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Supporting information for

# Solvation of a chiral carboxylic acid: Effects of hydrogen bonding on the IR and VCD spectra of α-Methoxyphenylacetic acid

Karoline Bünnemann, Christian Merten\*

Organic Chemistry 2, Ruhr-University Bochum, 44801 Bochum, Germany.

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## 1. Concentration dependent IR spectra



Figure S1. Concentration dependent IR spectra of MPAA in chloroform-d<sub>1</sub>

### 2. Conformational analysis

#### 2.1 Chloroform-d<sub>1</sub>

• •		B3I	LYP / 6-311+-	+G(2d,p) / IE	CFPCM		B3LY	P-GD3 / 6-31 IEFPC	1++G(2d M	G(2d,p) / ΔΕ popΔG 6 ] [%] 37.2 29.1 27.6 36.8	
	α	β	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G	
	[deg]	[deg]	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]	
<b>c</b> 1	166.2	99.0	0.00	0.00	44.1	45.7	0.00	0.14	37.2	29.1	
c2	72.0	103.6	0.39	0.45	22.9	21.3	0.18	0.00	27.6	36.8	
c3	167.7	-86.9	0.45	0.45	20.8	21.3	0.38	0.40	19.5	18.9	
c4	72.9	-85.1	0.79	0.83	11.6	11.3	0.60	0.60	13.4	13.4	
c5	-51.6	118.8	2.59	2.90	0.6	0.3	1.73	1.91	2.0	1.5	
c6	-54.5	-47.2	3.58	3.63	0.1	0.1	2.78	2.76	0.3	0.3	

Table S1. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the **IEFPCM of chloroform** 

<sup>a)</sup> Reference to  $E_h(c1)$ = -574.66133 hartree and  $G_h(c1)$ = -574.69993 hartree <sup>b)</sup> Reference to  $E_h(c1)$ = -574.6792 hartree and  $G_h(c2)$ = -574.71761hartree

Table S2. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of the 10 most populated dimeric structures (MPAA)<sub>2</sub> calculated within the **IEFPCM of chloroform** 

	B3LY	YP / 6-311++G	G(2d,p) / IEF	РСМ	B3LYP-	GD3 / 6-311+	+G(2d,p) / II	EFPCM
	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G
	[kcal/mol ]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
d11	0.00	0.00	24.8	23.1	0.00	0.00	20.67	19.44
d13	0.29	0.50	15.2	9.9	0.24	0.39	13.82	10.08
d12	0.32	0.33	14.4	13.2	0.20	0.24	14.72	12.99
d14	0.59	0.01	9.1	22.6	0.52	0.13	8.58	15.56
d22	0.65	0.75	8.3	6.5	0.43	0.41	10.05	9.76
d23	0.65	0.98	8.2	4.4	0.54	0.74	8.31	5.57
d33	0.68	0.47	7.9	10.4	0.63	0.80	7.09	5.01
d24	1.00	1.07	4.6	3.8	0.83	0.66	5.05	6.39
d34	1.03	1.04	4.4	4.0	0.83	0.77	5.09	5.26
d44	1.41	1.73	2.3	1.3	1.07	0.77	3.38	5.28

<sup>a)</sup> Reference to  $E_h(d11)$ = -1149.3405 hartree and  $G_h(d11)$  = -1149.39933 hartree

<sup>b)</sup> Reference to  $E_h(d11) = -1149.38127$  hartree and  $G_h(d11) = -1149.43971$  hartree

		B3I	.YP / 6-311+-	+G(2d,p) / IE	FPCM		B3LY	P-GD3 / 6-31 IEFPC	1++G(2d M	<b>,p</b> ) /
	α	β	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G
	[deg]	[deg]	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
c1	166.2	99.0	0.00	0.00	44.7	42.4	0.00	0.00	37.24	38.40
c2	72.1	103.8	0.25	0.18	29.2	31.5	0.06	0.05	33.85	35.28
c3	167.7	-86.7	0.61	0.63	16.0	14.5	0.50	0.58	15.95	14.33
c4	72.9	-84.8	0.91	0.78	9.6	11.3	0.72	0.76	11.01	10.65
c5	-51.6	119.1	2.75	2.99	0.4	0.3	1.86	2.11	1.60	1.08
c6	-54.5	-47.1	3.57	3.56	0.1	0.1	2.77	2.97	0.34	0.25

Table S3. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the IEFPCM of DMSO

<sup>a)</sup> Reference to  $E_{h}(c1) = -574.66468$  hartree and  $G_{h}(c1) = -574.70321$  hartree

<sup>b)</sup> Reference to  $E_h(c1) = -574.6825$  hartree and  $G_h(c1) = -574.721$  hartree

Table S4. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of monosolvated MPAA-DMSO calculated within the IEFPCM of DMSO

	B3LY	Z <b>P / 6-311</b> ++G	G(2d,p) / IEFI	РСМ	B3LYP-	-GD3 / 6-311+	+G(2d,p) / II	EFPCM
	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}^{b)}$	рор∆Е	pop∆G
_	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
bifur	cated MPAA	-DMSO			bifurcated 1	MPAA-DMSC	)	
c1	0.00	0.26	28.29	16.92	0.04	0.00	19.99	38.64
c2	0.20	0.56	20.15	10.18	0.19	0.37	15.39	20.81
c3	0.53	0.91	11.49	5.68	0.55	0.69	8.50	11.99
c4	0.82	0.91	7.13	5.68	0.82	0.91	5.39	8.37
c5	2.90	3.55	0.21	0.07	2.11	2.73	0.61	0.39
c6	3.63	4.38	0.06	0.02	2.82	3.37	0.18	0.13
linea	r MPAA-DM	ISO			angled MPA	AA-DMSO		
<b>c</b> 1	0.40	0.00	14.51	26.41	0.00	0.94	21.37	7.85
c2	0.62	0.04	9.91	24.52	0.13	1.04	17.29	6.70
c3	1.00	0.77	5.25	7.17	0.67	1.57	6.95	2.72
c4	1.36	1.26	2.84	3.14	0.97	1.77	4.18	1.94
c5	3.20	3.07	0.13	0.15	n/a <sup>c)</sup>			
c6	3.98	3.58	0.03	0.06	2.99	2.62	0.14	0.46

<sup>a)</sup> Reference to  $E_h(c1\text{-bifurcated}) = -1127.91603$  hartree and  $G_h(c1\text{-linear}) = -1127.96747$  hartree <sup>b)</sup> Reference to  $E_h(c1\text{-angled}) = -1127.9452$  hartree and  $G_h(c1\text{-bifurcated}) = -1127.995704$  hartree

c) angled form of c3-DMSO does not exist due to steric reasons

F · F ·												
		B3L	2YP / 6-311++	-G(2d,p) / IE	FPCM		B3LY	P-GD3 / 6-3 IEFP(	511++G(26 CM	<b>2d,p</b> ) / <b>pop∆G</b> [%] 39.4 35.0		
	α	β	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	ΔE <sub>ZPC</sub> <sup>b)</sup>	$\Delta G_{298K}^{b)}$	рор∆Е	pop∆G		
	[deg]	[deg]	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]		
c1	166.2	99.0	0.00	0.00	44.6	42.2	0.00	0.00	37.4	39.4		
c2	72.0	103.6	0.26	0.18	28.9	31.3	0.06	0.07	33.6	35.0		
c3	167.7	-86.9	0.60	0.61	16.3	14.9	0.50	0.61	16.0	13.9		
c4	72.9	-85.1	0.90	0.78	9.7	11.2	0.72	0.79	11.0	10.4		
c5	-51.6	118.8	2.75	2.97	0.4	0.3	1.86	2.13	1.6	1.1		
сб	-54.5	-47.2	3.57	3.56	0.1	0.1	2.78	3.01	0.3	0.2		

Table S5. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the IEFPCM of acetonitrile

<sup>a)</sup> Reference to  $E_h(c1)$ = -574.66454 hartree and  $G_h(c1)$  = -574.70306 hartree

<sup>b)</sup> Reference to  $E_h(c1) = -574.68237$  hartree and  $G_h(c1) = -574.72091$  hartree

Table S6. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of ACN-monosolvated MPAA calculated within the IEFPCM of acetonitrile

	B3LY	ZP / 6-311++0	G(2d,p) / IEFI	РСМ	B3LYP-	GD3 / 6-311+	-+G(2d,p) / II	EFPCM
	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G
	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
c1	0.00	0.04	44.2	32.7	0.00	0.23	36.2	23.1
c2	0.26	0.21	28.6	24.6	0.06	0.00	32.9	34.2
c3	0.55	0.00	17.6	35.2	0.43	0.17	17.6	25.7
c4	0.94	0.95	9.0	7.1	0.69	0.51	11.3	14.5
c5	2.80	2.90	0.4	0.3	1.87	1.61	1.5	2.2
c6	3.56	3.12	0.1	0.2	2.76	2.98	0.3	0.2

<sup>a)</sup> Reference to  $E_h(c1)$ = -707.44385 hartree and  $G_h(c3)$  = -707.49366 hartree <sup>b)</sup> Reference to  $E_h(c1)$ = -707.4647 hartree and  $G_h(c1)$  = -707.51453 hartree



pop	ulations		a calculated w		CWI OI IIIC	unanoi				
		B3I	LYP / 6-311+-	+G(2d,p) / IE	FPCM		B3LYI	P-GD3 / 6-31 IEFPC	1++G(2d M	,p) /
	α	β	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G
	[deg]	[deg]	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
<b>c</b> 1	166.3	98.9	0.00	0.00	44.2	42.0	0.00	0.00	37.4	39.3
c2	72.0	103.5	0.25	0.18	28.9	31.2	0.07	0.07	33.3	34.9
c3	167.8	-86.9	0.58	0.60	16.5	15.2	0.50	0.61	16.2	14.0
c4	72.9	-85.2	0.88	0.78	9.9	11.3	0.72	0.78	11.2	10.4
c5	-51.6	118.7	2.75	2.97	0.4	0.3	1.86	2.13	1.6	1.1
c6	-54.5	-47.3	3.55	3.56	0.1	0.1	2.77	3.01	0.3	0.2

**Table S7.** Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of MPAA calculated within the **IEFPCM of methanol** 

<sup>a)</sup> Reference to  $E_{b}(c1) = -574.66788$  hartree and  $G_{b}(c1) = -574.70656$  hartree

<sup>b)</sup> Reference to  $E_h(c1) = -574.68573$  hartree and  $G_h(c1) = -574.72443$  hartree

Table S8. Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of monosolvated MPAA-(CD<sub>3</sub>OD)<sub>1</sub> calculated within the IEFPCM of methanol

		B3LYP /	/ 6-311++G(2	<b>d,p) / IEF</b>	РСМ	B3LYP-GI	03 / 6-311++0	G(2d,p) / II	EFPCM
	OH <sup>a)</sup>	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{ b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G
		[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
c1	proR	0.00	0.00	23.81	22.69	0.00	0.07	18.64	18.77
c1	proS	0.03	0.10	22.82	19.16	0.02	0.00	18.06	21.09
c2	proR	0.24	0.29	15.75	13.79	0.07	0.10	16.59	17.80
c2	proS	0.41	0.55	11.83	9.03	0.13	0.15	15.08	16.35
c3	proS	0.65	0.38	7.99	11.89	0.40	0.67	9.46	6.79
c3	proR	0.66	0.36	7.82	12.27	0.46	0.67	8.60	6.79
c4	proR	0.93	0.75	4.91	6.43	0.65	0.72	6.26	6.30
c4	proS	0.98	0.97	4.56	4.39	0.72	0.88	5.51	4.73
c5	proS	2.80	3.12	0.21	0.12	1.90	2.05	0.75	0.67
c5	proR	2.81	2.94	0.21	0.16	1.97	2.42	0.67	0.36
c6	proS	3.67	3.89	0.05	0.03	2.68	2.65	0.20	0.24
c6	proR	3.67	3.78	0.05	0.04	2.72	3.03	0.19	0.13

<sup>a)</sup> Configuration of OH-group considering the nomenclature shown in the Scheme S1 below this table. <sup>b)</sup> Reference to  $E_h(c1\text{-proR}) = -690.4119$  hartree and  $G_h(c1\text{-proR}) = -690.46001$  hartree

<sup>c)</sup> Reference to  $E_h(c1\text{-proR}) = -690.4341$  hartree and  $G_h(c1\text{-proS}) = -690.48137$  hartree



Scheme S1. Definition of methanol-binding orientations with priorities  $CH_3 > H > Hbond > LP$ . Left: pro-S; right: pro-R.

populations of two	ioia solvatta		OD 12 culet	inuca with		in or methal	101	
	B3LYP	/ 6-311++G(2	d,p) / IEFI	РСМ	B3LYP-GI	03 / 6-311++0	G(2d,p) / I	EFPCM
	$\Delta E_{ZPC}^{a)}$	$\Delta G_{298K}{}^{a)}$	рор∆Е	pop∆G	$\Delta E_{ZPC}^{b)}$	$\Delta G_{298K}{}^{b)}$	рор∆Е	pop∆G
	[kcal/mol]	[kcal/mol]	[%]	[%]	[kcal/mol]	[kcal/mol]	[%]	[%]
c1-proR-trans	0.00	0.00	12.58	16.20	0.03	0.57	9.65	7.25
c1-proS-trans	0.03	0.21	12.02	11.34	0.00	0.22	10.12	13.03
c1-proR-cis	0.19	0.47	9.09	7.30	0.01	0.49	10.02	8.23
c1-proS-cis	0.20	0.41	8.94	8.10	0.15	0.97	7.83	3.64
c2-proS-trans	0.29	0.40	7.76	8.29	0.17	0.00	7.57	18.86
c2-proR-trans	0.29	0.56	7.66	6.28	0.15	0.55	7.84	7.41
c2-proR-cis	0.43	0.54	6.05	6.55	0.18	0.83	7.41	4.61
c2-proS-cis	0.48	0.65	5.62	5.37	0.33	1.02	5.82	3.36
c3-proR-trans	0.49	0.70	5.48	4.93	0.39	0.82	5.28	4.76
c3-proS-trans	0.50	0.52	5.41	6.71	0.41	0.81	5.05	4.79
c3-proS-cis	0.59	0.60	4.61	5.86	0.38	0.67	5.34	6.04
c3-proR-cis	0.69	0.92	3.92	3.42	0.53	1.22	4.13	2.38
c4-proR-trans	0.85	1.11	3.01	2.50	0.67	0.94	3.25	3.84
c4-proS-trans	0.88	1.18	2.86	2.21	0.70	0.76	3.11	5.26
c4-proR-cis	1.01	1.14	2.30	2.36	0.80	1.27	2.62	2.22
c4-proS-cis	1.01	1.16	2.27	2.29	0.67	1.02	3.28	3.34
c5-proS-trans	2.89	3.20	0.10	0.07	2.06	3.13	0.31	0.10
c5-proR-trans	2.89	3.43	0.09	0.05	2.01	2.72	0.34	0.19
c5-proS-cis	3.02	3.52	0.08	0.04	2.07	2.59	0.31	0.24
c5-proR-cis	3.11	3.54	0.07	0.04	2.05	2.86	0.32	0.15
c6-proR-trans	3.57	4.14	0.03	0.01	2.70	3.89	0.11	0.03
c6-proS-trans	3.58	3.95	0.03	0.02	2.69	2.72	0.11	0.19
c6-proR-cis	3.71	4.02	0.02	0.02	2.77	3.31	0.09	0.07
c6-proS-cis	3.74	4.14	0.02	0.01	2.74	3.81	0.10	0.03

**Table S9.** Geometries, zero-point-corrected electronic and Gibbs free energies and the corresponding Boltzmann populations of **twofold-solvated MPAA-(CD<sub>3</sub>OD)**<sub>2</sub> calculated within the **IEFPCM of methanol** 

<sup>a)</sup> Reference to  $E_h(c1\text{-proR-trans}) = -806.157489$  hartree and  $G_h(c1\text{-proR-trans}) = -806.21223$  hartree <sup>b)</sup> Reference to  $E_h(c1\text{-proS-trans}) = -806.185204$  hartree and  $G_h(c2\text{-proS-trans}) = -806.24003$  hartree

#### 3. Calculated IR and VCD spectra



**Figure S2.** Single conformer IR and VCD spectra of MPAA calculated at the B3LYP/6-311++G(2d,p)/ IEFPCM(chloroform) level of theory.



**Figure S3.** Comparison of calculated VCD spectra for MPAA··DMSO adducts: (A) Boltzmann weighted over all six conformers; (B) spectra for conformation c1



**Figure S4.** The structure of mono-solvated c1··(DMSO)<sub>1</sub> calculated by taking into account dispersion interactions with the B3LYP-GD3 functional under otherwise identical theoretical conditions.



**Figure S5.** Potential energy surface for the rotation of the DMSO molecule bond to c1 (expressed as the angle C-O(H) $\cdot$ O=S). The black line corresponds to calculations using B3LYP, the blue line represents energies obtained with B3LYP-GD3.



**Figure S6.** The structures of twofold-solvated c1··(DMSO)<sub>2</sub>. Left: Structures obtained with the B3LYP functional; Right: Representative structure obtained after including dispersion corrections (B3LYP-GD3)



**Figure S7.** Dependence of the calculated rotational strength  $R_{(C=O)}$  for the carbonyl stretching mode of c1··(DMSO)<sub>1</sub> on the spatial orientation of the DMSO molecules (expressed as the angle C-O(H)··O=S). The red stars mark the two localized minimum structures (B3LYP/6-311++G(2d,p)/IEFPCM(DMSO))



Figure S8. Calculated VCD spectra for conformer c1 of the MPAA··(CD<sub>3</sub>OD) and MPAA··(CD<sub>3</sub>OD)<sub>2</sub> adducts.

