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Computational and experimental studies of reactive intermediates in glycosylation reactions

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Computational and Experimental Studies of Reactive Intermediates in Glycosylation Reactions

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List of abbreviations |

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

[M]	metal leaving group	SSIP	solvent-separated ion pair
m	multiplet	t	triplet
MS ²	tandem-mass spectrometric	<i>t</i>	<i>tert</i>
m/z	mass over charge ratio	<i>T</i>	twist
min	minute(s)	T	temperature
Man	mannose	Ts	tosyl
ManA	mannuronic acid	TaIA	taluronic acid
<i>m</i> -CPBA	meta-chloroperoxybenzoic acid	TBAF	tetrabutylammonium fluoride
Me	methyl	TBS	<i>tert</i> -butyldimethylsilyl
MFE	monofluoroethanol	TES	triethylsilyl
MM	molecular mechanics	TEMPO	(2,2,6,6-tetramethylpiperidin-1-yl)oxyl
MMFF	Merck molecular force field	TFA	trifluoroacetic acid
MP	Møller-Plesset perturbation theory	TFE	trifluoroethanol
MPF	methyl(phenyl)formamide	Tf	triflyl; trifluoromethanesulfonyl
NAP	2-methylnaphthyl	THF	tetrahydrofuran
NBS	<i>N</i> -bromosuccinimide	TLC	thin layer chromatography
NFM	<i>N</i> -formylmorpholine	TMS	trimethylsilyl
Nico	nicotinate	Tol	tolyl; 4-methylphenyl
NGP	neighboring group participation	TOCSY	total correlation spectroscopy
NMR	nuclear magnetic resonance	TS	transition state
NOESY	nuclear Overhauser effect spectroscopy	td	triple doublet
Nu	nucleophile	tt	triple triplet
Nuc	nucleophile	TTBP	2,4,6-tri- <i>tert</i> -butylpyrimidine
<i>p</i>	<i>para</i>	UV	ultraviolet
P	protection group or product	<i>V</i> _{elstat}	electrostatic interaction energy
PC	product complex	VT	variable temperature
PCM	polarizable continuum model	ZPE	zero-point energy
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		
<i>R</i> _f	retention factor		
RRV	relative reactivity value		
RT	room temperature		
s	singlet		
S	skew boat		
sat.	saturated		
SCF	self-consistent field		
S _E 2'	bimolecular electrophilic substitution		
SMILES	simplified molecular input line entry system		
S _N 1	uni-molecular nucleophilic substitution		
S _N 2	bi-molecular nucleophilic substitution		
S _N 2-b	backside bi-molecular nucleophilic substitution		
S _N 2-f	frontside bi-molecular nucleophilic substitution		
S _N i	internal nucleophilic substitution		
SPh	thiophenyl		

