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METHOD Quickstep

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MULTIPLICITY 3
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REL__CUTOFF 40
NGRIDS 5
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SCF__GUESS RESTART
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EPS__SCF 1.0E-7
MAX__SCF 10
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PRECONDITIONER FULL__ALL
MINIMIZER DIIS
N__DIIS 7
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&VDW__POTENTIAL
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&SUBSYS
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PERIODIC XYZ

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&COORD

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