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Autore	McBride, A. C.
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Altri autori (Persone)	Roach, G. F.
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2. Record Nr.	UNINA9910346720003321
Autore	Bachorz Rafal A
Titolo	Implementation and application of the explicitly correlated coupled-cluster method in Turbomole
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Sommario/riassunto	In this thesis the implementation of the explicitly correlated coupled-cluster singles-and-doubles model is presented. This tool is capable of efficiently calculating CCSD energies at the basis set limit with relatively small orbital basis sets. The implementation supports RHF, UHF and ROHF reference wave functions. The usefulness of the developed tool is illustrated with selected chemical applications.