#### 4. Vibrational energy distribution

In the vibrational analysis, the following atom numbering given below is used:



Table S10. Vibrational energy distribution analysis for c1 (B3LYP/6-311++G(2d,p)/IEFPCM(chloroform)).
For better comparison, the range below 500 cm <sup>-1</sup> is removed from the list. The color coding highlights the
modes discussed in the main text, important vibrational contributions are printed in bold type.

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1	Vscaled	Contributing interna	coordination and cont	ribution in percentage			
	3658	v(OH) 100					
	3129	ν(C <sub>9</sub> -H <sub>13</sub> ) 62	ν(C <sub>12</sub> -H <sub>16</sub> ) 22	ν(C <sub>14</sub> -H <sub>17</sub> ) 10			
	3123	ν(C <sub>9</sub> -H <sub>13</sub> ) -24	ν(C <sub>10</sub> -H <sub>15</sub> ) 37	ν(C <sub>14</sub> -H <sub>17</sub> ) 30			
	3113	ν(C <sub>8</sub> -H <sub>11</sub> ) 20	ν(C <sub>10</sub> -H <sub>15</sub> ) 24	ν(C <sub>12</sub> -H <sub>16</sub> ) -29	ν(C <sub>14</sub> -H <sub>17</sub> ) -17		
	3105	ν(C <sub>8</sub> -H <sub>11</sub> ) 38	ν(C <sub>12</sub> -H <sub>16</sub> ) 36	ν(C <sub>14</sub> -H <sub>17</sub> ) -20			
	3099	v(C <sub>8</sub> -H <sub>11</sub> ) -34	ν(C <sub>10</sub> -H <sub>15</sub> ) 31	ν(C <sub>12</sub> -H <sub>16</sub> ) 12	ν(C <sub>14</sub> -H <sub>17</sub> ) -22		
	3064	ν(C <sub>19</sub> -H <sub>20</sub> ) 91					
	2999	ν(C <sub>19</sub> -H <sub>21</sub> ) -31	ν(C <sub>19</sub> -H <sub>22</sub> ) 67				
	2952	v(C <sub>1</sub> -H <sub>2</sub> ) 99					
	2940	v(C <sub>19</sub> -H <sub>21</sub> ) 65	ν(C <sub>19</sub> -H <sub>22</sub> ) 27				
	1749	v(O <sub>4</sub> -C <sub>3</sub> ) 87					
	1606	v(C <sub>8</sub> -C <sub>10</sub> ) 10	v(C9-C12) 29				
	1590	v(C <sub>7</sub> -C <sub>8</sub> ) -18	v(C14-C10) 27	δ(C7-C8-C10) 13			
	1499	δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 15	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 16	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> ) 17	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 18		
	1469	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) -31	δ(H <sub>22</sub> -C <sub>9</sub> -C <sub>21</sub> ) 48	$\tau$ (H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 13			
	1459	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> ) -11	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 10	δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>12</sub> ) -26			
	1454	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) -28	δ(H <sub>21</sub> -C <sub>19</sub> -H <sub>20</sub> ) 29	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) -19	τ(H <sub>20</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -12	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 11	
	1444	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 17	δ(H <sub>21</sub> -C <sub>19</sub> -H <sub>20</sub> ) 52	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 13			
	1361	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 57					
	1345	δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) -15	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 14	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 23			
	1318	ν(C <sub>8</sub> -C <sub>10</sub> ) -11	ν(C <sub>9</sub> -C <sub>12</sub> ) 14	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) -19	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) -11		
	1290	ν(C <sub>7</sub> -C <sub>8</sub> ) 10	δ(H <sub>6</sub> -O <sub>5</sub> -C <sub>3</sub> ) 25	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 16			
	1257	δ(H <sub>6</sub> -O <sub>5</sub> -C <sub>3</sub> ) -12	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 33				
	1192	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> )-25	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 25			
	1192 1187	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12 ν(C <sub>1</sub> -C <sub>7</sub> ) 30	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> )-25	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 25			
	1192 1187 1177	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12 ν(C <sub>1</sub> -C <sub>7</sub> ) 30 δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> )-25 δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 22	$\tau$ (H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 25 $\delta$ (H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> ) -16	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) -14		
	1192 1187 1177 1157	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12 <b>ν(C<sub>1</sub>-C<sub>7</sub>) 30</b> δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23 ν(C <sub>12</sub> -C <sub>14</sub> ) 10	$\begin{split} \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}25\\ \\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12})\text{-}22\\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14})\text{-}18 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & 25 \\ \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14}) & -16 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 19 \end{split}$	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) -14 δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>12</sub> ) 35		
	1192 1187 1177 1157 1149	$\begin{split} \delta(H_{22}\text{-}C_{19}\text{-}H_{21}) \ 12 \\ \hline \textbf{v(C_1-C_7) 30} \\ \delta(H_{11}\text{-}C_8\text{-}C_{10}) \ 23 \\ \nu(C_{12}\text{-}C_{14}) \ 10 \\ \delta(H_{20}\text{-}C_{19}\text{-}H_{22}) \ 14 \end{split}$	$\begin{split} \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}25\\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12})\text{-}22\\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14})\text{-}18\\ \delta(H_{21}\text{-}C_{19}\text{-}H_{20})\text{-}12 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & 25 \\ \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14}) & -16 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 19 \\ \tau(H_{20}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & 34 \end{split}$	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) -14 δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>12</sub> ) 35 τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -21	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -16	
	1192 1187 1177 1157 1149 1118	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12 <b>v(C<sub>1</sub>-C<sub>7</sub>) 30</b> δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23 v(C <sub>12</sub> -C <sub>14</sub> ) 10 δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 14 <b>v(O<sub>5</sub>-C<sub>3</sub>) 27</b>	$\begin{array}{c} \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}25\\ \\ \\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12})\text{-}22\\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14})\text{-}18\\ \\ \delta(H_{21}\text{-}C_{19}\text{-}H_{20})\text{-}12\\ \\ \nu(O_{18}\text{-}C_{1})\text{-}14 \end{array}$	$\begin{array}{c} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\ 25\\ \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14})\ -16\\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14})\ 19\\ \tau(H_{20}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\ 34\\ \\ \delta(H_{6}\text{-}O_{5}\text{-}C_{3})\ -17 \end{array}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14})\text{-}14\\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{12})\text{-}35\\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}21 \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -16	
	1192 1187 1177 1157 1149 1118 1089	$\begin{split} \delta(H_{22}-C_{19}-H_{21}) & 12 \\ \hline v(C_1-C_7) & 30 \\ \delta(H_{11}-C_8-C_{10}) & 23 \\ v(C_{12}-C_{14}) & 10 \\ \delta(H_{20}-C_{19}-H_{22}) & 14 \\ \hline v(O_5-C_3) & 27 \\ v(O_5-C_3) & -25 \end{split}$	$\begin{array}{c} \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}25\\ \\ \\ \\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12})\text{-}22\\ \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14})\text{-}18\\ \\ \delta(H_{21}\text{-}C_{19}\text{-}H_{20})\text{-}12\\ \\ \\ \nu(O_{18}\text{-}C_{1})\text{-}14\\ \\ \nu(O_{18}\text{-}C_{1})\text{-}23\\ \end{array}$	$\begin{array}{c} \tau(H_{22}-C_{19}-O_{18}-C_{1})\ 25\\ \\ \\ \\ \delta(H_{15}-C_{10}-C_{14})\ -16\\ \\ \delta(H_{16}-C_{12}-C_{14})\ 19\\ \\ \tau(H_{20}-C_{19}-O_{18}-C_{1})\ 34\\ \\ \\ \hline \\ \delta(H_{6}-O_{5}-C_{3})\ -17\\ \\ \\ \nu(O_{18}-C_{19})\ -25\\ \end{array}$	$\begin{split} \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & -14 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{12}) & 35 \\ \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -21 \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -16	
	1192 1187 1177 1157 1149 1118 1089 1080	$\begin{split} \delta(H_{22}-C_{19}-H_{21}) & 12 \\ \hline v(C_1-C_7) & 30 \\ \delta(H_{11}-C_8-C_{10}) & 23 \\ v(C_{12}-C_{14}) & 10 \\ \delta(H_{20}-C_{19}-H_{22}) & 14 \\ \hline v(O_5-C_3) & 27 \\ v(O_5-C_3) & -25 \\ v(C_8-C_{10}) & 20 \\ \end{split}$	$\begin{array}{c} \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}25\\ \\ \\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12})\text{-}22\\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14})\text{-}18\\ \\ \delta(H_{21}\text{-}C_{19}\text{-}H_{20})\text{-}12\\ \\ \hline \nu(O_{18}\text{-}C_{1})\text{-}14\\ \\ \nu(O_{18}\text{-}C_{1})\text{-}23\\ \\ \nu(C_{9}\text{-}C_{12})\text{-}14 \end{array}$	$\begin{array}{c} \tau(H_{22}-C_{19}-O_{18}-C_{1})25\\ \\ \\ \delta(H_{15}-C_{10}-C_{14})-16\\ \delta(H_{16}-C_{12}-C_{14})19\\ \\ \tau(H_{20}-C_{19}-O_{18}-C_{1})34\\ \\ \hline \delta(H_{6}-O_{5}-C_{3})-17\\ \\ \nu(O_{18}-C_{19})-25\\ \\ \delta(H_{13}-C_{9}-C_{12})-13\\ \end{array}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -16	
	1192 1187 1177 1157 1149 1118 1089 1080 1028	$\begin{split} \delta(H_{22}-C_{19}-H_{21}) & 12 \\ \hline v(C_1-C_7) & 30 \\ \delta(H_{11}-C_8-C_{10}) & 23 \\ v(C_{12}-C_{14}) & 10 \\ \delta(H_{20}-C_{19}-H_{22}) & 14 \\ \hline v(O_5-C_3) & 27 \\ v(O_5-C_3) & 25 \\ v(C_8-C10) & 20 \\ v(C_{12}-C_{14}) & 18 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12})& 22\\ \delta(H_{15}-C_{10}-C_{14})& -18\\ \delta(H_{21}-C_{19}-H_{20})& -12\\ \hline \nu(O_{18}-C_{1})& 14\\ \nu(O_{18}-C_{1})& 23\\ \nu(C_{9}-C_{12})& -14\\ \nu(C_{14}-C_{10})& 16 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1})\ 25\\ \\ (H_{15}-C_{10}-C_{14})\ -16\\ \delta(H_{16}-C_{12}-C_{14})\ 19\\ \tau(H_{20}-C_{19}-O_{18}-C_{1})\ 34\\ \hline \delta(H_{6}-O_{5}-C_{3})\ -17\\ \nu(O_{18}-C_{19})\ -25\\ \delta(H_{13}-C_{9}-C_{12})\ -13\\ \delta(C_{9}-C_{12}-C_{14})\ -18\\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \delta(H_{6}-O_{5}-C_{3}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -16 δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 11	δ(C8-C10-C14) -10
	1192 1187 1177 1157 1149 1148 1089 1080 1028 1000	$\begin{split} \delta(H_{22}-C_{19}-H_{21}) & 12 \\ \hline v(C_1-C_7) & 30 \\ \delta(H_{11}-C_8-C_{10}) & 23 \\ v(C_{12}-C_{14}) & 10 \\ \delta(H_{20}-C_{19}-H_{22}) & 14 \\ \hline v(O_5-C_3) & 27 \\ v(O_5-C_3) & -25 \\ v(C_8-C10) & 20 \\ v(C_{12}-C_{14}) & 18 \\ v(C_{12}-C_{14}) & 15 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25 \\ (H_{13}-C_{9}-C_{12}) & 22 \\ \delta(H_{15}-C_{10}-C_{14}) & -18 \\ \delta(H_{21}-C_{19}-H_{20}) & -12 \\ (VO_{18}-C_{1}) & 14 \\ (VO_{18}-C_{1}) & 23 \\ (VO_{18}-C_{1}) & -14 \\ (VC_{14}-C_{10}) & 16 \\ (VC_{14}-C_{10}) & 12 \\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1})\ 25\\ \\ & \\ \delta(H_{15}-C_{10}-C_{14})\ -16\\ & \\ \delta(H_{16}-C_{12}-C_{14})\ 19\\ \\ \tau(H_{20}-C_{19}-O_{18}-C_{1})\ 34\\ \hline & \\ \delta(H_{6}-O_{5}-C_{3})\ -17\\ \\ & \\ \nu(O_{18}-C_{19})\ -25\\ & \\ \delta(H_{13}-C_{9}-C_{12})\ -13\\ \\ & \\ \delta(C_{9}-C_{12}-C_{14})\ -18\\ \\ & \\ \delta(C_{9}-C_{12}-C_{14})\ 24 \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \end{split}$	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}16$ $\delta(H_{16}\text{-}C_{12}\text{-}C_{14})\text{ 11}$ $\delta(C_{12}\text{-}C_{14}\text{-}C_{10})\text{-}16$	δ(C8-C10-C14) -10
	1192 1187 1177 1157 1149 1118 1089 1080 1028 1000 988	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ & \bullet(C_1-C_7)\ 30\\ &\delta(H_{11}-C_8-C_{10})\ 23\\ &\nu(C_{12}-C_{14})\ 10\\ &\delta(H_{20}-C_{19}-H_{22})\ 14\\ & \bullet(O_5-C_3)\ 27\\ & \nu(O_5-C_3)\ 27\\ &\nu(C_8-C_{10})\ 20\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 15\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25 \\ (H_{13}-C_{9}-C_{12}) & 22 \\ \delta(H_{15}-C_{10}-C_{14}) & -18 \\ \delta(H_{21}-C_{19}-H_{20}) & -12 \\ (H_{15}-C_{10}) & 14 \\ (H_{16}-C_{1}) & 23 \\ (H_{16}-C_{12}) & -14 \\ (H_{16}-C_{10}) & 12 \\ (H_{16}-C_{12}-C_{14}-C_{10}) & 24 \\ (H_{16}-C_{12}-C_{14}-C_{10}) & 24 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline \delta(H_{6}-O_{5}-C_{3}) \ -17 \\ \nu(O_{18}-C_{19}) \ -25 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ 24 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 28 \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \delta(H_{6}-O_{5}-C_{3}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \delta(C_{8}-C_{10}-C_{14}) & 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) & -13 \\ \end{split}$	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \text{-}16$ $\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \text{-}11$ $\delta(C_{12}\text{-}C_{14}\text{-}C_{10}) \text{-}16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	1192 1187 1177 1157 1149 1118 1089 1080 1028 1000 988 977	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ &\textbf{V(C_1-C_7)\ 30}\\ &\delta(H_{11}-C_8-C_{10})\ 23\\ &\nu(C_{12}-C_{14})\ 10\\ &\delta(H_{20}-C_{19}-H_{22})\ 14\\ &\textbf{V(O_5-C_3)\ 27}\\ &\textbf{V(O_5-C_3)\ 27}\\ &\textbf{V(O_5-C_3)\ -25}\\ &\nu(C_{8}-C10)\ 20\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 15\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ &\nu(O_{18}-C_{1})\ 19 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1})\ 25\\ \\ (H_{15}-C_{10}-C_{14})\ -16\\ \delta(H_{16}-C_{12}-C_{14})\ 19\\ \tau(H_{20}-C_{19}-O_{18}-C_{1})\ 34\\ \hline \delta(H_{6}-O_{5}-C_{3})\ -17\\ (H_{10}-C_{10})\ -25\\ \delta(H_{13}-C_{9}-C_{12})\ -13\\ \delta(C_{9}-C_{12}-C_{14})\ -18\\ \delta(C_{9}-C_{12}-C_{14})\ 24\\ \tau(H_{17}-C_{14}-C_{12}-C_{9})\ 28\\ \delta(O_{18}-C_{1}-C_{7})\ -10\\ \end{split}$	$\begin{split} &\delta(H_{16}-C_{12}-C_{14})-14\\ &\delta(H_{17}-C_{14}-C_{12})35\\ &\tau(H_{21}-C_{19}-O_{18}-C_{1})-21\\ & \\ &\delta(H_6-O_5-C_3)10\\ &\delta(H_{17}-C_{14}-C_{17})-13\\ &\delta(H_{15}-C_{10}-C_{14})10\\ &\delta(C_8-C_{10}-C_{14})12\\ &\tau(C_9-C_{12}-C_{14}-C_{10})-13 \end{split}$	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\text{-}16$ $\delta(H_{16}\text{-}C_{12}\text{-}C_{14})\text{ 11}$ $\delta(C_{12}\text{-}C_{14}\text{-}C_{10})\text{-}16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	1192 1187 1177 1157 1149 1089 1080 1028 1000 988 977 967	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ & \textbf{V}(\textbf{C}_1-\textbf{C}_7)\ \textbf{30}\\ & \delta(H_{11}-C_8-C_{10})\ 23\\ & \nu(C_{12}-C_{14})\ 10\\ & \delta(H_{20}-C_{19}-H_{22})\ 14\\ & \textbf{V}(\textbf{O}_5-\textbf{C}_3)\ \textbf{27}\\ & \textbf{V}(\textbf{O}_5-\textbf{C}_3)\ \textbf{-25}\\ & \nu(C_8-C10)\ 20\\ & \nu(C_{12}-C_{14})\ 18\\ & \nu(C_{12}-C_{14})\ 15\\ & \tau(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ & \nu(\textbf{O}_{18}-\textbf{C}_1)\ \textbf{19}\\ & \tau(H_{11}-C_8-C_{10}-C_{14})\ -17\end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline (H_{16}-O_{5}-C_{3}) \ -17 \\ (O_{18}-C_{19}) \ -25 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ 24 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 28 \\ \delta(O_{18}-C_{1}-C_{7}) \ -10 \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ 