
11. \text{U}(i,j) + \text{B} + \text{missing TF}
12. \text{U} + \text{missing TF}
13. \text{Beta}(i,j) + \text{U} + \text{missing TF}
14. \text{U}(i,j) + \text{U} + \text{missing TF}
15. \text{B} + \text{U} + \text{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