Computational and experimental studies of reactive intermediates in glycosylation reactions

Remmerswaal, W.A.

Computational and Experimental Studies of Reactive Intermediates in Glycosylation Reactions

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Promotor	Prof.dr. J. D. C. Codée
Co-promotor	Dr. T. Hansen
Promotiecommissie:	Prof. dr. M. Ubbink
	Dr. D. V. Filippov
	Prof. dr. H. S. Overkleeft
	Prof. dr. Célia Fonseca Guerra, VU Amsterdam
	Prof. dr. K. A. Woerpel, New York University

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Ac	acetyl
All	allyl
ADF	Amsterdam density functional
APT	attached proton test
aq.	aqueous
Ar	aryl
Arom	aromatic
ASD	activation strain diagram
ASM	activation strain model
AMS	Amsterdam modelling suite
B	boat
BAIB	(diacetoxyiodo)benzene
BAr_4^F	tetrakis[3,5-bis(trifluoromethyl)phenyl]-borate
Bis	bisected
Bn	benzyl
bs	broad singlet
BSP	benzenesulfinyl piperidine
Bu	butyl
Bz	benzoyl
C	chair
cal	calorie
calcd	calculated
cat.	Catalytic
CBS	complete basis set
CEL	conformational energy landscape
CEST	chemical exchange saturation transfer
CG	consistent geometry
CID	collision induced dissociation
CIP	contact ion pair
COSY	correlation spectroscopy
Cq	quaternary carbon atom
CSA	camphor-10-sulfonic acid
δ	chemical shift (ppm)
d	doublet
DCM	dichloromethane
dd	double doublet
ddd	doublet of double doublets
dddd	double doublet of double doublets
ddt	doublet of double triplets
DFE	difluorethanol
DFT	density function theory
Diox	dioxolenium
DMAP	4-dimethylaminopyridine
DMF	dimethylformamide
DMNPA	2,2-dimethyl-2-(*ortho*-nitrophenyl) DMNPAA 2,2-dimethyl-2-(*ortho*-nitrophenyl) anhydride
DMSO	dimethylsulfoxide
dq	double quartet
dt	double
dtd	doublet of triple doublets
DTBMP	2,6-di-*tert*-butyl-4-methylpyridine
DTBS	di-*tert*-butylsilylidene
E	electronic energy or envelope
E_{int}	interaction energy
E_{Pauli}	Pauli repulsion energy
E_{oi}	orbital interaction energy
EDA	energy decomposition analysis
EDC	1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide
Eq.	equation
equiv	molar equivalent
ESI	electrospray ionization
est.	estimate
Et	ethyl
E-X	electrophilic activator system
EXSY	exchange NMR spectroscopy
FELIX	free electron laser for infrared experiments
FMO	frontier molecular orbital
FT	Fourier transform
gg	gauche-gauche
gt	gauche-trans
G	Gibbs free energy
GATED	proton decoupling applied only during relaxation
GalA	galacturonic acid
GlcA	glucuronic acid
Glu	glucose
h	hour(s)
H	half-chair or enthalpy
HAD	hydrogen bond mediated aglycone delivery
HFIP	hexafluoro-*iso*-propanol
HMBC	heteronuclear multiple-bond correlation spectroscopy
HOMO	highest occupied molecular orbital
HMPA	hexamethylphosphoric triamide
HPLC	high performance liquid chromatography
HRMS	high-resolution mass spectroscopy
HSQC	heteronuclear single quantum Coherence
i-Nico	*iso*-nicotinate
INT	intermediate
IR	infrared
IRIS	infrared ion spectroscopy
IRC	intrinsic reaction coordinate
IRMPD	infrared multi-photon dissociation
J	coupling constant
K	Kelvin
KIE	kinetic isotope effect
KHMDS	potassium bis(trimethylsilyl)amide
KS-MO	Kohn-Sham molecular orbital theory
LC-MS	liquid chromatography mass spectrometry
LG	leaving group
LTQ	linear trap quadropole
LUMO	lowest unoccupied molecular orbital
LRP	long-range participation
M	molar

[M]	metal leaving group
m	multiplet
MS^2	tandem-mass spectrometric
m/z	mass over charge ratio
min	minute(s)
Man	mannose
ManA	mannuronic acid
m-CPBA	meta-chloroperoxybenzoic acid
Me	methyl
MFE	monofluoroethanol
MM	molecular mechanics
MMFF	Merck molecular force field
MP	Møller-Plesset perturbation theory
MPF	methyl(phenyl)formamide
NAP	2-methylnaphthyl
NBS	*N*-bromosuccinimide
NFM	N-formylmorpholine
Nico	nicotinate
NGP	neighboring group participation
NMR	nuclear magnetic resonance
NOESY	nuclear Overhauser effect spectroscopy
Nu	nucleophile
Nuc	nucleophile
p	*para*
P	protection group or product
PC	product complex
PCM	polarizable continuum model
PES	potential energy surface
PG	protection group
Ph	phenyl
Pico	picoloyl ester
PM	parametric method
PMB	4-methoxybenzyl
PNBz	4-nitrobenzoyl
PMBz	4-methoxybenzoyl
PMP	4-methoxyphenyl
ppm	parts per million
q	quartet
qd	quartet of doublets
QH	quasi-harmonic
QM	quantum mechanics
R	reactant
RC	reaction complex
R*f*	retention factor
RRV	relative reactivity value
RT	room temperature
s	singlet
S	skew boat
sat.	saturated
SCF	self-consistent field
S_E2'	bimolecular electrophilic substitution
SMILES	simplified molecular input line entry system
S_N1	uni-molecular nucleophilic substitution
S_N2	bi-molecular nucleophilic substitution
S_N2-b	backside bi-molecular nucleophilic substitution
S_N2-f	frontside bi-molecular nucleophilic substitution
S_Ni	internal nucleophilic substitution
SPh	thiophenyl
SSIP	solvent-separated ion pair
t	triplet
t	*tert*
T	twist
T	temperature
Ts	tosyl
TalA	taluronic acid
TBAF	tetrabutylammonium fluoride
TBS	*tert*-butyldimethylsilyl
TES	triethylsilyl
TEMPO	(2,2,6,6-tetramethylpiperidin-1-yl)oxyl
TFA	trifluoroacetic acid
TFE	trifluoroethanol
Tf	triflyl; trifluoromethanesulfonyl
THF	tetrahydrofuran
TLC	thin layer chromatography
TMS	trimethylsilyl
Tol	tolyl; 4-methylphenyl
TOCSY	total correlation spectroscopy
TS	transition state
td	triple doublet
tt	triple triplet
TTBP	2,4,6-tri-*tert*-butylpyrimidine
UV	ultraviolet
V_{elstat}	electrostatic interaction energy
VT	variable temperature
ZPE	zero-point energy