31 \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \delta(H_{6}-O_{5}-C_{5}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \delta(C_{8}-C_{10}-C_{14}) & 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) & -13 \\ \hline \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 21 \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1}) -16$ $\delta(H_{16}-C_{12}-C_{14}) 11$ $\delta(C_{12}-C_{14}-C_{10}) -16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	1192       1187       1177       1157       1149       1089       1080       1080       1088       9988       977       967       924	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ &\mathbf{V(C_1-C_7)\ 30}\\ &\delta(H_{11}-C_8-C_{10})\ 23\\ &\nu(C_{12}-C_{14})\ 10\\ &\delta(H_{20}-C_{19}-H_{22})\ 14\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\mathbf{V(O_5-C_3)\ 25}\\ &\nu(C_8-C10)\ 20\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 15\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ &\nu(O_{18}-C_{1})\ 19\\ &\tau(H_{11}-C_8-C_{10}-C_{14})\ -23\\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) & 22\\ \delta(H_{15}-C_{10}-C_{14}) & -18\\ \delta(H_{21}-C_{19}-H_{20}) & -12\\ \hline v(O_{18}-C_{1}) & 44\\ v(O_{18}-C_{1}) & 23\\ v(C_{9}-C_{12}) & -14\\ v(C_{14}-C_{10}) & 16\\ v(C_{14}-C_{10}) & 12\\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 24\\ v(O_{18}-C_{1}) & 38\\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) & -20\\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) & 18 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline & (H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline & (O_{18}-C_{19}) \ -25 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ 24 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 28 \\ \delta(O_{18}-C_{1}-C_{7}) \ -10 \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ 31 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \delta(H_{6}-O_{5}-C_{3}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \delta(C_{8}-C_{10}-C_{14}) & 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) & -13 \\ \hline \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 21 \end{split}$	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \text{-}16$ $\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \text{11}$ $\delta(C_{12}\text{-}C_{14}\text{-}C_{10}) \text{-}16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	1192         1187         1177         1157         1149         1089         1080         1028         1000         988         977         967         924         878	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12           ν(C <sub>1</sub> -C <sub>7</sub> ) 30           δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23           ν(C <sub>12</sub> -C <sub>14</sub> ) 10           δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 14           ν(O <sub>5</sub> -C <sub>3</sub> ) 27           ν(O <sub>5</sub> -C <sub>3</sub> ) -25           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 19           τ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> -C <sub>10</sub> ) -13           ν(O <sub>18</sub> -C <sub>1</sub> ) 19           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -23           ν(C <sub>1-</sub> C <sub>1</sub> ) 25	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) & 22\\ \delta(H_{15}-C_{10}-C_{14}) & -18\\ \delta(H_{21}-C_{19}-H_{20}) & -12\\ \hline v(O_{18}-C_{1}) & 44\\ v(O_{18}-C_{1}) & 23\\ v(C_{9}-C_{12}) & -14\\ v(C_{14}-C_{10}) & 16\\ v(C_{14}-C_{10}) & 16\\ v(C_{14}-C_{10}) & 12\\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 24\\ v(O_{18}-C_{19}) & 38\\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) & 18\\ \delta(C_{12}-C_{14}-C_{10}) & -10\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_1) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_1) \ 34 \\ \hline & (H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_1) \ 34 \\ \hline & (O_{18}-C_{19}) \ -25 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ 24 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 28 \\ \delta(O_{18}-C_{1}-O_{1}) \ -10 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) &-14\\ \delta(H_{17}-C_{14}-C_{12}) &35\\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) &-21\\ \hline \\ \delta(H_6-O_5-C_3) &10\\ \delta(H_{17}-C_{14}-C_{17}) &-13\\ \delta(H_{15}-C_{10}-C_{14}) &10\\ \delta(C_8-C_{10}-C_{14}) &12\\ \tau(C_9-C_{12}-C_{14}-C_{10}) &-13\\ \hline \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) &21 \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1}) -16$ $\delta(H_{16}-C_{12}-C_{14}) 11$ $\delta(C_{12}-C_{14}-C_{10}) -16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	1192       1187       1177       1157       1149       1080       1080       1080       988       977       967       924       878       871	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12           ν(C <sub>1</sub> -C <sub>7</sub> ) 30           δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23           ν(C <sub>12</sub> -C <sub>14</sub> ) 10           δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 14           ν(O <sub>5</sub> -C <sub>3</sub> ) 27           ν(O <sub>5</sub> -C <sub>3</sub> ) -25           ν(C <sub>8</sub> -C10) 20           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 15           τ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> -C <sub>10</sub> ) -13           ν(O <sub>18</sub> -C <sub>1</sub> ) 19           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -23           ν(C <sub>12</sub> -C <sub>14</sub> ) 25           δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 10	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12})&22\\ \delta(H_{15}-C_{10}-C_{14})&-18\\ \delta(H_{21}-C_{19}-H_{20})&-12\\ \hline v(O_{18}-C_{1})&14\\ \hline v(O_{18}-C_{1})&23\\ v(C_{9}-C_{12})&-14\\ v(C_{14}-C_{10})&16\\ v(C_{14}-C_{10})&16\\ v(C_{14}-C_{10})&12\\ \tau(H_{15}-C_{12}-C_{14}-C_{10})&24\\ r(H_{13}-C_{9}-C_{12}-C_{14})&-20\\ \tau(H_{13}-C_{9}-C_{12}-C_{14})&-18\\ \delta(C_{12}-C_{16}-C_{10})&-10\\ \theta(O_{4}-C_{1}-O_{5}-C_{3})&20\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ (H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ (H_{16}-C_{12}-C_{14}) \ 34 \\ (H_{17}-C_{19}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ 24 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 28 \\ \delta(O_{18}-C_{1}-C_{7}) \ -10 \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ 31 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \\ \phi(C_{3}-C_{7}-O_{18}-C_{1}) \ 19 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{22}-C_{19}-O_{18}-C_{1}) & -21 \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1}) -16$ $\delta(H_{16}-C_{12}-C_{14}) 11$ $\delta(C_{12}-C_{14}-C_{10}) -16$	δ(C8-C10-C14) -10
	1192       1187       1177       1149       1149       1089       1080       1080       1080       988       977       967       924       878       871       839	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 12           ν(C <sub>1</sub> -C <sub>7</sub> ) 30           δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23           ν(C <sub>12</sub> -C <sub>14</sub> ) 10           δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 14           ν(O <sub>5</sub> -C <sub>3</sub> ) 27           ν(O <sub>5</sub> -C <sub>3</sub> ) -25           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 15           τ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> -C <sub>10</sub> ) -13           ν(O <sub>18</sub> -C <sub>1</sub> ) 19           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -23           ν(C <sub>12</sub> -C <sub>14</sub> ) C <sub>10</sub>	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) & 22\\ \delta(H_{15}-C_{10}-C_{14}) & -18\\ \delta(H_{21}-C_{19}-H_{20}) & -12\\ \\ (H_{15}-C_{10}) & 12\\ \\ (H_{16}-C_{1}) & 23\\ \\ (H_{16}-C_{12}) & -14\\ \\ (H_{16}-C_{12}-C_{14}-C_{10}) & 24\\ \\ (H_{16}-C_{12}-C_{14}-C_{10}) & 24\\ \\ (H_{16}-C_{12}-C_{14}-C_{10}) & 24\\ \\ (H_{13}-C_{9}-C_{12}-C_{14}) & 18\\ \\ \delta(C_{12}-C_{14}-C_{10}) & -10\\ \\ (H_{13}-C_{9}-C_{12}-C_{14}) & 25\\ \\ (H_{13}-C_{13}-C_{14}-C_{14}) & 25\\ \\ (H_{13}-C_{14}-C_{14}-C_{14}) & 25\\ \\ (H_{13}-C_{14}-C_{14}-C_{14}) & 25\\ \\ (H_{13}-C_{14}-C_{14}-C_{14}-C_{14}) & 25\\ \\ (H_{13}-C_{14}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline (H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline (H_{16}-O_{5}-C_{3}) \ -17 \\ \tau(H_{20}-C_{10}) \ -25 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -28 \\ \delta(O_{18}-C_{1}-C_{7}) \ -10 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \\ \hline (H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \\ \hline (H_{17}-C_{10}-C_{14}-C_{10}) \ -28 \\ \hline (H_{15}-C_{10}-C_{14}-C_{10}) \ -28 \\ \hline (H_{15}-C_{10}-C_{$	$\begin{split} &\delta(H_{16}-C_{12}-C_{14})-14\\ &\delta(H_{17}-C_{14}-C_{12})35\\ &\tau(H_{21}-C_{19}-O_{18}-C_{1})-21\\ \hline &\delta(H_{6}-O_{5}-C_{3})10\\ &\delta(H_{17}-C_{14}-C_{17})-13\\ &\delta(H_{15}-C_{10}-C_{14})10\\ &\delta(C_{8}-C_{10}-C_{14})12\\ &\tau(C_{9}-C_{12}-C_{14}-C_{10})-13\\ \hline &\tau(H_{16}-C_{12}-C_{14}-C_{10})21\\ \end{split}$	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \text{-}16$ $\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \text{11}$ $\delta(C_{12}\text{-}C_{14}\text{-}C_{10}) \text{-}16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	1192 1187 1177 1157 1149 1089 1080 1028 1000 988 977 967 967 924 878 871 839	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ &V(C_1-C_7)\ 30\\ &\delta(H_{11}-C_8-C_{10})\ 23\\ &V(C_{12}-C_{14})\ 10\\ &\delta(H_{20}-C_{19}-H_{22})\ 14\\ \hline &V(O_5-C_3)\ 27\\ &V(O_5-C_3)\ 27\\ &V(O_5-C_3)\ 27\\ &V(C_8-C_{10})\ 20\\ &V(C_{12}-C_{14})\ 18\\ &V(C_{12}-C_{14})\ 18\\ &V(C_{12}-C_{14})\ 15\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ &V(O_{18}-C_{1})\ 19\\ &\tau(H_{11}-C_8-C_{10}-C_{14})\ -23\\ &V(C_{12}-C_{14})\ 25\\ &\delta(C_{12}-C_{14}-C_{10})\ 10\\ &\tau(H_{11}-C_8-C_{10}-C_{14})\ 27\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ 12\\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) 22\\ \\ \delta(H_{15}-C_{10}-C_{14}) -18\\ \\ \delta(H_{21}-C_{19}-H_{20}) -12\\ \\ (VO_{18}-C_{1}) 23\\ \\ V(O_{18}-C_{1}) 23\\ \\ V(O_{18}-C_{1}) 23\\ \\ V(C_{14}-C_{10}) 16\\ \\ V(C_{14}-C_{10}) 16\\ \\ V(C_{14}-C_{10}) 12\\ \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) -20\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) -20\\ \\ \delta(C_{12}-C_{14}-C_{10}) -10\\ \\ \Theta(O_{4}-C_{1}-O_{5}-C_{3}) 20\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) -21\\ \\ \end{array}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25\\ \\ (H_{15}-C_{10}-C_{14}) \ -16\\ \\ \delta(H_{16}-C_{12}-C_{14}) \ 19\\ \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34\\ \hline (H_{16}-O_{5}-C_{3}) \ -17\\ \\ (H_{10}-C_{10}-C_{10}) \ -25\\ \\ \delta(H_{13}-C_{9}-C_{12}) \ -13\\ \\ \delta(C_{9}-C_{12}-C_{14}) \ -18\\ \\ \delta(C_{9}-C_{12}-C_{14}) \ -18\\ \\ \delta(C_{9}-C_{12}-C_{14}) \ -18\\ \\ \delta(C_{9}-C_{12}-C_{14}) \ -18\\ \\ \delta(C_{18}-C_{1}-C_{7}) \ -10\\ \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ -31\\ \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ -28\\ \\ e(C_{3}-C_{7}-O_{18}-C_{1}) \ 19\\ \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ -28\\ \hline \end{cases}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \\ \delta(H_{6}-O_{5}-C_{5}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \delta(C_{8}-C_{10}-C_{14}) & 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) & -13 \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 21 \\ \end{split}$	$τ(H_{22}-C_{19}-O_{18}-C_1)$ -16 δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 11 δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> )-16	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	<ol> <li>1192</li> <li>1187</li> <li>1177</li> <li>1157</li> <li>1149</li> <li>1089</li> <li>1089</li> <li>1080</li> <li>1088</li> <li>907</li> <li>967</li> <li>967</li> <li>924</li> <li>878</li> <li>871</li> <li>839</li> <li>757</li> <li>717</li> </ol>	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ &\mathbf{V(C_1-C_7)\ 30}\\ &\delta(H_{11}-C_8-C_{10})\ 23\\ &\nu(C_{12}-C_{14})\ 10\\ &\delta(H_{20}-C_{19}-H_{22})\ 14\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\mathbf{V(O_5-C_3)\ 27}\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 18\\ &\nu(C_{12}-C_{14})\ 19\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ &\nu(C_{12}-C_{14}-C_{10})\ -13\\ &\nu(C_{12}-C_{14}-C_{10})\ 10\\ &\tau(H_{11}-C_8-C_{10}-C_{14})\ 27\\ &\tau(H_{15}-C_{10}-C_{14}-C_{10})\ 12\\ &\delta(C_{12}-C_{14}-C_{10})\ 18\\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) 22\\ \delta(H_{15}-C_{10}-C_{14})-18\\ \delta(H_{21}-C_{19}-H_{20})-12\\ \\ (VO_{18}-C_{1}) 44\\ \\ (VO_{18}-C_{1}) 23\\ (VC_{9}-C_{12})-14\\ \\ (C_{14}-C_{10}) 16\\ \\ (VC_{14}-C_{10}) 12\\ \\ (C_{14}-C_{10}) 12\\ \\ (H_{16}-C_{12}-C_{14}-C_{10}) 24\\ \\ (VO_{18}-C_{19}) 38\\ \\ (H_{13}-C_{9}-C_{12}-C_{14}) 18\\ \\ \delta(C_{12}-C_{14}-C_{10})-10\\ \\ (O(0_{4}-C_{1}-O_{5}-C_{3}) 20\\ \\ (H_{13}-C_{9}-C_{12}-C_{14}) 25\\ \\ (H_{16}-C_{12}-C_{14}-C_{10}) -11\\ \\ (O(0_{4}-C_{1}-O_{5}-C_{3})-30\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ 25 \\ (H_{15}-C_{10}-C_{14}) \ -16 \\ \delta(H_{16}-C_{12}-C_{14}) \ 19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) \ 34 \\ \hline & \delta(H_{16}-O_{5}-C_{3}) \ -17 \\ \nu(O_{18}-C_{19}) \ -25 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -18 \\ \delta(C_{9}-C_{12}-C_{14}) \ -28 \\ \delta(O_{18}-C_{1}-C_{12}) \ -20 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 28 \\ \delta(O_{18}-C_{1}-C_{7}) \ -10 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \\ \hline & \Theta(C_{3}-C_{7}-O_{18}-C_{1}) \ 19 \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) \ 23 \\ \hline & \Theta(C_{3}-C_{7}-O_{18}-C_{1}) \ 19 \\ \tau(H_{15}-C_{10}-C_{14}-C_{10}) \ 23 \\ \tau(C_{7}-C_{8}-C_{10}-C_{14}) \ -27 \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \\ \delta(H_{6}-O_{5}-C_{3}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \delta(C_{8}-C_{10}-C_{14}) & 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) & -13 \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 21 \\ \end{split}$	$\tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \text{-}16$ $\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \text{11}$ $\delta(C_{12}\text{-}C_{14}\text{-}C_{10}) \text{-}16$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	<ol> <li>1192</li> <li>1187</li> <li>1177</li> <li>1149</li> <li>1148</li> <li>1089</li> <li>1080</li> <li>1028</li> <li>1000</li> <li>988</li> <li>907</li> <li>967</li> <li>924</li> <li>878</li> <li>871</li> <li>839</li> <li>757</li> <li>717</li> <li>696</li> </ol>	$\begin{split} &\delta(H_{22}-C_{19}-H_{21})\ 12\\ &V(C_1-C_7)\ 30\\ &\delta(H_{11}-C_8-C_{10})\ 23\\ &V(C_{12}-C_{14})\ 10\\ &\delta(H_{20}-C_{19}-H_{22})\ 14\\ &V(O_5-C_3)\ 27\\ &V(O_5-C_3)\ 27\\ &V(O_5-C_3)\ 27\\ &V(O_5-C_3)\ 27\\ &V(O_5-C_3)\ 27\\ &V(C_{12}-C_{14})\ 18\\ &V(C_{12}-C_{14})\ 18\\ &V(C_{12}-C_{14})\ 18\\ &V(C_{12}-C_{14})\ 15\\ &T(H_{15}-C_{10}-C_{14}-C_{10})\ -13\\ &V(O_{18}-C_{1})\ 19\\ &T(H_{11}-C_8-C_{10}-C_{14})\ -23\\ &V(C_{12}-C_{14},C_{10})\ 10\\ &T(H_{11}-C_8-C_{10}-C_{14})\ 27\\ &T(H_{15}-C_{10}-C_{14}-C_{10})\ 12\\ &\delta(C_{12}-C_{14}-C_{10})\ 18\\ &T(H_{11}-C_8-C_{10}-C_{14})\ -11\end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) 22\\ \\ \delta(H_{15}-C_{10}-C_{14}) -18\\ \\ \delta(H_{21}-C_{19}-H_{20}) -12\\ \\ (VO_{18}-C_{1}) 14\\ \\ (VO_{18}-C_{1}) 23\\ \\ (VO_{18}-C_{1}) 23\\ \\ (VO_{14}-C_{10}) 