

Electronic Supplementary Information

Vibrational spectroscopy and DFT calculations of the di-amino acid peptide L-aspartyl-L-glutamic acid in the zwitterionic state

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Table S1

Comparison of computed (B3-LYP/cc-pVDZ) bond angles, and dihedral angles for different L-Asp-L-Glu models.

$\theta / ^\circ$	CPCM cluster with 10H ₂ O	CPCM peptide only	Gas-phase cluster with 10H ₂ O
$\theta(\text{H2N1C3})$	111.48	108.64	111.97
$\theta(\text{H2N1H29})$	106.74	111.27	109.57
$\theta(\text{H2N1H32})$	109.03	109.28	107.80
$\theta(\text{C3N1H29})$	110.49	108.65	108.02
$\theta(\text{C3N1H32})$	110.46	111.76	111.76
$\theta(\text{N1C3H4})$	107.79	107.54	107.76
$\theta(\text{N1C3C5})$	108.06	106.48	106.81
$\theta(\text{N1C3C7})$	110.32	109.98	109.86
$\theta(\text{H29N1H32})$	108.53	107.26	107.63
$\theta(\text{H4C3C5})$	108.26	111.78	109.05
$\theta(\text{H4C3C7})$	108.78	110.73	109.24
$\theta(\text{C5C3C7})$	113.47	110.21	113.93
$\theta(\text{C3C5O6})$	120.21	118.40	119.60
$\theta(\text{C3C5N13})$	114.95	115.63	116.80
$\theta(\text{C3C7H8})$	111.01	109.81	110.40
$\theta(\text{C3C7H9})$	109.51	109.27	111.22
$\theta(\text{C3C7C10})$	113.15	113.70	114.54
$\theta(\text{O6C5N13})$	124.81	125.93	123.60
$\theta(\text{C5N13H14})$	120.15	122.07	119.73
$\theta(\text{C5N13C15})$	124.31	124.77	119.73
$\theta(\text{H8C7H9})$	107.53	106.89	105.87
$\theta(\text{H8C7C10})$	110.62	107.26	109.71
$\theta(\text{H9C7C10})$	104.69	109.67	104.63
$\theta(\text{C7C10O11})$	113.01	112.51	113.00
$\theta(\text{C7C10O12})$	121.54	123.64	122.96
$\theta(\text{O11C10O12})$	125.39	123.83	124.02
$\theta(\text{C10O11H30})$	112.27	108.55	112.26

$\theta(\text{H14N13C15})$	114.97	112.89	113.14
$\theta(\text{N13C15H16})$	107.34	108.54	108.07
$\theta(\text{N13C15C17})$	109.02	107.92	107.77
$\theta(\text{N13C15C19})$	107.82	110.51	109.17
$\theta(\text{H16C15C17})$	107.49	108.24	106.82
$\theta(\text{H16C15C19})$	110.59	108.29	110.77
$\theta(\text{C17C15C19})$	114.35	113.23	114.03
$\theta(\text{C15C17O18})$	117.00	116.65	117.43
$\theta(\text{C15C17O28})$	116.67	115.52	115.75
$\theta(\text{C15C19H20})$	107.16	107.22	107.78
$\theta(\text{C15C19H21})$	109.14	109.12	109.63
$\theta(\text{C15C19C22})$	116.59	114.79	115.45
$\theta(\text{O18C17O28})$	126.33	127.83	126.82
$\theta(\text{H20C19H21})$	106.89	107.46	106.44
$\theta(\text{H20C19C22})$	108.25	108.96	108.90
$\theta(\text{H21C19C22})$	108.41	109.03	108.27
$\theta(\text{C19C22H23})$	111.21	112.23	111.52
$\theta(\text{C19C22H24})$	107.00	109.37	107.97
$\theta(\text{C19C22C25})$	111.03	114.25	111.70
$\theta(\text{H23C22H24})$	109.78	106.54	108.52
$\theta(\text{H23C22C25})$	110.41	108.77	109.49
$\theta(\text{H24C22C25})$	107.26	105.18	107.49
$\theta(\text{C22C25O26})$	122.51	125.23	122.67
$\theta(\text{C22C25O27})$	114.39	111.92	113.84
$\theta(\text{O26C25O27})$	123.06	122.66	123.46
$\theta(\text{C25O27H31})$	109.12	107.24	109.76

