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SUPPORTING INFORMATION

Title: Fluorinated Furan-2(5*H*)-ones: Reactivity and Stereoselectivity in Diels–Alder Reactions
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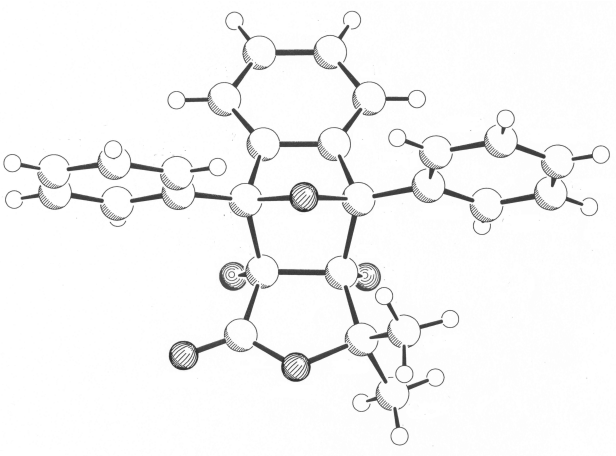
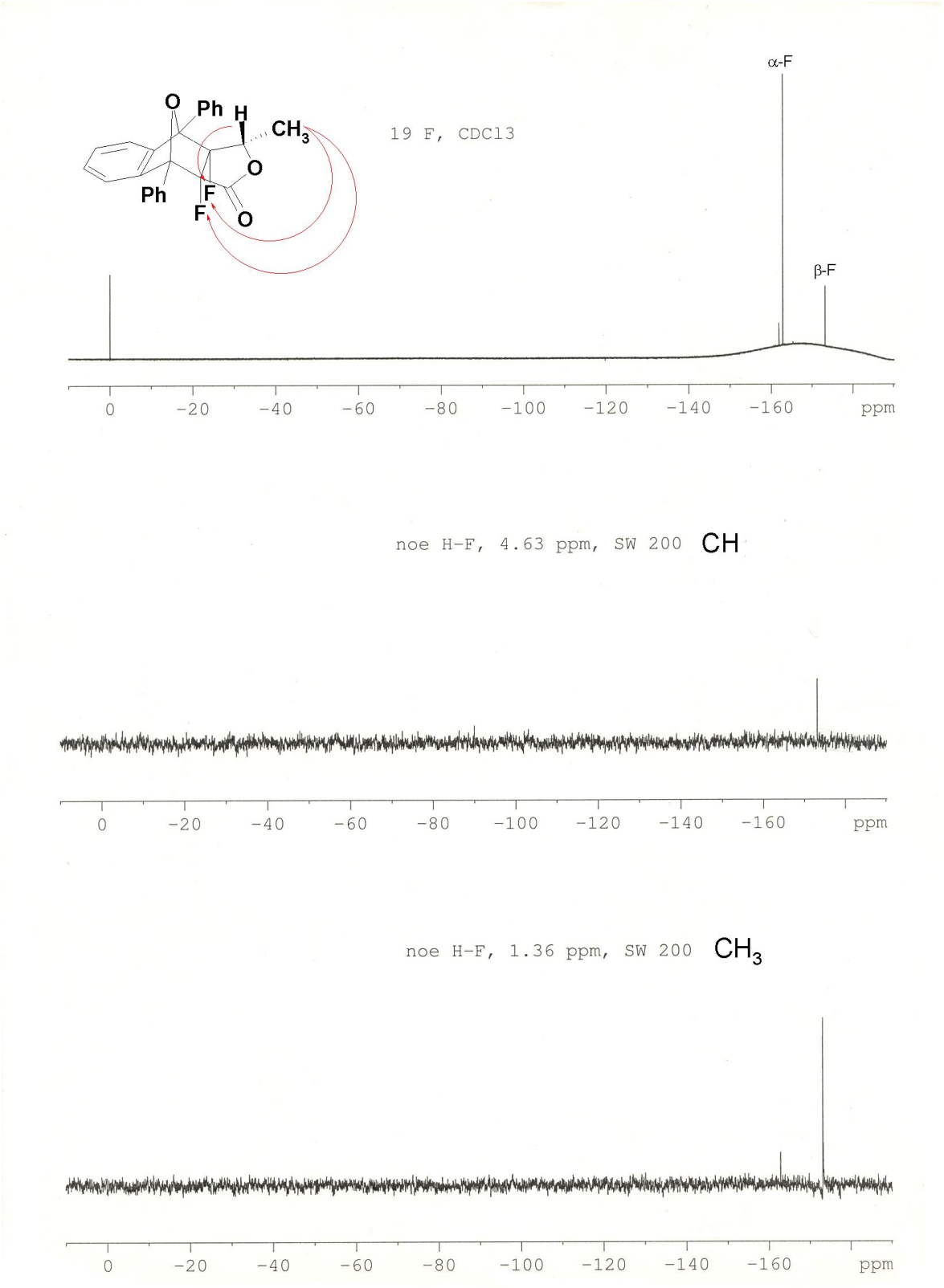
Ref. No.: O200700543

X-ray structure of *exo*-4,9-Epoxy-3a,9a-difluoro-3,3-dimethyl-4,9-diphenyl-3a,4,9,9a-tetrahydro-naphtho[2,3-*c*]furan-2(3*H*)-one (9):

