

## Supplementary Material

### *FraGen*: a computer program for real space structure solution of extended inorganic frameworks

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List of output files:

\*.out: main output files produced by *FraGen*; all input keywords, parameters, restraints, and constraints are listed, as well as the atomic coordinates of each generated structure model;

\*.csq: coordination sequences of each generated structure model are stored in these files;

\*.lst: various cost terms of each generated model are stored in these files;

\*.xls: the “Unique” sheet lists the cost, the rank of the cost ordered from lowest to highest, the frequency of occurrence, and the rank of frequency ordered from highest to lowest for each unique models; the “All” sheet lists the costs of all generated models;

cj19a.\*: the CJ-19 example without knowing the exact coordination of each atom;

cj19b.\*: the CJ-19 example using the coordination of each atom as additional input;

zsm18.\*: the ZSM-18 example;

ssz51a.\*: the SSZ-51 example without early exit;

ssz51b.\*: the SSZ-51 example with early exit;

ssz51c.\*: the SSZ-51 example without early exit; three reflection intensities are introduced;

ssz51d.\*: the SSZ-51 example with early exit; three reflection intensities are introduced;

ssz51e.\*: the SSZ-51 example without early exit; a structure envelope is introduced;

ssz51f.\*: the SSZ-51 example with early exit; a structure envelope is introduced.