Molecular simulated annealing algorithm for inverting x-ray or electron scattering data to nuclear coordinates

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Abstract

1

1.1 Outline of code

The SA function reads in the following inputs:

1. starting_xyz # The starting xyz coordinates of the molecule
2. displacements # The molecular displacement unit vectors (e.g. from a normal modes calculation)
3. target_array # The target function array, e.g. for time-resolved x-ray scattering, it would be a $N_q \times N_t$ sized array
4. qvector # q-vector (Å^{-1})
5.

```
import numpy
```