16\\ \\ (VC_{14}-C_{10}) 16\\ \\ (VC_{14}-C_{10}) 12\\ \\ (H_{16}-C_{12}-C_{14}-C_{10}) 24\\ \\ (VO_{18}-C_{19}) 38\\ \\ (H_{13}-C_{9}-C_{12}-C_{14}) 18\\ \\ \delta(C_{12}-C_{14}-C_{10}) -10\\ \\ (H_{13}-C_{9}-C_{12}-C_{14}) 25\\ \\ (H_{13}-C_{14}-C_{12}-C_{14}-C_{10}) 25\\ \\ (H_{13}-C_{14}-C_{14}-C_{14}-C_{14}) 25\\ \\ (H_{13}-C_{14}-C$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) 25\\ \\ (H_{15}-C_{10}-C_{14}) -16\\ \delta(H_{16}-C_{12}-C_{14}) 19\\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) 34\\ \hline (H_{16}-O_{5}-C_{3}) -17\\ \hline (H_{10}-C_{10}) -25\\ \delta(H_{13}-C_{9}-C_{12}) -13\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -24\\ \hline (H_{17}-C_{14}-C_{12}-C_{9}) 28\\ \delta(O_{18}-C_{1}-O_{1}) -10\\ \hline (H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \hline (H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \hline (H_{15}-C_{10}-C_{14}-C_{10}) 23\\ \hline (H_{15}-C_{10}-C_{14}-C_{10}) 23\\ \hline (H_{17}-C_{14}-C_{12}-C_{9}) -17\\ \end{split}$	$\begin{split} &\delta(H_{16}-C_{12}-C_{14})-14\\ &\delta(H_{17}-C_{14}-C_{12})35\\ &\tau(H_{21}-C_{19}-O_{18}-C_{1})-21\\ \hline \\ &\delta(H_{6}-O_{5}-C_{3})10\\ &\delta(H_{17}-C_{14}-C_{17})-13\\ &\delta(H_{15}-C_{10}-C_{14})10\\ &\delta(C_{8}-C_{10}-C_{14})12\\ &\tau(C_{9}-C_{12}-C_{14}-C_{10})-13\\ \hline \\ &\tau(H_{16}-C_{12}-C_{14}-C_{10})21\\ \hline \\ &\tau(H_{16}-C_{12}-C_{14}-C_{10})25\\ \hline \\ &\tau(C_{7}-C_{8}-C_{10}-C_{14})-35\\ \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1})-16$ $\delta(H_{16}-C_{12}-C_{14}) \ 11$ $\delta(C_{12}-C_{14}-C_{10})-16$ $\tau(C_{9}-C_{12}-C_{14}-C_{10})-10$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	<ol> <li>1192</li> <li>1187</li> <li>1177</li> <li>1157</li> <li>1149</li> <li>1089</li> <li>1080</li> <li>1080</li> <li>1080</li> <li>988</li> <li>977</li> <li>967</li> <li>967</li> <li>957</li> <li>958</li> <li>957</li> <li>9</li></ol>	$\delta(H_{22}-C_{19}-H_{21})$ 12 $v(C_1-C_7)$ 30 $\delta(H_{11}-C_8-C_{10})$ 23 $v(C_{12}-C_{14})$ 10 $\delta(H_{20}-C_{19}-H_{22})$ 14 $v(O_5-C_3)$ 27 $v(O_5-C_3)$ 27 $v(O_5-C_3)$ -25 $v(C_8-C10)$ 20 $v(C_{12}-C_{14})$ 18 $v(C_{12}-C_{14})$ 15 $t(H_{15}-C_{10}-C_{14}-C_{10})$ -13 $v(O_{18}-C_1)$ 19 $t(H_{11}-C_8-C_{10}-C_{14})$ -13 $v(C_1-C_1)$ 25 $\delta(C_{12}-C_{14}-C_{10})$ 10 $t(H_{11}-C_8-C_{10}-C_{14})$ 27 $t(H_{15}-C_{10}-C_{14}-C_{10})$ 12 $\delta(C_{12}-C_{14}-C_{10})$ 18 $t(H_{11}-C_8-C_{10}-C_{14})$ -11 $v(O_5-C_3)$ 15 t	<ul> <li>τ(H<sub>21</sub>-C<sub>19</sub>-O<sub>18</sub>-C<sub>1</sub>)-25</li> <li>δ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>) 22</li> <li>δ(H<sub>15</sub>-C<sub>10</sub>-C<sub>14</sub>) -18</li> <li>δ(H<sub>21</sub>-C<sub>19</sub>-H<sub>20</sub>) -12</li> <li>ν(O<sub>18</sub>-C<sub>1</sub>) 23</li> <li>ν(O<sub>18</sub>-C<sub>1</sub>) 23</li> <li>ν(C<sub>9</sub>-C<sub>12</sub>) -14</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 16</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 16</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 12</li> <li>τ(H<sub>16</sub>-C<sub>12</sub>-C<sub>14</sub>-C<sub>10</sub>) 24</li> <li>δ(C<sub>12</sub>-C<sub>19</sub>) 38</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 18</li> <li>δ(C<sub>12</sub>-C<sub>14</sub>-C<sub>10</sub>) -10</li> <li>Θ(O<sub>4</sub>-C<sub>1</sub>-O<sub>5</sub>-C<sub>3</sub>) 20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -11</li> <li>Θ(O<sub>4</sub>-C<sub>1</sub>-O<sub>5</sub>-C<sub>3</sub>) -30</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 11</li> <li>δ(O<sub>4</sub>-C<sub>3</sub>-O<sub>5</sub>) 40</li> </ul>	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) 25\\ \\ S(H_{15}-C_{10}-C_{14}) -16\\ \\ \delta(H_{16}-C_{12}-C_{14}) 19\\ \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) 34\\ \hline (H_{10}-C_{12}-C_{14}) -18\\ \\ S(H_{13}-C_{9}-C_{12}) -13\\ \\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \\ \delta(C_{9}-C_{12}-C_{14}) -28\\ \\ \delta(O_{18}-C_{1}-C_{7}) -10\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \\ \tau(C_{7}-C_{8}-C_{10}-C_{14}) -27\\ \\ \end{array}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{22}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline & 5(H_6-O_5-C_3) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{17}-C_{10}-C_{14}) & 10 \\ \delta(C_8-C_{10}-C_{14}) & 12 \\ \tau(C_9-C_{12}-C_{14}-C_{10}) & -13 \\ \hline & \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 21 \\ \hline & \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 25 \\ \hline & \tau(C_7-C_8-C_{10}-C_{14}) & -35 \\ \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1})-16$ $\delta(H_{16}-C_{12}-C_{14}) 11$ $\delta(C_{12}-C_{14}-C_{10})-16$ $\tau(C_{9}-C_{12}-C_{14}-C_{10})-10$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	<ol> <li>1192</li> <li>1187</li> <li>1187</li> <li>1149</li> <li>1089</li> <li>1089</li> <li>1080</li> <li>1088</li> <li>1000</li> <li>988</li> <li>977</li> <li>967</li> <li>967</li> <li>957</li> <li>957</li> <li>957</li> <li>957</li> <li>957</li> <li>957</li> <li>957</li> <li>957</li> <li>958</li> <li>959</li> <li>959</li> <li>959</li> <li>959</li> <li>959</li> <li>959</li> <li>950</li> <li>951</li> <li>950</li> <li>951</li> <li>951</li> <li>951</li> <li>951</li> <li>951</li> <li>951</li> <li>951</li> <li>951</li> <li>952</li> <li>953</li> <li>954</li> <li>954</li> <li>955</li> <li>954</li> <li>955</li> <li>95</li> <li< th=""><th><math>\delta(H_{22}-C_{19}-H_{21})</math> 12 <math>v(C_1-C_7)</math> 30 <math>\delta(H_{11}-C_8-C_{10})</math> 23 <math>v(C_{12}-C_{14})</math> 10 <math>\delta(H_{20}-C_{19}-H_{22})</math> 14 <math>v(O_5-C_3)</math> 27 <math>v(O_5-C_3)</math> 27 <math>v(O_5-C_3)</math> 27 <math>v(C_5-C_1)</math> 20 <math>v(C_{12}-C_{14})</math> 18 <math>v(C_{12}-C_{14})</math> 15 <math>\tau(H_{15}-C_{10}-C_{14}-C_{10})</math> -13 <math>v(O_{18}-C_1)</math> 19 <math>\tau(H_{11}-C_8-C_{10}-C_{14})</math> -13 <math>v(C_1-C_1)</math> 25 <math>\delta(C_{12}-C_{14}-C_{10})</math> 10 <math>\tau(H_{11}-C_8-C_{10}-C_{14})</math> 27 <math>\tau(H_{15}-C_{10}-C_{14}-C_{10})</math> 12 <math>\delta(C_{12}-C_{14}-C_{10})</math> 18 <math>\tau(H_{11}-C_8-C_{10}-C_{14})</math> -11 <math>v(O_5-C_3)</math> 15 <math>\delta(C_9-C_{12}-C_{14})</math> -22 -z</th><th><ul> <li>τ(H<sub>21</sub>-C<sub>19</sub>-O<sub>18</sub>-C<sub>1</sub>)-25</li> <li>δ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>) 22</li> <li>δ(H<sub>15</sub>-C<sub>10</sub>-C<sub>14</sub>) -18</li> <li>δ(H<sub>21</sub>-C<sub>19</sub>-H<sub>20</sub>) -12</li> <li>ν(O<sub>18</sub>-C<sub>1</sub>) 14</li> <li>ν(O<sub>18</sub>-C<sub>1</sub>) 23</li> <li>ν(C<sub>9</sub>-C<sub>12</sub>) -14</li> <li>ν(C<sub>9</sub>-C<sub>12</sub>) -14</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 16</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 16</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 13</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 18</li> <li>δ(C<sub>12</sub>-C<sub>14</sub>-C<sub>10</sub>) -10</li> <li>Θ(O<sub>4</sub>-C<sub>1</sub>-O<sub>5</sub>-C<sub>3</sub>) 20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 25</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 13</li> <li>Θ(O<sub>4</sub>-C<sub>1</sub>-O<sub>5</sub>-C<sub>3</sub>) -30</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 14</li> <li>δ(O<sub>4</sub>-C<sub>3</sub>-O<sub>5</sub>) 40</li> <li>δ(O<sub>4</sub>-C<sub>10</sub>-C<sub>14</sub>) 22</li> </ul></th><th><math display="block">\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) 25\\ \\ (H_{15}-C_{10}-C_{14}) -16\\ \delta(H_{16}-C_{12}-C_{14}) 19\\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) 34\\ \\ (H_{16}-C_{12}-C_{14}) 19\\ \\ \tau(H_{20}-C_{19}-C_{10}) -25\\ \delta(H_{13}-C_{9}-C_{12}) -13\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -28\\ \delta(C_{9}-C_{12}-C_{14}) -28\\ \delta(O_{18}-C_{1}-C_{7}) -10\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) -23\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) -17\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) -17\\ \\ \tau(H_{6}-O_{5}-C_{3}-C_{1}) -10\\ \end{split}</math></th><th><math display="block">\begin{split} \delta(H_{16}-C_{12}-C_{14}) &amp; -14 \\ \delta(H_{17}-C_{14}-C_{12}) &amp; 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) &amp; -21 \\ \hline \\ \delta(H_{6}-O_{5}-C_{3}) &amp; 10 \\ \delta(H_{17}-C_{14}-C_{17}) &amp; -13 \\ \delta(H_{15}-C_{10}-C_{14}) &amp; 10 \\ \delta(C_{8}-C_{10}-C_{14}) &amp; 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) &amp; -13 \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) &amp; 21 \\ \hline \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) &amp; 25 \\ \tau(C_{7}-C_{8}-C_{10}-C_{14}) &amp; -35 \\ \end{split}</math></th><th><math display="block">\tau(H_{22}-C_{19}-O_{18}-C_{1})-16</math> <math display="block">\delta(H_{16}-C_{12}-C_{14}) 11</math> <math display="block">\delta(C_{12}-C_{14}-C_{10})-16</math> <math display="block">\tau(C_{9}-C_{12}-C_{14}-C_{10})-10</math></th><th>δ(C<sub>8</sub>-C<sub>10</sub>-C<sub>14</sub>) -10</th></li<></ol>	$\delta(H_{22}-C_{19}-H_{21})$ 12 $v(C_1-C_7)$ 30 $\delta(H_{11}-C_8-C_{10})$ 23 $v(C_{12}-C_{14})$ 10 $\delta(H_{20}-C_{19}-H_{22})$ 14 $v(O_5-C_3)$ 27 $v(O_5-C_3)$ 27 $v(O_5-C_3)$ 27 $v(C_5-C_1)$ 20 $v(C_{12}-C_{14})$ 18 $v(C_{12}-C_{14})$ 15 $\tau(H_{15}-C_{10}-C_{14}-C_{10})$ -13 $v(O_{18}-C_1)$ 19 $\tau(H_{11}-C_8-C_{10}-C_{14})$ -13 $v(C_1-C_1)$ 25 $\delta(C_{12}-C_{14}-C_{10})$ 10 $\tau(H_{11}-C_8-C_{10}-C_{14})$ 27 $\tau(H_{15}-C_{10}-C_{14}-C_{10})$ 12 $\delta(C_{12}-C_{14}-C_{10})$ 18 $\tau(H_{11}-C_8-C_{10}-C_{14})$ -11 $v(O_5-C_3)$ 15 $\delta(C_9-C_{12}-C_{14})$ -22 -z	<ul> <li>τ(H<sub>21</sub>-C<sub>19</sub>-O<sub>18</sub>-C<sub>1</sub>)-25</li> <li>δ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>) 22</li> <li>δ(H<sub>15</sub>-C<sub>10</sub>-C<sub>14</sub>) -18</li> <li>δ(H<sub>21</sub>-C<sub>19</sub>-H<sub>20</sub>) -12</li> <li>ν(O<sub>18</sub>-C<sub>1</sub>) 14</li> <li>ν(O<sub>18</sub>-C<sub>1</sub>) 23</li> <li>ν(C<sub>9</sub>-C<sub>12</sub>) -14</li> <li>ν(C<sub>9</sub>-C<sub>12</sub>) -14</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 16</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 16</li> <li>ν(C<sub>14</sub>-C<sub>10</sub>) 13</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) -20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 18</li> <li>δ(C<sub>12</sub>-C<sub>14</sub>-C<sub>10</sub>) -10</li> <li>Θ(O<sub>4</sub>-C<sub>1</sub>-O<sub>5</sub>-C<sub>3</sub>) 20</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 25</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 13</li> <li>Θ(O<sub>4</sub>-C<sub>1</sub>-O<sub>5</sub>-C<sub>3</sub>) -30</li> <li>τ(H<sub>13</sub>-C<sub>9</sub>-C<sub>12</sub>-C<sub>14</sub>) 14</li> <li>δ(O<sub>4</sub>-C<sub>3</sub>-O<sub>5</sub>) 40</li> <li>δ(O<sub>4</sub>-C<sub>10</sub>-C<sub>14</sub>) 22</li> </ul>	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) 25\\ \\ (H_{15}-C_{10}-C_{14}) -16\\ \delta(H_{16}-C_{12}-C_{14}) 19\\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) 34\\ \\ (H_{16}-C_{12}-C_{14}) 19\\ \\ \tau(H_{20}-C_{19}-C_{10}) -25\\ \delta(H_{13}-C_{9}-C_{12}) -13\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -18\\ \delta(C_{9}-C_{12}-C_{14}) -28\\ \delta(C_{9}-C_{12}-C_{14}) -28\\ \delta(O_{18}-C_{1}-C_{7}) -10\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) 23\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) -23\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) -17\\ \\ \tau(H_{17}-C_{14}-C_{12}-C_{9}) -17\\ \\ \tau(H_{6}-O_{5}-C_{3}-C_{1}) -10\\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & -14 \\ \delta(H_{17}-C_{14}-C_{12}) & 35 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -21 \\ \hline \\ \delta(H_{6}-O_{5}-C_{3}) & 10 \\ \delta(H_{17}-C_{14}-C_{17}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 10 \\ \delta(C_{8}-C_{10}-C_{14}) & 12 \\ \tau(C_{9}-C_{12}-C_{14}-C_{10}) & -13 \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 21 \\ \hline \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) & 25 \\ \tau(C_{7}-C_{8}-C_{10}-C_{14}) & -35 \\ \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1})-16$ $\delta(H_{16}-C_{12}-C_{14}) 11$ $\delta(C_{12}-C_{14}-C_{10})-16$ $\tau(C_{9}-C_{12}-C_{14}-C_{10})-10$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
	<ol> <li>1192</li> <li>1187</li> <li>1177</li> <li>1149</li> <li>1148</li> <li>1089</li> <li>1080</li> <li>1080</li> <li>988</li> <li>977</li> <li>967</li> <li>924</li> <li>878</li> <li>871</li> <li>839</li> <li>757</li> <li>717</li> <li>696</li> <li>650</li> <li>621</li> <li>617</li> </ol>	δ(H <sub>22</sub> -C <sub>13</sub> -H <sub>21</sub> ) 12           ν(C <sub>1</sub> -C <sub>7</sub> ) 30           δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 23           ν(C <sub>12</sub> -C <sub>14</sub> ) 10           δ(H <sub>20</sub> -C <sub>13</sub> -H <sub>22</sub> ) 14           ν(O <sub>5</sub> -C <sub>3</sub> ) 27           ν(O <sub>5</sub> -C <sub>3</sub> ) -25           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 18           ν(C <sub>12</sub> -C <sub>14</sub> ) 15           τ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> -C <sub>10</sub> ) -13           ν(C <sub>18</sub> -C <sub>1</sub> ) 19           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -23           ν(C <sub>1-</sub> C <sub>1</sub> ) 25           δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 10           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) 27           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) 18           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -11           δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 18           τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -11           δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 15           δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 14	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-25\\ \\ (H_{13}-C_{9}-C_{12}) 22\\ \\ \delta(H_{15}-C_{10}-C_{14}) -18\\ \\ \delta(H_{21}-C_{19}-H_{20}) -12\\ \\ (VO_{18}-C_{1}) 23\\ \\ V(O_{18}-C_{1}) 23\\ \\ V(C_{9}-C_{12}) -14\\ \\ V(C_{14}-C_{10}) 16\\ \\ V(C_{14}-C_{10}) 16\\ \\ V(C_{14}-C_{10}) 12\\ \\ \tau(H_{16}-C_{12}-C_{14}-C_{10}) 24\\ \\ V(O_{18}-C_{19}) 38\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) -20\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) -20\\ \\ \delta(C_{12}-C_{14}-C_{10}) -10\\ \\ \theta(O_{4}-C_{1}-O_{5}-C_{3}) 20\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) 25\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) 25\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) -10\\ \\ \theta(O_{4}-C_{1}-O_{5}-C_{3}) -30\\ \\ \tau(H_{13}-C_{9}-C_{12}-C_{14}) 11\\ \\ \delta(O_{4}-C_{3}-O_{3}) 40\\ \\ \delta(C_{8}-C_{10}-C_{14}) 22\\ \\ \tau(H_{6}-O_{5}-C_{3}-C_{1}) 27\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) 25\\ \\ (H_{15}-C_{10}-C_{14}) -16\\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $	$\begin{split} &\delta(H_{16}-C_{12}-C_{14})-14\\ &\delta(H_{17}-C_{14}-C_{12})35\\ &\tau(H_{21}-C_{19}-O_{18}-C_{1})-21\\ \hline & & & \\ &\delta(H_{6}-O_{5}-C_{3})10\\ &\delta(H_{17}-C_{14}-C_{17})-13\\ &\delta(H_{15}-C_{10}-C_{14})10\\ &\delta(C_{8}-C_{10}-C_{14})12\\ &\tau(C_{9}-C_{12}-C_{14}-C_{10})-13\\ \hline & & \\ &\tau(H_{16}-C_{12}-C_{14}-C_{10})21\\ \hline & & \\ &\tau(H_{16}-C_{12}-C_{14}-C_{10})25\\ \hline & & \\ &\tau(C_{7}-C_{8}-C_{10}-C_{14})-35\\ \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1})-16$ $\delta(H_{16}-C_{12}-C_{14}) 11$ $\delta(C_{12}-C_{14}-C_{10})-16$ $\tau(C_{9}-C_{12}-C_{14}-C_{10})-10$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10