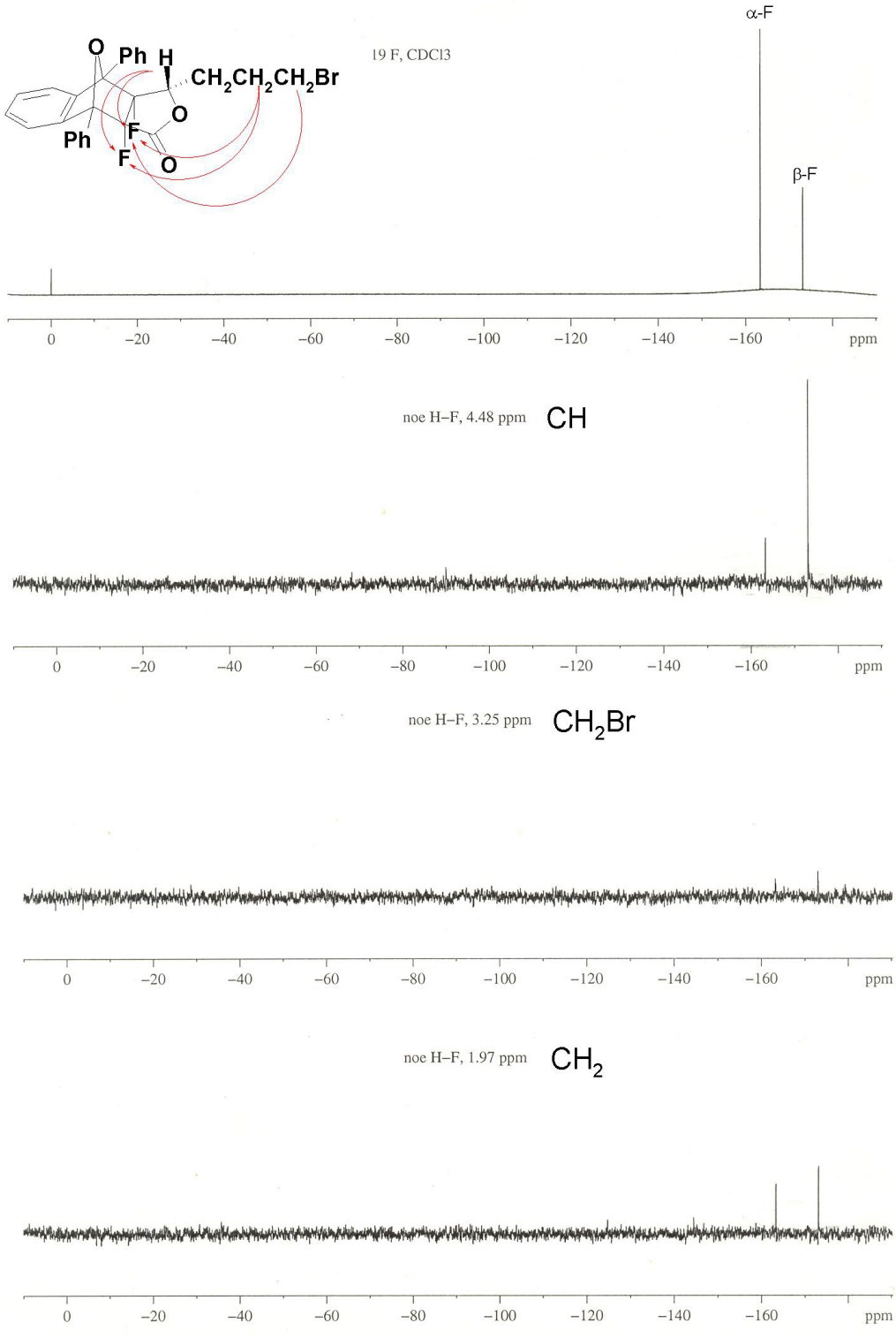


Results of the $^{19}F^{1}H$ NOE experiments:

$^{19}F - \{^{1}H\}$ NOE experiment for compound **7**



$^{19}F - \{^{1}H\}$ NOE experiment for compound **8**



Note: Methylene group with shift 1,69-1,97 ppm was not irradiated. Its multiplet is very complicated.

Transition state relative energies and activation energies of the reactions of cyclopentadiene with some 2(5*H*)-furanones:

Cyclopentadiene and 2(5*H*)-furanone				
Method/relative energies (kJ/mol)	*exo*		*endo*	
mPW1PW91/6-311++G(d,p)	1.5	E_A 80	0	E_A 76
MP2/6-311++G(d,p)	4.9		0.0	
BMK/aug-pc-2	**1.7**		**0.0**	
Cyclopentadiene and 3-fluoro-2(5*H*)-furanone				
Method/relative energies (kJ/mol)	*exo*		*endo*	
mPW1PW91/6-311++G(d,p)	0.0	E_A 86	0.2	E_A 84
MP2/6-311++G(d,p)	3.3		0.0	
BMK/aug-pc-2	**0.5**		**0.0**	
Cyclopentadiene and 3,4-difluoro-2(5*H*)-furanone				
Method/relative energies (kJ/mol)	*exo*		*endo*	
mPW1PW91/6-311++G(d,p)	0.0	E_A 87	4.5	E_A 90
MP2/6-311++G(d,p)	2.2		0.0	
BMK/aug-pc-2	**0.0**		**3.5**	