sb_ncbr_partial_atomic_charges

'Partial atomic charges for each atom of the structure'

type_id [PK] [FK] [code]

'Type of the charge calculation method'

atom_id [PK] [FK] [int]

'ID of an atom'

charge [float] [e] (-5.0..5.0)

'The value of partial atomic charge'

type_id → id

atom_id → id

sb_ncbr_partial_atomic_charges_meta

'Information about the type of charges'

id [PK] [code]

'Unique ID of a charge set'

method [text]

'Charge calculation method'

type [code] {QM | empirical | other}

'Type of the charge calculation method'

atom_site