**Table S11.** Vibrational energy distribution analysis for c1··ACN (B3LYP/6-311++G(2d,p)/IEFPCM(<sub>ACN</sub>)). For better comparison, modes involving ACN and the range below 500 cm<sup>-1</sup> are removed from the list. The color coding highlights the modes discussed in the main text, important vibrational contributions are printed in bold type.

$\nu_{scaled}$	Contributing internal coordination and contribution in percentage				
3252	ν(OH)97				
3128	ν(C <sub>9</sub> -H <sub>13</sub> ) 40	ν(C <sub>10</sub> -H <sub>15</sub> ) 12	ν(C <sub>12</sub> -H <sub>16</sub> ) 26	v(C <sub>14</sub> -H <sub>17</sub> ) 20	
3122	n(C <sub>9</sub> -H <sub>13</sub> ) -39	ν(C <sub>10</sub> -H <sub>15</sub> ) 34	ν(C <sub>14</sub> -H <sub>17</sub> ) 19		
3113	ν(C <sub>8</sub> -H <sub>11</sub> ) -20	ν(C <sub>9</sub> -H <sub>13</sub> ) -13	ν(C <sub>10</sub> -H <sub>15</sub> ) -22	v(C <sub>12</sub> -H <sub>16</sub> ) 23	ν(C <sub>14</sub> -H <sub>17</sub> ) 22
3105	ν(C <sub>8</sub> -H <sub>11</sub> ) 37	ν(C <sub>12</sub> -H <sub>15</sub> ) 37	ν(C <sub>14</sub> -H <sub>17</sub> ) -17		
3100	ν(C <sub>8</sub> -H <sub>11</sub> ) -33	ν(C <sub>10</sub> -H <sub>15</sub> ) 30	ν(C <sub>12</sub> -H <sub>16</sub> ) 13	v(C <sub>14</sub> -H <sub>17</sub> ) -22	
3062	ν(C <sub>19</sub> -H <sub>20</sub> ) 90				
2999	ν(C <sub>19</sub> -H <sub>21</sub> ) -33	ν(C <sub>19</sub> -H <sub>22</sub> ) 65			
2957	ν(C <sub>1</sub> -H <sub>2</sub> ) 98				
2941	ν(C <sub>19</sub> -H <sub>21</sub> ) 62	ν(C <sub>19</sub> -H <sub>22</sub> ) 29			
1715	ν(O <sub>4</sub> -C <sub>3</sub> ) 86				
1605	ν(C <sub>8</sub> -C <sub>10</sub> ) 10	v(C <sub>9</sub> -C <sub>12</sub> ) 30			
1589	n(C <sub>7</sub> -C <sub>8</sub> ) -19	ν(C <sub>10</sub> -C <sub>14</sub> ) 28	δ(C <sub>9</sub> -C <sub>12</sub> -C <sub>14</sub> ) 10		
1499	δ(H <sub>11</sub> -C <sub>8</sub> -H <sub>10</sub> ) -15	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) -16	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>8</sub> ) 18	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) -18	
1467	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) -30	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 49	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 13		
1458	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) -10	δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>11</sub> ) 26			
1451	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) -28	δ(H <sub>21</sub> -C <sub>19</sub> -H <sub>20</sub> ) 31	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) -16	τ(H <sub>20</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -12	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 11
1442	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 18	δ(H <sub>21</sub> -C <sub>19</sub> -H <sub>20</sub> ) 49	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 16		
1382	ν(O <sub>5</sub> -C <sub>3</sub> ) 15	δ(H <sub>6</sub> -O <sub>5</sub> -C <sub>3</sub> ) 33	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) -17	δ(O <sub>4</sub> -C <sub>3</sub> -O <sub>5</sub> ) -11	
1351	δ(H <sub>11</sub> -C <sub>8</sub> -H <sub>10</sub> ) 14	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>8</sub> ) -10	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 24	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 11	
1326	δ(H <sub>11</sub> -C <sub>8</sub> -H <sub>10</sub> ) -12	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 16	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 30		
1306	ν(C <sub>7</sub> -C <sub>8</sub> ) -12	ν(C <sub>8</sub> -C <sub>10</sub> )11	v(C <sub>9</sub> -C <sub>12</sub> ) -11	v(C <sub>12</sub> -C <sub>14</sub> ) 10	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 23
1263	ν(C <sub>7</sub> -C <sub>8</sub> ) 11	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 27			
1193	ν(O <sub>5</sub> -C <sub>3</sub> ) -12	ν(C <sub>1</sub> -C <sub>7</sub> ) 24			
1190	ν(O <sub>18</sub> -C <sub>1</sub> ) 10	δ(H <sub>22</sub> -C <sub>19</sub> -H <sub>21</sub> ) 11	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -23	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 25	
1175	δ(H <sub>11</sub> -C <sub>8</sub> -H <sub>10</sub> ) 22	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 22	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>8</sub> ) 18	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) -14	
1165	ν(O <sub>5</sub> -C <sub>3</sub> ) 35	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) -13			
1156	ν(C <sub>12</sub> -C <sub>14</sub> ) 10	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>8</sub> ) 17	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 19	δ( <sub>H17-</sub> C <sub>14</sub> -C <sub>11</sub> ) 36	
1145	δ(H <sub>20</sub> -C <sub>19</sub> -H <sub>22</sub> ) 14	δ(H <sub>21</sub> -C <sub>19</sub> -H <sub>20</sub> ) -12	τ(H <sub>20</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 33	$\tau$ (H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -18	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -16
1091	ν(O <sub>18</sub> -C <sub>1</sub> ) 36	ν(O <sub>18</sub> -C <sub>19</sub> ) -31			
1078	ν(C <sub>8</sub> -C <sub>10</sub> ) 19	v(C <sub>9</sub> -C <sub>12</sub> ) -13	v(O <sub>18</sub> -C <sub>19</sub> ) 10	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) -11	δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>11</sub> ) -11
1027	ν(C <sub>10</sub> -C <sub>14</sub> ) 17	ν(C <sub>12</sub> -C <sub>14</sub> ) 19	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 11	δ(C <sub>9</sub> -C <sub>12</sub> -C <sub>14</sub> ) -18	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -12
999	ν(C <sub>10</sub> -C <sub>14</sub> ) -13	v(C <sub>12</sub> -C <sub>14</sub> ) -15	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -12	δ(C <sub>9</sub> -C <sub>12</sub> -C <sub>14</sub> ) -24	δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 17
990	$\tau(H_{15}-C_{10}-C_8-C_7)$ 14	$\tau$ (H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 16	τ(H <sub>17</sub> -C <sub>14</sub> -C <sub>12</sub> -C <sub>9</sub> ) 21	$\tau$ (C <sub>7</sub> -C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -12	τ(C <sub>9</sub> -C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) -11
976	ν(O <sub>18</sub> -C <sub>1</sub> ) 18	v(O <sub>18</sub> -C <sub>19</sub> ) 38			
970	τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>7</sub> -C <sub>1</sub> ) 21	τ(H <sub>13</sub> -C <sub>9</sub> -C <sub>7</sub> -C <sub>1</sub> ) 23	τ(H <sub>15</sub> -C <sub>10</sub> -C <sub>8</sub> -C <sub>7</sub> ) -22	$\tau$ (H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 22	
925	τ(H <sub>11</sub> -C <sub>8</sub> -C <sub>7</sub> -C <sub>1</sub> ) -22	τ(H <sub>13</sub> -C <sub>9</sub> -C <sub>7</sub> -C <sub>1</sub> ) 19	τ(H <sub>17</sub> -C <sub>14</sub> -C <sub>12</sub> -C <sub>9</sub> ) -17		
887	ν(C <sub>3</sub> -C <sub>1</sub> ) 28				
873	δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) -14	τ(O <sub>4</sub> -C <sub>1</sub> -O <sub>5</sub> -C <sub>3</sub> ) -22			
858	$\tau$ (H <sub>6</sub> -O <sub>5</sub> -C <sub>3</sub> -C <sub>1</sub> ) 41	τ(N <sub>28</sub> -H <sub>6</sub> -O <sub>5</sub> -C <sub>3</sub> ) 45			
840	$\tau(H_{11}-C_8-C_7-C_1)$ -26	$\tau$ (H <sub>13</sub> -C <sub>9</sub> -C <sub>7</sub> -C <sub>1</sub> ) -26	τ(H <sub>15</sub> -C <sub>10</sub> -C <sub>8</sub> -C <sub>7</sub> ) -23	$\tau$ (H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 24	
762	$\tau(H_{15}-C_{10}-C_8-C_7)$ -16	$\tau$ (H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) -13	$\tau$ (C <sub>7</sub> -C8-C <sub>10</sub> -C <sub>14</sub> ) -14		
714	δ(C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) 16	τ(O <sub>4</sub> -C <sub>1</sub> -O <sub>5</sub> -C <sub>3</sub> ) -20			
697	$\tau$ (H <sub>17</sub> -C <sub>14</sub> -C <sub>12</sub> -C <sub>9</sub> ) -28	$\tau(C_7 - C_8 - C_{10} - C_{14}) - 23$	$\tau$ (C <sub>9</sub> -C <sub>12</sub> -C <sub>14</sub> -C <sub>10</sub> ) -10	τ(C <sub>1</sub> -C <sub>9</sub> -C <sub>8</sub> -C <sub>7</sub> ) 12	
662	ν(O <sub>5</sub> -C <sub>3</sub> ) 10	δ(O <sub>4</sub> -C <sub>3</sub> -O <sub>5</sub> ) 39	δ(O <sub>18</sub> -C <sub>1</sub> -C <sub>3</sub> ) 12		
620	δ(C <sub>7</sub> -C <sub>8</sub> -C <sub>10</sub> ) 18	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -35	δ(C <sub>9</sub> -C <sub>12</sub> -C <sub>14</sub> ) 25		
595	δ(C <sub>7</sub> -C <sub>8</sub> -C <sub>10</sub> ) 14	τ(O <sub>4</sub> -C <sub>1</sub> -O <sub>5</sub> -C <sub>3</sub> ) -13	τ(O <sub>18</sub> -C <sub>3</sub> -C <sub>7</sub> -C <sub>1</sub> ) 15		
514	δ(C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 11	τ(O <sub>4</sub> -C <sub>1</sub> -O <sub>5</sub> -C <sub>3</sub> ) 13	τ(C <sub>1</sub> -C <sub>9</sub> -C <sub>8</sub> -C <sub>7</sub> ) -19		

<b>Table S12.</b> Vibrational energy distribution analysis for c1 <sub>1</sub> ··DMSO (B3LYP/6-311++G(2d,p)/IEFPCM( <sub>DMSO</sub> )).
Modes involving DMSO and the range below 500 cm <sup>-1</sup> are removed from the list. The color coding highlights
the modes discussed in the main text, important vibrational contributions are printed in bold type.

