

**Neutral and Cationic Zirconium Alkyl and Hydride
Complexes Supported by a Macrocycle Based on Cyclen:
Synthesis, Characterization and Reactivity**

Von der Fakultät für Mathematik, Informatik und Naturwissenschaften der
RWTH Aachen University
zur Erlangung des akademischen Grades eines
Doktors der Naturwissenschaften genehmigte Dissertation

vorgelegt von

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Berichte aus der Chemie

Heiko Kulinna

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Prof. Dr. Jun Okuda

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List of Abbreviations

br	broad
COE	cyclooctene
COSY	correlated spectroscopy
Cp	cyclopentadienyl (C ₅ H ₅ ⁻)
Cp [*]	pentamethylcyclopentadienyl (C ₅ Me ₅ ⁻)
d	doublet
DCM	dichloromethane
DFT	density functional theory
DME	1,2-dimethoxyethane
dmpe	1,2-bis(dimethylphosphino)ethane
DO3A	1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid with an alkyl group
DOTA	1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid
equiv	equivalent
HMPA	hexamethylphosphoramide
HSQC	heteronuclear multiple bond correlation
<i>i</i>	<i>iso-</i>
<i>J</i>	coupling constant
m	multiplet
<i>n</i>	<i>normal-</i>
NMR	nuclear magnetic resonance
Ph	phenyl
ppm	parts per million
q	quartet
quint	quintet
<i>r</i> (H)	radius of the macrocyclic hole
s	singlet
time (s)	time in seconds
t	triplet
<i>t</i>	<i>tert.-</i>
TACN	triazacyclononane

(Me ₂ TACD)H ₂	1,7-dimethyl-1,4,7,10-tetraazacyclododecane
(Me ₃ TACD)H	1,4,7-trimethyl-1,4,7,10-tetraazacyclododecane
Me ₃ TAMC ₂	2,5,8-trimethyl-2,5,8-triaza[9]metacyclophane
Me ₃ TAMC ₃	2,6,10-trimethyl-2,6,10-triaza[11]metacyclophane
TMEDA	tetramethylethylenediamine
THF	tetrahydrofuran
TMP	2,2,6,6-tetramethylpiperidine
TREN	tris(2-aminoethyl)amine
VE	valence electron(s)

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