Vscaled	Contributing interna	l coordination and cont	ribution in percentage			
3121	v(C <sub>9</sub> -H <sub>13</sub> ) -44	v(C <sub>10</sub> -H <sub>15</sub> ) 31	v(C <sub>14</sub> -H <sub>17</sub> ) 14			
3113	v(C <sub>8</sub> -H <sub>11</sub> ) -19	v(C <sub>9</sub> -H <sub>13</sub> ) -16	v(C <sub>10</sub> -H <sub>15</sub> ) -21	v(C <sub>12</sub> -H <sub>16</sub> ) 19	v(C <sub>14</sub> -H <sub>17</sub> ) 23	
3105	ν(C <sub>8</sub> -H <sub>11</sub> ) 35	v(C <sub>12</sub> -H <sub>16</sub> ) 38	ν(C <sub>14</sub> -H <sub>17</sub> ) -16			
3099	v(C <sub>8</sub> -H <sub>11</sub> ) 36	v(C <sub>10</sub> -H <sub>15</sub> ) -30	ν(C <sub>12</sub> -H <sub>16</sub> ) -12	v(C <sub>14</sub> -H <sub>17</sub> ) 20		
3060	v(C <sub>19</sub> -H <sub>20</sub> ) 90					
2999	v(C <sub>19</sub> -H <sub>21</sub> ) -32	v(C <sub>19</sub> -H <sub>22</sub> ) 66				
2957	v(C <sub>1</sub> -H <sub>2</sub> ) 99					
2941	v(C <sub>19</sub> -H <sub>21</sub> ) 64	v(C <sub>19</sub> -H <sub>22</sub> ) 27				
2864	v(OH) 92					
1702	v(O <sub>4</sub> -C <sub>3</sub> ) 85					
1605	ν(C <sub>8</sub> -C <sub>10</sub> ) 10	v(C <sub>9</sub> -C <sub>12</sub> ) 30				
1588	v(C <sub>7</sub> -C <sub>8</sub> ) -18	ν(C <sub>14</sub> -C <sub>10</sub> ) 28	δ(C <sub>7</sub> -C <sub>8</sub> -C <sub>10</sub> ) 11			
1498	δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 16	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 16	δ(H <sub>15</sub> -C <sub>10</sub> -C <sub>14</sub> ) 17	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 18		
1467	δ(H <sub>20</sub> -C <sub>19</sub> -C <sub>22</sub> ) -31	δ(H <sub>22</sub> -C <sub>19</sub> -C <sub>21</sub> ) 48	$\tau$ (H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 13			
1458	$\delta(H_{15}-C_{10}-C_{14})$ -11	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 10	δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>10</sub> ) 26			
1451	δ(H <sub>20</sub> -C <sub>19</sub> -C <sub>22</sub> ) 28	δ(H <sub>21</sub> -C <sub>19</sub> -C <sub>20</sub> ) -30	δ(H <sub>22</sub> -C <sub>19</sub> -C <sub>21</sub> ) 17	$\tau$ (H <sub>20</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 12	$\tau$ (H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -11	
1442	δ(H <sub>20</sub> -C <sub>19</sub> -C <sub>22</sub> ) 16	δ(H <sub>21</sub> -C <sub>19</sub> -C <sub>20</sub> ) 50	δ(H <sub>22</sub> -C <sub>19</sub> -C <sub>21</sub> ) 15			
1425	δ(O <sub>DMSO</sub> -H <sub>6</sub> -C <sub>5</sub> ) 14	δ(H <sub>6</sub> -O <sub>5</sub> -C <sub>3</sub> ) 30				
1354	δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) 11	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 43				
1332	δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) -12	δ(H <sub>13</sub> -C <sub>9</sub> -C <sub>12</sub> ) 14	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 29	$\tau$ (H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) -11		
1311	ν(C <sub>8</sub> -C <sub>10</sub> ) 13	v(C <sub>9</sub> -C <sub>12</sub> ) -15	v(C <sub>12</sub> -C <sub>14</sub> ) 10	$\tau$ (H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 24		
1266	ν(C <sub>7</sub> -C <sub>8</sub> ) 12	τ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> -C <sub>19</sub> ) 20				
1208	ν(O <sub>5</sub> -C <sub>3</sub> ) 40	ν(C <sub>1</sub> -C <sub>7</sub> ) -12	δ(H <sub>2</sub> -C <sub>1</sub> -O <sub>18</sub> ) 11			
1191	δ(H <sub>22</sub> -C <sub>19</sub> -C <sub>21</sub> ) 11	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -23	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) 25			
1191 1179	δ(H <sub>22</sub> -C <sub>19</sub> -C <sub>21</sub> ) 11 ν(O <sub>5</sub> -C <sub>3</sub> ) 13	τ(H <sub>21</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -23 ν(C <sub>1</sub> -C <sub>7</sub> ) 20	$\tau(H_{22}-C_{19}-O_{18}-C_{1}) 25$ $\tau(H_{2}-C_{1}-O_{18}-C_{19}) -13$			
1191 1179 1174	δ(H <sub>22</sub> -C <sub>19</sub> -C <sub>21</sub> ) 11 <b>v(O<sub>5</sub>-C<sub>3</sub>) 13</b> δ(H <sub>11</sub> -C <sub>8</sub> -C <sub>10</sub> ) -19	$\begin{aligned} \tau(H_{21}-C_{19}-O_{18}-C_{1}) &-23 \\ \hline v(C_1-C_7) & 20 \\ \delta(H_{13}-C_9-C_{12}) &-20 \end{aligned}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & 25 \\ \tau(H_2\text{-}C_1\text{-}O_{18}\text{-}C_{19}) & -13 \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14}) & 19 \end{split}$	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 15		
1191 1179 1174 1155	$\begin{split} \delta(H_{22}-C_{19}-C_{21}) & 11 \\ \hline \nu(O_5-C_3) & 13 \\ \delta(H_{11}-C_8-C_{10}) & -19 \\ \nu(C_{12}-C_{14}) & -10 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1}) &-23\\ \hline \nu(C_{1}-C_{7}) &20\\ \delta(H_{13}-C_{9}-C_{12}) &-20\\ \delta(H_{15}-C_{10}-C_{14}) &17 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_{2}-C_{1}-O_{18}-C_{19}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \delta(H_{16}-C_{12}-C_{14}) & -19 \end{split}$	δ(H <sub>16</sub> -C <sub>12</sub> -C <sub>14</sub> ) 15 δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>10</sub> ) 36		
1191 1179 1174 1155 1145	$\begin{array}{c} \delta(H_{22}\text{-}C_{19}\text{-}C_{21})11\\ \hline\\ \nu(O_5\text{-}C_3)13\\ \delta(H_{11}\text{-}C_8\text{-}C_{10})-19\\ \nu(C_{12}\text{-}C_{14})-10\\ \delta(H_{20}\text{-}C_{19}\text{-}C_{22})14 \end{array}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_1)-23 \\ \hline \nu(C_1-C_7) \ 20 \\ \delta(H_{13}-C_9-C_{12})-20 \\ \delta(H_{15}-C_{10}-C_{14}) \ 17 \\ \delta(H_{21}-C_{19}-C_{20})-12 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_{2}-C_{1}-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \end{split}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ 15 \\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ 36 \\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ \text{-}18 \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -18	
1191 1179 1174 1155 1145 1090	$\begin{array}{c} \delta(H_{22}-C_{19}-C_{21})11\\ \hline \\ \nu(0_5-C_8)13\\ \hline \\ \delta(H_{11}-C_8-C_{10})-19\\ \nu(C_{12}-C_{14})-10\\ \hline \\ \delta(H_{20}-C_{19}-C_{22})14\\ \nu(O_{18}-C_1)37 \end{array}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_1)-23 \\ \hline \nu(C_1-C_7)\ 20 \\ \delta(H_{13}-C_9-C_{12})-20 \\ \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_1) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_1) & 34 \end{split}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ 15 \\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ 36 \\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ \text{-}18 \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -18	
1191 1179 1174 1155 1145 1090 1077	$\begin{array}{c} \delta(H_{22}-C_{19}-C_{21}) \ 11 \\ \hline \nu(O_5-C_3) \ 13 \\ \delta(H_{11}-C_8-C_{10}) \ -19 \\ \nu(C_{12}-C_{14}) \ -10 \\ \delta(H_{20}-C_{19}-C_{22}) \ 14 \\ \nu(O_{18}-C_1) \ 37 \\ \nu(C_8-C_{10}) \ 19 \end{array}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_1) &-23 \\ \hline \nu(C_1-C_7) & 20 \\ \delta(H_{13}-C_9-C_{12}) &-20 \\ \delta(H_{15}-C_{10}-C_{14}) & 17 \\ \delta(H_{21}-C_{19}-C_{20}) &-12 \\ \nu(O_{18}-C_{19}) &-32 \\ \nu(C_9-C_{12}) &-13 \\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \tau(H_{22}-C_{1}-O_{18}-C_{19}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \nu(O_{18}-C_{19}) & 10 \end{split}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14})\;15\\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{10})\;36\\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\;\text{-}18\\ &\delta(H_{13}\text{-}C_{9}\text{-}C_{12})\;\text{-}13 \end{split}$	τ(H <sub>22</sub> -C <sub>19</sub> -O <sub>18</sub> -C <sub>1</sub> ) -18 δ(H <sub>17</sub> -C <sub>14</sub> -C <sub>10</sub> ) 11	
1191 1179 1174 1155 1145 1090 1077 1026	$\begin{array}{c} \delta(H_{22}-C_{19}-C_{21})11\\ \hline\\ \nu(O_5-C_3)13\\ \hline\\ \delta(H_{11}-C_8-C_{10})-19\\ \nu(C_{12}-C_{14})-10\\ \hline\\ \delta(H_{20}-C_{19}-C_{22})14\\ \nu(O_{18}-C_{1})37\\ \nu(C_8-C_{10})19\\ \nu(C_{12}-C_{14})18\\ \end{array}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})\ -12 \\ \nu(O_{18}-C_{19})\ -32 \\ \nu(C_{9}-C_{12})\ -13 \\ \nu(C_{14}-C_{10})\ 15 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) & 15 \\ \delta(H_{17}-C_{14}-C_{10}) & 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) & -18 \\ \delta(H_{13}-C_{9}-C_{12}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 11 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ \text{-}18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ \text{11} \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ \text{10} \end{split}$	δ(C8-C10-C14) -10
1191 1179 1174 1155 1145 1090 1077 1026 999	$\begin{array}{c} \delta(H_{22}-C_{19}-C_{21})11\\ \hline\\ \hline\\ \nu(O_5-C_9)13\\ \hline\\ \delta(H_{11}-C_8-C_{10})-19\\ \nu(C_{12}-C_{14})-10\\ \hline\\ \delta(H_{20}-C_{19}-C_{22})14\\ \nu(O_{18}-C_1)37\\ \nu(C_8-C_{10})19\\ \nu(C_{12}-C_{14})18\\ \nu(C_{12}-C_{14})-16\\ \hline\end{array}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ -13 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_{2}-C_{1}-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_{9}-C_{12}-C_{14}) & -17 \\ \hline \delta(C_{9}-C_{12}-C_{14}) & -23 \\ \end{split}$	$\begin{split} \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ 15 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ 36 \\ \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ -18 \\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12}) \ -13 \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14}) \ 11 \\ \delta(C_8\text{-}C_{10}\text{-}C_{14}) \ -12 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999	$\begin{split} &\delta(H_{22}-C_{19}-C_{21})11\\ \hline &V(O_5-C_3)13\\ &\delta(H_{11}-C_8-C_{10})-19\\ &v(C_{12}-C_{14})-10\\ &\delta(H_{20}-C_{19}-C_{22})14\\ &v(O_{18}-C_1)37\\ &v(C_8-C_{10})19\\ &v(C_{12}-C_{14})18\\ &v(C_{12}-C_{14})-16\\ &\tau(H_{15}-C_{10}-C_8-C_7)-13 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_1)-23 \\ \hline \nu(C_1-C_7) \ 20 \\ \hline \delta(H_{13}-C_9-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14}) \ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_9-C_{12})-13 \\ \nu(C_{14}-C_{10}) \ 15 \\ \nu(C_{14}-C_{10})-13 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 18 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \tau(O_{18}-C_{19}) & 10 \\ \delta(C_9-C_{12}-C_{14}) & -17 \\ \delta(C_9-C_{12}-C_{14}) & -23 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977	$\begin{split} &\delta(H_{22}-C_{19}-C_{21})11\\ \hline &V(O_5-C_3)13\\ \hline &\delta(H_{11}-C_8-C_{10})-19\\ &v(C_{12}-C_{14})-10\\ \hline &\delta(H_{20}-C_{19}-C_{22})14\\ &v(O_{18}-C_1)37\\ &v(C_8-C_{10})19\\ &v(C_8-C_{10})19\\ &v(C_{12}-C_{14})18\\ &v(C_{12}-C_{14})-16\\ \hline &\tau(H_{15}-C_{10}-C_8-C_7)-13\\ &v(O_{18}-C_1)17 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})\ -12 \\ \nu(O_{18}-C_{19})\ -32 \\ \nu(C_{9}-C_{12})\ -13 \\ \nu(C_{9}-C_{12})\ -13 \\ \nu(C_{14}-C_{10})\ -13 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \end{split}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14})\ 15\\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{10})\ 36\\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1})\ -18\\ &\delta(H_{13}\text{-}C_{9}\text{-}C_{12})\ -13\\ &\delta(H_{15}\text{-}C_{10}\text{-}C_{14})\ 11\\ &\delta(C_8\text{-}C_{10}\text{-}C_{14})\ -12\\ &\tau(C_7\text{-}C_8\text{-}C_{10}\text{-}C_{14})\ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1) & -18\\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11\\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10\\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977 970	$\begin{split} &\delta(H_{22}-C_{19}-C_{21})11\\ \hline &V(O_5-C_9)13\\ \hline &\delta(H_{11}-C_8-C_{10})-19\\ &V(C_{12}-C_{14})-10\\ \hline &\delta(H_{20}-C_{19}-C_{22})14\\ &V(O_{18}-C_1)37\\ &V(C_8-C_{10})19\\ &V(C_{12}-C_{14})18\\ &V(C_{12}-C_{14})-16\\ \hline &\tau(H_{15}-C_{10}-C_8-C_7)-13\\ &V(O_{18}-C_1)17\\ \hline &\tau(H_{11}-C_8-C_{10}-C_{14})17 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ -13 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -13 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 22 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1090 1077 1026 999 990 977 970	$\begin{split} &\delta(H_{22}-C_{19}-C_{21})11\\ \hline &V(O_5-C_3)13\\ \hline &\delta(H_{11}-C_8-C_{10})-19\\ &v(C_{12}-C_{14})-10\\ \hline &\delta(H_{20}-C_{19}-C_{22})14\\ &v(O_{18}-C_1)37\\ &v(C_8-C_{10})19\\ &v(C_{12}-C_{14})18\\ &v(C_{12}-C_{14})-16\\ &\tau(H_{15}-C_{10}-C_8-C_7)-13\\ &v(O_{18}-C_1)17\\ &\tau(H_{11}-C_8-C_{10}-C_{14})17\\ &\tau(H_{6}-O_5-C_{2}-C_{1})31 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})-13 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23 \\ \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 22 \\ \hline \tau(S=O-H_6-O_5) & -19 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ -16 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8}) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977 970 970 963	$\begin{split} & \delta(H_{22}-C_{19}-C_{21})11 \\ \hline & V(O_5-C_3)13 \\ & \delta(H_{11}-C_8-C_{10})-19 \\ & v(C_{12}-C_{14})-10 \\ & \delta(H_{20}-C_{19}-C_{22})14 \\ & v(O_{18}-C_1)37 \\ & v(C_8-C_{10})19 \\ & v(C_8-C_{10})19 \\ & v(C_{12}-C_{14})18 \\ & v(C_{12}-C_{14})-16 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-13 \\ & v(O_{18}-C_1)17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_6-O_5-C_3-C_1)31 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})19 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23\\ \hline \nu(C_{1}-C_{7})\ 20\\ \hline \delta(H_{13}-C_{9}-C_{12})-20\\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17\\ \hline \delta(H_{21}-C_{19}-C_{20})-12\\ \nu(O_{18}-C_{19})-32\\ \nu(C_{9}-C_{12})-13\\ \nu(C_{9}-C_{12})-13\\ \nu(C_{14}-C_{10})\ 15\\ \nu(C_{14}-C_{10})\ 15\\ \nu(C_{14}-C_{10})-13\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18\\ \nu(O_{18}-C_{19})\ 35\\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23\\ \hline \tau(O_{DMS0}-H_{6}-O_{5}-C_{3})\ 41\\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(S=O-H_6-O_5) & -19 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1) & -18\\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11\\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10\\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977 970 970 963 924 891	$\begin{split} &\delta(H_{22}-C_{19}-C_{21})11\\ \hline &V(O_5-C_3)13\\ \hline &\delta(H_{11}-C_8-C_{10})-19\\ &V(C_{12}-C_{14})-10\\ &\delta(H_{20}-C_{19}-C_{22})14\\ &V(O_{18}-C_1)37\\ &V(C_8-C_{10})19\\ &V(C_{12}-C_{14})18\\ &V(C_{12}-C_{14})-16\\ &\tau(H_{15}-C_{10}-C_8-C_7)-13\\ &V(O_{18}-C_1)17\\ &\tau(H_{11}-C_8-C_{10}-C_{14})17\\ &\tau(H_{11}-C_8-C_{10}-C_{14})19\\ &V(C_3-C_1)28\\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_1)-23 \\ \hline \nu(C_1-C_7) \ 20 \\ \hline \delta(H_{13}-C_9-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14}) \ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_9-C_{12})-13 \\ \nu(C_{14}-C_{10}) \ 15 \\ \nu(C_{14}-C_{10}) \ 15 \\ \nu(C_{14}-C_{10})-13 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 18 \\ \nu(O_{18}-C_{19}) \ 35 \\ \tau(H_{13}-C_9-C_7-C_1)-23 \\ \tau(O_{DMSO}-H_6-O_5-C_3) \ 41 \\ \tau(H_{13}-C_9-C_7-C_1) \ 20 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_1) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \tau(H_{20}-C_{19}-O_{18}-C_1) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) & 22 \\ \hline \tau(H_{15}-C_{10}-C_8-C_7) & 22 \\ \tau(S=O-H_6-O_5) & -19 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \end{split}$	$\begin{split} \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ 15 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ 36 \\ \tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ -18 \\ \delta(H_{13}\text{-}C_{9}\text{-}C_{12}) \ -13 \\ \delta(H_{15}\text{-}C_{10}\text{-}C_{14}) \ 11 \\ \delta(C_8\text{-}C_{10}\text{-}C_{14}) \ -12 \\ \tau(C_7\text{-}C_8\text{-}C_{10}\text{-}C_{14}) \ 16 \\ \tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18\\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11\\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10\\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1090 1077 1026 999 990 977 970 963 924 891	$\begin{split} & \delta(H_{22}-C_{19}-C_{21})11 \\ \hline & v(O_5-C_3)13 \\ \hline & \delta(H_{11}-C_8-C_{10})-19 \\ & v(C_{12}-C_{14})-10 \\ & \delta(H_{20}-C_{19}-C_{22})14 \\ & v(O_{18}-C_1)37 \\ & v(C_8-C_{10})19 \\ & v(C_8-C_{10})19 \\ & v(C_{12}-C_{14})18 \\ & v(C_{12}-C_{14})-16 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-13 \\ & v(O_{18}-C_1)17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & v(C_3-C_1)28 \\ & \delta(C_{12}-C_{14}-C_{10})15 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ -13 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23 \\ \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20 \\ \hline o(O_{4}-C_{1}-O_{5}-C_{3})\ 19 \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_1) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_1) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 22 \\ \hline \tau(H_{15}-C_{10}-C_8-C_7) & 22 \\ \hline \tau(S=O-H_6-O_5) & -19 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \end{split}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ 15 \\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ 36 \\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ -18 \\ &\delta(H_{13}\text{-}C_{9}\text{-}C_{12}) \ -13 \\ &\delta(H_{15}\text{-}C_{10}\text{-}C_{14}) \ 11 \\ &\delta(C_8\text{-}C_{10}\text{-}C_{14}) \ -12 \\ &\tau(C_7\text{-}C_8\text{-}C_{10}\text{-}C_{14}) \ 16 \\ &\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18\\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11\\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10\\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1090 1077 1026 999 990 977 970 963 924 891 874	$\begin{split} & (H_{22}-C_{19}-C_{21})11 \\ \hline & (O_5-C_3)13 \\ \hline & (H_{11}-C_8-C_{10})-19 \\ & (V(C_{12}-C_{14})-10 \\ \hline & (H_{20}-C_{19}-C_{22})14 \\ & (V(O_{18}-C_1)37 \\ & (V(O_{18}-C_1)37 \\ & (V(C_{8}-C_{10})19 \\ & (V(C_{12}-C_{14})18 \\ & (V(C_{12}-C_{14})-16 \\ \hline & (H_{15}-C_{10}-C_8-C_7)-13 \\ & (V(O_{18}-C_1)17 \\ & (T(H_{11}-C_8-C_{10}-C_{14})17 \\ & (T(H_{11}-C_8-C_{10}-C_{14})17 \\ \hline & (T(H_{11}-C_8-C_{10}-C_{14})19 \\ & (V(C_{12}-C_{14}-C_{10})15 \\ & (U(H_{11}-C_8-C_{10}-C_{14})-26 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})-13 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23 \\ \hline \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20 \\ \hline o(O_{4}-C_{1}-O_{5}-C_{3})\ 19 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 27 \\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(S=O-H_6-O_5) & -19 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 20 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 20 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 23 \\ \hline \end{array}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1) & -18\\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11\\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10\\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977 970 970 970 973 970 973 874 891 874 840 765	$\begin{split} & \delta(H_{22}-C_{19}-C_{21})11 \\ \hline & V(O_5-C_3)13 \\ \hline & \delta(H_{11}-C_8-C_{10})-19 \\ & V(C_{12}-C_{14})-10 \\ & \delta(H_{20}-C_{19}-C_{22})14 \\ & V(O_{18}-C_1)37 \\ & V(C_{8}-C_{10})19 \\ & V(C_{12}-C_{14})18 \\ & V(C_{12}-C_{14})18 \\ & V(C_{12}-C_{14})-16 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-13 \\ & V(O_{18}-C_1)17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})19 \\ & V(C_{3}-C_{1})28 \\ & \delta(C_{12}-C_{14}-C_{10})15 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})-26 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-17 \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 13 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20 \\ \hline 0(O_{4}-C_{1}-O_{5}-C_{3})\ 41 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20 \\ \hline 0(O_{4}-C_{1}-O_{5}-C_{3})\ 19 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 27 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 17 \\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 22 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 20 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 23 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & -11 \\ \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \\ \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977 970 963 924 891 874 840 765 720	$\begin{split} & \delta(H_{22}-C_{19}-C_{21})11 \\ \hline & v(O_5-C_8)13 \\ \hline & \delta(H_{11}-C_8-C_{10})-19 \\ & v(C_{12}-C_{14})-10 \\ & \delta(H_{20}-C_{19}-C_{22})14 \\ & v(O_{18}-C_1)37 \\ & v(C_8-C_{10})19 \\ & v(C_{12}-C_{14})18 \\ & v(C_{12}-C_{14})-16 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-13 \\ & v(O_{18}-C_1)17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})19 \\ & v(C_3-C_1)28 \\ & \delta(C_{12}-C_{14}-C_{10})15 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-17 \\ & \delta(O_4-C_3-O_5)12 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ -13 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23 \\ \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41 \\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20 \\ \hline 0(O_{4}-C_{1}-O_{5}-C_{3})\ 19 \\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 17 \\ \delta(C_{12}-C_{14}-C_{10})\ 15 \\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_1) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_1) & 34 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_1) & 34 \\ \hline \tau(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 22 \\ \hline \tau(H_{17}-C_{16}-C_8-C_7) & 22 \\ \hline \tau(H_{17}-C_{16}-C_8-C_7) & 22 \\ \hline \tau(H_{17}-C_{16}-C_8-C_7) & 23 \\ \hline \tau(H_{17}-C_{16}-C_8-C_8-C_7) & 23 \\ \hline \tau(H_{17}-C_8-C_8-C_8-C_8-C_8-C_8-C_8-C_8-C_8-C_8$	$\begin{split} &\delta(H_{16}-C_{12}-C_{14}) \ 15 \\ &\delta(H_{17}-C_{14}-C_{10}) \ 36 \\ &\tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ &\delta(H_{13}-C_{9}-C_{12}) \ -13 \\ &\delta(H_{15}-C_{10}-C_{14}) \ 11 \\ &\delta(C_8-C_{10}-C_{14}) \ -12 \\ &\tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ &\tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \\ &\tau(H_{17}-C_{14}-C_{10}-C_8) \ 24 \\ &o(C_1-C_8-C_9-C_7) \ -10 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 990 977 970 970 970 963 924 891 874 840 765 720 697	$\begin{split} & (H_{22}-C_{19}-C_{21})11 \\ \hline & (O_5-C_3)13 \\ \hline & (H_{11}-C_8-C_{10})-19 \\ & (V(C_{12}-C_{14})-10 \\ \hline & (H_{20}-C_{19}-C_{22})14 \\ & (V(O_{18}-C_1)37 \\ & (V(O_{18}-C_1)37 \\ & (V(C_{8}-C_{10})19 \\ & (V(C_{12}-C_{14})18 \\ & (V(C_{12}-C_{14})-16 \\ \hline & (H_{15}-C_{10}-C_8-C_7)-13 \\ & (V(O_{18}-C_1)17 \\ & (T(H_{11}-C_8-C_{10}-C_{14})17 \\ & (T(H_{11}-C_8-C_{10}-C_{14})17 \\ \hline & (T(H_{11}-C_8-C_{10}-C_{14})19 \\ & (V(C_{12}-C_{14}-C_{10})15 \\ & (T(H_{11}-C_8-C_{10}-C_{14})-12 \\ \hline & (H_{11}-C_8-C_{10}-C_{14})-12 \\ \hline & (U(H_{11}-C_8-C_{10}-C_{14})-12 \\ \hline & (U(H_{11}-C_8-C_{14}-C_{14})$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23 \\ \hline \nu(C_{1}-C_{7})\ 20 \\ \hline \delta(H_{13}-C_{9}-C_{12})-20 \\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17 \\ \hline \delta(H_{21}-C_{19}-C_{20})-12 \\ \nu(O_{18}-C_{19})-32 \\ \nu(C_{9}-C_{12})-13 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})\ 15 \\ \nu(C_{14}-C_{10})-13 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18 \\ \nu(O_{18}-C_{19})\ 35 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23 \\ \hline \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20 \\ \hline 0(O_{4}-C_{1}-O_{5}-C_{3})\ 19 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 27 \\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 27 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 15 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 19 \\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{12}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(S=O-H_6-O_5) & -19 \\ \hline \tau(H_{15}-C_{10}-C_8-C_7) & 23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \hline \end{array}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{27}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \\ \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 970 970 970 970 970 973 874 891 874 840 765 720 697 670	$\begin{split} & \delta(H_{22}-C_{19}-C_{21})11 \\ \hline & v(O_5-C_3)13 \\ & \delta(H_{11}-C_8-C_{10})-19 \\ & v(C_{12}-C_{14})-10 \\ & \delta(H_{20}-C_{19}-C_{22})14 \\ & v(O_{18}-C_1)37 \\ & v(C_{12}-C_{14})13 \\ & v(C_{12}-C_{14})19 \\ & v(C_{12}-C_{14})-16 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-13 \\ & v(O_{18}-C_1)17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})19 \\ & v(C_3-C_1)28 \\ & \delta(C_{12}-C_{14}-C_{10})15 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})-26 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-17 \\ & \delta(O_4-C_3-O_5)12 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})-12 \\ & \delta(O_4-C_3-O_5)35 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23\\ \hline \nu(C_{1}-C_{7})\ 20\\ \hline \delta(H_{13}-C_{9}-C_{12})-20\\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17\\ \hline \delta(H_{21}-C_{19}-C_{20})-12\\ \nu(O_{18}-C_{19})-32\\ \nu(C_{9}-C_{12})-13\\ \nu(C_{14}-C_{10})\ 15\\ \nu(C_{14}-C_{10})\ 15\\ \nu(C_{14}-C_{10})\ 13\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18\\ \nu(O_{18}-C_{19})\ 35\\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23\\ \hline \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41\\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20\\ \hline 0\\ (O_{4}-C_{1}-O_{5}-C_{3})\ 19\\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 25\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 19\\ \hline \delta(C_{12}-C_{14}-C_{10})\ 15\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 19\\ \hline \delta(O_{18}-C_{1}-C_{3})\ 13\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \nu(O_{18}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -17 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 22 \\ \hline \tau(S=O-H_6-O_5) & -19 \\ \hline \tau(H_{15}-C_{10}-C_{8}-C_{7}) & 23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 20 \\ \hline \end{split}$	$\begin{split} &\delta(H_{16}\text{-}C_{12}\text{-}C_{14}) \ 15 \\ &\delta(H_{17}\text{-}C_{14}\text{-}C_{10}) \ 36 \\ &\tau(H_{21}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) \ -18 \\ &\delta(H_{13}\text{-}C_{9}\text{-}C_{12}) \ -13 \\ &\delta(H_{15}\text{-}C_{10}\text{-}C_{14}) \ 11 \\ &\delta(C_8\text{-}C_{10}\text{-}C_{14}) \ -12 \\ &\tau(C_7\text{-}C_8\text{-}C_{10}\text{-}C_{14}) \ 16 \\ &\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8) \ 16 \\ &\tau(H_{17}\text{-}C_{14}\text{-}C_{10}\text{-}C_8) \ 24 \\ &o(C_1\text{-}C_8\text{-}C_9\text{-}C_7) \ -10 \\ &\tau(C_9\text{-}C_{12}\text{-}C_{14}\text{-}C_{10}) \ -19 \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_{1}) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
1191 1179 1174 1155 1145 1090 1077 1026 999 970 970 970 970 963 924 891 874 874 874 874 870 65 720 697 670 620	$\begin{split} & \delta(H_{22}-C_{19}-C_{21})11 \\ \hline & v(O_5-C_3)13 \\ \hline & \delta(H_{11}-C_8-C_{10})-19 \\ & v(C_{12}-C_{14})-10 \\ & \delta(H_{20}-C_{19}-C_{22})14 \\ & v(O_{18}-C_1)37 \\ & v(C_8-C_{10})19 \\ & v(C_{12}-C_{14})18 \\ & v(C_{12}-C_{14})-16 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-13 \\ & v(O_{18}-C_1)17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})17 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})19 \\ & v(C_3-C_1)28 \\ & \delta(C_{12}-C_{14}-C_{10})15 \\ & \tau(H_{15}-C_{10}-C_8-C_7)-17 \\ & \delta(O_4-C_3-O_5)12 \\ & \tau(H_{11}-C_8-C_{10}-C_{14})-12 \\ & \delta(O_4-C_3-O_5)35 \\ & \delta(C_9-C_{12}-C_{14})-25 \\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23\\ \hline \nu(C_{1}-C_{7})\ 20\\ \hline \delta(H_{13}-C_{9}-C_{12})-20\\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17\\ \hline \delta(H_{21}-C_{19}-C_{20})-12\\ \nu(O_{18}-C_{19})-32\\ \nu(C_{9}-C_{12})-13\\ \nu(C_{14}-C_{10})\ 15\\ \nu(C_{14}-C_{10})\ 15\\ \nu(C_{14}-C_{10})\ -13\\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18\\ \nu(O_{18}-C_{19})\ 35\\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23\\ \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41\\ \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20\\ \hline 0(O_{4}-C_{1}-O_{5}-C_{3})\ 19\\ \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 17\\ \delta(C_{12}-C_{14}-C_{10}-C_{8})\ 19\\ \delta(O_{18}-C_{1}-O_{3})\ 13\\ \delta(O_{18}-C_{1}-O_{3})\ 13\\ \hline \delta(O_{18}-C_{1}-O_{3})\ 13\\ \end{split}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25 \\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13 \\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19 \\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19 \\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34 \\ \hline \tau(H_{20}-C_{19}) & 10 \\ \hline \delta(C_9-C_{12}-C_{14}) & -23 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 22 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 22 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & 20 \\ \hline \tau(H_{17}-C_{14}-C_{10}-C_8) & -11 \\ \hline \sigma(O_4-C_1-O_5-C_3) & -19 \\ \hline \tau(C_7-C_8-C_{10}-C_{14}) & -23 \\ \hline \sigma(O_4-C_1-O_5-C_3) & 11 \\ \hline \delta(C_8-C_{10}-C_{14}) & 37 \\ \end{split}$	$\begin{split} &\delta(H_{16}-C_{12}-C_{14}) \ 15 \\ &\delta(H_{17}-C_{14}-C_{10}) \ 36 \\ &\tau(H_{21}-C_{19}-O_{18}-C_{1}) \ -18 \\ &\delta(H_{13}-C_{9}-C_{12}) \ -13 \\ &\delta(H_{15}-C_{10}-C_{14}) \ 11 \\ &\delta(C_8-C_{10}-C_{14}) \ 12 \\ &\tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ &\tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \\ &\tau(H_{17}-C_{14}-C_{10}-C_8) \ 24 \\ &o(C_1-C_8-C_9-C_7) \ -10 \\ &\tau(C_9-C_{12}-C_{14}-C_{10}) \ -19 \end{split}$	$\tau(H_{22}-C_{19}-O_{18}-C_{1})-18$ $\delta(H_{17}-C_{14}-C_{10}) 11$ $\delta(H_{16}-C_{12}-C_{14}) 10$ $\delta(C_{12}-C_{14}-C_{10}) 16$ $\tau(C_{12}-C_{14}-C_{10}-C_{8}) 14$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10
<ul> <li>11191</li> <li>1179</li> <li>1174</li> <li>1155</li> <li>1145</li> <li>1090</li> <li>1077</li> <li>1026</li> <li>999</li> <li>990</li> <li>977</li> <li>970</li> <li>963</li> <li>924</li> <li>891</li> <li>874</li> <li>840</li> <li>765</li> <li>720</li> <li>697</li> <li>670</li> <li>620</li> <li>596</li> </ul>	$\begin{split} \delta(H_{22}-C_{19}-C_{21})11\\ \hline V(O_5-C_3)13\\ \hline \delta(H_{11}-C_8-C_{10})-19\\ v(C_{12}-C_{14})-10\\ \hline \delta(H_{20}-C_{19}-C_{22})14\\ v(O_{18}-C_1)37\\ v(C_8-C_{10})19\\ v(C_{12}-C_{14})18\\ v(C_{12}-C_{14})-16\\ \hline t(H_{15}-C_{10}-C_8-C_7)-13\\ v(O_{18}-C_1)17\\ \hline t(H_{11}-C_8-C_{10}-C_{14})17\\ \hline t(H_{11}-C_8-C_{10}-C_{14})17\\ \hline t(H_{1-}C_8-C_{10}-C_{14})19\\ v(C_{12}-C_{14},C_{10})15\\ \hline t(H_{1-}C_8-C_{10}-C_{14})-12\\ \hline t(H_{1-}C_8-C_{10}-C_{14})-12\\ \hline t(H_{1-}C_8-C_{10}-C_{14})-25\\ \hline \delta(O_4-C_3-O_5)35\\ \hline \delta(C_7-C_8-C_{10})14\\ \end{split}$	$\begin{split} \tau(H_{21}-C_{19}-O_{18}-C_{1})-23\\ \hline v(C_{1}-C_{7})\ 20\\ \hline \delta(H_{13}-C_{9}-C_{12})-20\\ \hline \delta(H_{15}-C_{10}-C_{14})\ 17\\ \hline \delta(H_{21}-C_{19}-C_{20})-12\\ v(O_{18}-C_{19})-32\\ v(C_{9}-C_{12})-13\\ v(C_{14}-C_{10})\ 15\\ v(C_{14}-C_{10})\ 15\\ v(C_{14}-C_{10})-13\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 18\\ v(O_{18}-C_{19})\ 35\\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ -23\\ \hline \tau(O_{DMSO}-H_{6}-O_{5}-C_{3})\ 41\\ \hline \tau(H_{13}-C_{9}-C_{7}-C_{1})\ 20\\ \hline o(O_{4}-C_{1}-O_{5}-C_{3})\ 19\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 17\\ \hline \delta(C_{12}-C_{14}-C_{10})\ 15\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8})\ 19\\ \hline \delta(O_{18}-C_{1}-C_{3})\ 13\\ \hline \delta(C_{7}-C_{8}-C_{10})\ -13\\ \hline o(O_{4}-C_{1}-O_{5}-C_{3})\ -13\\ \hline o(O_{4}-C_{1}-O_{5}-C_{3})\ -13\\ \hline \end{cases}$	$\begin{split} \tau(H_{22}-C_{19}-O_{18}-C_{1}) & 25\\ \hline \tau(H_2-C_1-O_{18}-C_{19}) & -13\\ \hline \delta(H_{15}-C_{10}-C_{14}) & 19\\ \hline \delta(H_{16}-C_{12}-C_{14}) & -19\\ \hline \tau(H_{20}-C_{19}-O_{18}-C_{1}) & 34\\ \hline \nu(O_{18}-C_{19}) & 10\\ \hline \delta(C_9-C_{12}-C_{14}) & -17\\ \hline \delta(C_9-C_{12}-C_{14}) & -23\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 22\\ \hline \tau(S=O-H_6-O_5) & -19\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 20\\ \hline r(H_{17}-C_{14}-C_{10}-C_{8}) & 20\\ \hline r(H_{17}-C_{16}-C_{8}-C_{7}) & 23\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & 20\\ \hline r(H_{17}-C_{16}-C_{8}-C_{7}) & 23\\ \hline \tau(H_{17}-C_{14}-C_{10}-C_{8}) & -11\\ \hline o(O_4-C_1-O_5-C_3) & -19\\ \hline \tau(C_7-C_8-C_{10}-C_{4}) & -23\\ \hline o(O_4-C_1-O_5-C_{3}) & 11\\ \hline \delta(C_8-C_{10}-C_{14}) & 37\\ \hline o(O_{18}-C_{3}-C_{7}-C_{1}) & 16\\ \hline \end{split}$	$\begin{split} \delta(H_{16}-C_{12}-C_{14}) \ 15 \\ \delta(H_{17}-C_{14}-C_{10}) \ 36 \\ \tau(H_{22}-C_{19}-O_{18}-C_{1}) \ -18 \\ \delta(H_{13}-C_{9}-C_{12}) \ -13 \\ \delta(H_{15}-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ 11 \\ \delta(C_8-C_{10}-C_{14}) \ -12 \\ \tau(C_7-C_8-C_{10}-C_{14}) \ 16 \\ \tau(H_{17}-C_{14}-C_{10}-C_8) \ 16 \\ \end{split}$	$\begin{split} \tau(H_{22}\text{-}C_{19}\text{-}O_{18}\text{-}C_1) & -18 \\ \delta(H_{17}\text{-}C_{14}\text{-}C_{10}) & 11 \\ \delta(H_{16}\text{-}C_{12}\text{-}C_{14}) & 10 \\ \delta(C_{12}\text{-}C_{14}\text{-}C_{10}) & 16 \end{split}$	δ(C <sub>8</sub> -C <sub>10</sub> -C <sub>14</sub> ) -10

# 5. Cartesian coordinates of selected structures

conformer cl			
C	0.90122100	-0.15044500	-0.49631400
H C	1.08504000	0.08207000	-1.55193/00
0	1.5054/000	0.95912700	1 202/5300
0	1 42863300	2 15872600	-0 26133900
Н	1.80975700	2.83317300	0.32505800
C	-0.59416400	-0.14043700	-0.24034600
C	-1.47198100	0.35000800	-1.20505200
С	-1.10151200	-0.61699600	0.96982000
С	-2.84316200	0.36519500	-0.96618700
Н	-1.08491600	0.71837500	-2.14828200
C	-2.47161700	-0.60741000	1.20526200
Н	-0.42337300	-1.00242200	1.72074600
C	-3.34545000	-0.11426600	0.23919200
H	-3.51725100	0.74555900	-1.72431600
H	-2.85/91300	-0.98402500	2.14489800
H O	-4.41200100	-0.10000400	-0 16710400
C	2 75263600	-1 63218000	-0 62446200
Н	3.01003400	-2.65606200	-0.36033400
H	2.81434700	-1.51271200	-1.71203500
Н	3.45757700	-0.94947500	-0.14170700
dimer d11			
С	-3.44736000	-1.04045800	-0.00451400
Н	-3.78489100	-1.62561900	-0.86780400
С	-1.91376100	-1.13114900	0.02630000
0	-1.38403900	-1.15573000	-1.17925800
0	-4.02228300	-1.52589900	1.18498200
C	-3.94303900	-2.94180000	1.32772000
H	-2.905/0600	-3.28044700	1.40556600
H U	-4.40809200	-3.19134400	2.24/38800
С	-3 84831200	0 41021400	-0 20029700
C	-4.29096500	0.85693900	-1,44388300
C	-3.76449300	1.31107900	0.86288900
С	-4.64762600	2.18984000	-1.62613700
Н	-4.36108900	0.16198200	-2.27282800
С	-4.12685400	2.64096100	0.68136400
H	-3.42443100	0.96716700	1.83148300
C	-4.56679000	3.08405500	-0.56359500
H	-4.99362200	2.52639500	-2.59609300
H	-4.063/8/00	3.33312600 4 10110000	1.51256500
п О	-4.84748400	-1 15468400	1 06500500
C	3,44735400	-1.04045800	0.00464300
H	3.78488100	-1.62551300	0.86800600
С	1.91375500	-1.13114700	-0.02616300
0	1.26965500	-1.15480500	-1.06486700
0	4.02227900	-1.52604700	-1.18479100
C	3.94303800	-2.94196500	-1.32735200
Н	2.90570500	-3.28062300	-1.40516500
H	4.46870000	-3.19162500	-2.24698300
H	4.42913400	-3.44569000	-0.48440400
C	3.84831100	0.41023700	1 44276700
C	3 76445000	1.31098100	-0.86303800
C	4.64767800	2.19002600	1.62585500
- H	4.36116600	0.16224200	2.27278800
С	4.12681900	2.64088400	-0.68167800
Н	3.42435000	0.96695800	-1.83157800
С	4.56680200	3.08411900	0.56321400
Н	4.99371100	2.52669200	2.59575900
Н	4.06371900	3.33295300	-1.51295600
Н	4.84748100	4.12126100	0.70278600
0	1.38403100	-1.15558300	1.17939600

0.38139200	-1.15405800	1.12691700
-0.38140000	-1.15419500	-1.12678000
0		
-1.38911300	1.22621600	0.39081000
-1.50811400	1.57144900	1.42383800
0.07186400	0.76131500	0.23073500
0.72039800	0.91033200	-0.78484300
0.51465000	0.16343500	1.32570900
1.45767600	-0.18907700	1.20548200
-2.32138100	0.05478700	0.15083700
-3.02811800	-0.51369600	1.20946900
-2.47806400	-0.46964200	-1.13433700
-3.88031200	-1.59295600	0.99050000
-2.91590800	-0.11009300	2.20928600
-3.33415200	-1.54311000	-1.35444400
-1.93347100	-0.03302200	-1.96231000
-4.03583800	-2.10912700	-0.29213500
-4.42592000	-2.02473400	1.82102400
-3.45222000	-1.94026200	-2.35566800
-4.70133900	-2.94651400	-0.46474300
-1.71036200	2.26260600	-0.51410800
-1.10823100	3.51319100	-0.18600400
-1.46537500	4.23415800	-0.91921500
-1.40832400	3.83749200	0.81643700
-0.01712900	3.45875800	-0.23775400
3.98467600	-0.91891900	0.21843600
2.91397100	-0.83987600	1.31811500
4.21331100	0.77571100	-0.39234200
4.64803500	1.34671200	0.42597000
4.90743700	0.74042200	-1.23181300
3.24597800	1.17849400	-0.68762000
3.16442300	-1.62060900	-1.24162300
2.28129000	-1.02700200	-1.47184300
3.87815900	-1.61314800	-2.06524800
2.89881200	-2.64536800	-0.98858400
	0.38139200 -0.38140000 -0.38140000 -1.38911300 -1.50811400 0.07186400 0.72039800 0.51465000 1.45767600 -2.32138100 -3.02811800 -2.47806400 -3.88031200 -2.91590800 -3.33415200 -1.93347100 -4.03583800 -4.42592000 -3.45222000 -4.70133900 -1.71036200 -1.10823100 -1.46537500 -1.40832400 -0.01712900 3.98467600 2.91397100 4.21331100 4.64803500 4.90743700 3.24597800 3.16442300 2.28129000 3.87815900 2.89881200	$\begin{array}{ccccc} 0.38139200 & -1.15405800 \\ -0.38140000 & -1.15419500 \end{array} \\ \begin{array}{c} 0 \\ -1.50811400 & 1.57144900 \\ 0.07186400 & 0.76131500 \\ 0.72039800 & 0.91033200 \\ 0.51465000 & 0.16343500 \\ 1.45767600 & -0.18907700 \\ -2.32138100 & 0.05478700 \\ -3.02811800 & -0.51369600 \\ -2.47806400 & -0.46964200 \\ -3.88031200 & -1.59295600 \\ -2.91590800 & -0.11009300 \\ -3.33415200 & -1.54311000 \\ -1.93347100 & -0.03302200 \\ -4.03583800 & -2.10912700 \\ -4.42592000 & -2.02473400 \\ -3.45222000 & -1.94026200 \\ -4.70133900 & -2.94651400 \\ -1.71036200 & 2.26260600 \\ -1.10823100 & 3.51319100 \\ -1.46537500 & 4.23415800 \\ -1.40832400 & 3.83749200 \\ -0.01712900 & 3.45875800 \\ 3.98467600 & -0.91891900 \\ 2.91397100 & -0.83987600 \\ 4.21331100 & 0.77571100 \\ 4.64803500 & 1.34671200 \\ 4.90743700 & 0.74042200 \\ 3.24597800 & 1.17849400 \\ 3.16442300 & -1.62060900 \\ 2.28129000 & -1.02700200 \\ 3.87815900 & -1.61314800 \\ 2.89881200 & -2.64536800 \end{array}$

### Linear c1-DMSO (only stable without GD3)

С	-1.56147200	1.09889500	0.48068000
Н	-1.29903200	1.17355900	1.54196200
С	-0.24097600	1.06071500	-0.31419600
0	-0.08025400	1.60853100	-1.38354700
0	0.67842300	0.33853700	0.31207100
Н	1.53388800	0.27071700	-0.22329200
С	-2.33133600	-0.18716800	0.25262000
С	-2.49391900	-1.10648100	1.28784700
С	-2.88544900	-0.46428600	-0.99937400
С	-3.19942400	-2.28862200	1.07805900
Н	-2.07064000	-0.89773900	2.26378500
С	-3.59539000	-1.64165100	-1.20764200
Н	-2.76415100	0.24458100	-1.80921200
С	-3.75240800	-2.55804700	-0.16985700
Н	-3.32075600	-2.99432200	1.89119400
Н	-4.02449800	-1.84582500	-2.18143600
Н	-4.30447400	-3.47578600	-0.33380800
0	-2.37136000	2.19164600	0.09716500
С	-1.88302800	3.45247500	0.55135600
Н	-2.60972600	4.20020100	0.23861000
Н	-1.79816700	3.46522000	1.64353300
Н	-0.91113500	3.68894800	0.10929100
S	4.26243600	-0.39676200	-0.41385400
0	2.93333800	0.10339400	-0.99685600
С	3.96509800	-2.09127000	0.16672200
H(Iso=2)	3.76788700	-2.69489400	-0.71709700
H(Iso=2)	4.86968800	-2.44108500	0.66389000
H(Iso=2)	3.11294800	-2.10278600	0.84461700
С	4.45239200	0.41054900	1.20136600
H(Iso=2)	3.56843900	0.22649900	1.81008700
H(Iso=2)	5.34743100	0.00935400	1.67599400
H(Iso=2)	4.57760800	1.47403800	1.00738400

#### Angled c1-DMSO (only stable with GD3)

~ °	1 02595100	0 55752200	0 52656500
	-1.92585100	0.55752200	0.53050500
Н	-2.04483400	0.73187200	1.61246900
C	-0.81787300	1.49882900	0.02534200
0	-0.81885600	2.00940800	-1.07312400
0	0.16451600	1.59944900	0.91104200
н	1.02790300	1,90913500	0.47233300
C	_1 /1/1/000		0 20128800
c	-1.41414000	-0.85087800	0.30136600
C	-0./12//500	-1.52010/00	1.30415800
C	-1.55749700	-1.45012900	-0.95080700
C	-0.15736400	-2.77204200	1.05874500
H	-0.59333500	-1.05759300	2.27677500
С	-1.00855800	-2.70563600	-1.19307300
U U	-2 09394700	_0 92824500	_1 73235200
п	-2.09394700	-0.92824500	-1.73235200
C	-0.30309600	-3.36/45900	-0.19130500
Н	0.38868300	-3.28101800	1.84380200
H	-1.12442000	-3.16312800	-2.16829200
H	0.13066200	-4.34131500	-0.38373000
0	-3.14463700	0.74381300	-0.14200600
C	-3 78865300	1 97618800	0 17886900
U U	-1 72499600	1 99380700	_0 37598000
11	4.00011000	2.02617700	1 25212200
11		2.0301//UU	1105000
Н	-3.1//81200	2.83388500	-U.II759900
S	3.20635400	0.66572100	-0.32668400
0	2.48775400	2.01275900	-0.12763400
С	2.09455500	-0.37197800	-1.32339700
H(Iso=2)	1.97796400	0.12416700	-2.28471200
$H(T_{SO}=2)$	2 57525400	-1 34108700	-1 45496500
II(ISO-2)	1 12567400	0 40207000	0 02142000
H(ISO=Z)	1.13507400	-0.4030/900	-0.02142900
C	3.03627200	-0.23110700	1.24491700
H(Iso=2)	1.98372600	-0.26378100	1.52263600
H(Iso=2)	3.43782500	-1.23466300	1.10663900
H(Iso=2)	3.62177500	0.31148800	1.98458800
н С О	0.97822000 0.96090400 -0.47916600 -0.94465900 -1.15170800	1.11742700 1.32040700 0.86816200 1.22769900 0.18653600	-0.43878400 -1.51347500 0.00181500 1.05917200 -0.92454100
H	-2.07147800	-0.01839100	-0.61603400
С	1.80105900	-0.12941900	-0.18099000
С	2,24279300	-0.91386600	-1.24528300
C	2 12039400	-0 50742000	1 12518800
C	2 99361300	-2 06279100	_1 01070400
TT T	2.00070400	0 62561200	2 26224000
п	2.002/2400	-0.02501500	-2.20234000
C	2.8/569000	-1.65129100	1.35920400
Н	1.78262800	0.09746300	1.95754300
C	3.31228600	-2.43325600	0.29196900
H	3.33340000	-2.66320500	-1.84611100
H	3.12195100	-1.93422400	2.37574700
H	3.89945300	-3.32505100	0.47586500
0	1.54955200	2.20186300	0.26188400
C	1 04774100	3 47407700	-0 14392300
U U	1 59226000	1 22102200	0.12074600
п	1.00041000	4.22102300	1 01072200
H	1.22341000	3.63/52000	-1.212/3300
H	-0.02109400	3.56969600	0.06707900
C	-6.22904000	-1.20597000	0.28087200
H(Iso=2)	-6.36181400	-2.27609500	0.11965000
H(Iso=2)	-6.43656600	-0.97181800	1.32544100
H(Iso=2)	-6.92518200	-0.65826800	-0.35488400
с. — — — /	-4.86504500	-0.82631500	-0.04412000
N	-3 78663500	-0.52558000	-0.30002800
	3.,0000000		0.00002000
c1.(CD.OD)			
C	0 35503000	1 04583000	-0 48065600
с ц	0.33302300	1 10705700	_1 56003000
	0.10202000	1.12/33/UU	-14001500
	-0.95605300	0.530/4500	0.14291500
U	-1.38949600	0.89284500	1.21465500

0	-1.53962500	-0.37744500	-0.63351100
H(Tso=2)	-2 36232600	-0 73531800	-0 18903400
C C	1 46436200	0 04377100	-0 22505100
C	1 97236300	-0 72867700	-1 26831300
	1.97230300	-0.72807700	-1.20031300
C	1.98402300	-0.118/8400	1.00120200
C	2.98602400	-1.65371500	-1.03246800
H	1.57774300	-0.60573600	-2.27044200
C	3.00083900	-1.03788700	1.29565100
H	1.59614900	0.47914700	1.87656400
С	3.50278400	-1.80957300	0.24988000
Н	3.37442800	-2.24675500	-1.85180500
н	3,40046300	-1.15402900	2,29608900
 H	4 29391700	-2 52650800	0 43428400
0	0 73076600	2.22630300	0.05664700
9	0.73070000	2.29030300	0.00004700
	-0.08528800	3.3/880200	-0.38/09800
H	0.32939400	4.28348400	0.05381600
H	-0.05821200	3.46304800	-1.47900100
H	-1.12147100	3.26100100	-0.05772500
C	-4.92413000	-1.47772700	-0.32927600
H(Iso=2)	-4.65397500	-1.98432900	-1.25329000
H(Iso=2)	-5.29029400	-0.47515300	-0.55849300
H(Iso=2)	-5.70197900	-2.04837800	0.18011400
0	-3.73146500	-1.42328500	0.47583900
H(Tso=2)	-3 93469800	-0 98189100	1 3100000
11(100 2)	5.95109000	0.90109100	1.51000000
$c1-(CD_3OD)_2$			
C	1.04169700	1.07064700	-0.72553700
H	1.17399400	1.10380000	-1.81273900
С	-0.36812100	0.51213100	-0.45845900
0	-1.07272300	0.90134700	0.45668900
0	-0.69168400	-0.43501000	-1.31676900
H(Tso=2)	-1 59513900	-0 85360200	-1 11720600
C C	2 07320000	0 13152600	_0 12941900
C	2 97610700	0.15152000	0.12011000
C	2.87010700	-0.05140900	-0.95716800
C	2.22431200	1 51720000	1.25000700
	3.81945800	-1.51/39000	-0.41039500
Н	2.76783300	-0.58284100	-2.03354000
C	3.17075100	-0.82095900	1.80192000
H	1.60529800	0.64523100	1.90594600
C	3.96919200	-1.60307700	0.97017800
Н	4.43985700	-2.11905600	-1.06379400
Н	3.28394400	-0.88281400	2.87772400
Н	4.70523600	-2.27383100	1.39700700
0	1,21021200	2.35534200	-0.16693800
C	0 50604500	3 38135600	-0 86473500
U U	0 75640000	1 32023300	-0 37/31700
11	0.75040000	2 42471100	1 01272000
п	0.82154800	3.424/1100	-1.912/3000
H	-0.57586400	3.22882700	-0.81/1/200
C	-3.01306600	-2.9/648500	-0.69405500
H(Iso=2)	-2.55398000	-3.44173100	-1.56479400
H(Iso=2)	-4.03388500	-3.34919900	-0.58863700
H(Iso=2)	-2.43719000	-3.23733800	0.19735000
0	-3.01706800	-1.55891300	-0.91591000
H(Iso=2)	-3.40207600	-1.10214300	-0.13090400
C	-4.64211200	0.96270200	1.21627700
H(Iso=2)	-5.58491100	0.44103500	1.37357000
H(Iso=2)	-4 68216500	1 48817800	0 25824700
$H(T_{20}-2)$	-4 5007/200	1 68020200	2 02011200
0	2 60244200	1.00929300	1 22026700
	-3.00244300	-0.02203900	1.23026/00
H(1so=2)	-2./432/200	0.41108000	1.05925300