$\tau / ^\circ$	CPCM cluster with 10H ₂ O	CPCM peptide only	Gas-phase cluster with 10H ₂ O
$\tau(\text{H2N1C3H4})$	-60.50	-79.06	-55.44
$\tau(\text{H2N1C3C5})$	-177.29	160.99	-172.48
$\tau(\text{H2N1C3C7})$	58.14	41.59	63.49
$\tau(\text{H4C3N1H29})$	-179.02	159.75	-176.17
$\tau(\text{C5C3N1H29})$	64.20	39.80	66.79
$\tau(\text{C7C3N1H29})$	-60.37	-79.60	-57.24
$\tau(\text{H4C3N1H32})$	60.88	41.59	65.62
$\tau(\text{C5C3N1H32})$	-55.91	-78.36	-51.43
$\tau(\text{C7C3N1H32})$	179.52	162.25	-175.45
$\tau(\text{N1C3C5O6})$	-1.97	-28.55	5.66
$\tau(\text{N1C3C5N13})$	176.28	153.72	-175.27
$\tau(\text{N1C3C7H8})$	48.57	64.35	46.62
$\tau(\text{N1C3C7H9})$	167.15	-178.71	163.84
$\tau(\text{N1C3C7C10})$	-76.49	-55.82	-77.80
$\tau(\text{H4C3C5O6})$	-118.45	-145.72	-110.53

$\tau(\text{H4C3C5N13})$	59.80	36.56	68.53
$\tau(\text{H4C3C7H8})$	166.60	-176.94	164.63
$\tau(\text{H4C3C7H9})$	-74.82	-59.99	-78.15
$\tau(\text{H4C3C7C10})$	41.54	62.89	40.21
$\tau(\text{O6C5C3C7})$	120.70	90.70	127.15
$\tau(\text{N13C5C3C7})$	-61.06	-87.03	-53.78
$\tau(\text{C5C3C7H8})$	-72.84	-52.74	-73.16
$\tau(\text{C5C3C7H9})$	45.74	64.20	44.06
$\tau(\text{C5C3C7C10})$	162.10	-172.91	162.42
$\tau(\text{C3C5N13H14})$	7.84	-1.01	16.68
$\tau(\text{C3C5N13C15})$	178.75	172.54	164.58
$\tau(\text{C3C7C10O11})$	147.46	-151.23	168.05
$\tau(\text{C3C7C10O12})$	-35.19	30.41	-13.61
$\tau(\text{O6C5N13H14})$	-174.00	-178.54	-164.29
$\tau(\text{O6C5N13C15})$	-3.09	-4.99	-16.39
$\tau(\text{C5N13C15H16})$	13.18	-41.43	40.12
$\tau(\text{C5N13C15C17})$	-102.97	-158.52	-74.98
$\tau(\text{C5N13C15C19})$	132.35	77.18	160.67
$\tau(\text{H8C7C10O11})$	22.19	87.17	43.26
$\tau(\text{H8C7C10O12})$	-160.46	-91.19	-138.40
$\tau(\text{H9C7C10O11})$	-93.36	-28.56	-69.92
$\tau(\text{H9C7C10O12})$	83.98	153.08	108.42
$\tau(\text{C7C10O11H30})$	173.14	-176.54	176.53
$\tau(\text{H30O11C10O12})$	-4.08	1.81	-1.79
$\tau(\text{H14N13C15H16})$	-175.49	132.64	-170.01
$\tau(\text{H14N13C15C17})$	68.36	15.56	74.90
$\tau(\text{H14N13C15C19})$	-56.32	-108.75	-49.45
$\tau(\text{N13C15C17O18})$	-67.22	-13.24	-54.04
$\tau(\text{N13C15C17O28})$	112.38	167.22	125.29
$\tau(\text{N13C15C19H20})$	-59.71	-57.54	-73.50
$\tau(\text{N13C15C19H21})$	55.69	58.56	41.96
$\tau(\text{N13C15C19C22})$	178.89	-178.73	164.53
$\tau(\text{H16C15C17O18})$	176.73	-130.52	-169.96
$\tau(\text{H16C15C17O28})$	-3.67	49.93	9.38
$\tau(\text{H16C15C19H20})$	57.37	61.22	45.38
$\tau(\text{H16C15C19H21})$	172.78	177.32	160.84
$\tau(\text{H16C15C19C22})$	-64.03	-59.97	-76.58
$\tau(\text{O18C17C15C19})$	53.54	109.42	67.32
$\tau(\text{O28C17C15C19})$	-126.87	-70.13	-113.34
$\tau(\text{C17C15C19H20})$	178.87	-178.75	165.91
$\tau(\text{C17C15C19H21})$	-65.72	-62.64	-78.62
$\tau(\text{C17C15C19C22})$	57.47	60.06	43.95
$\tau(\text{C15C19C22H23})$	45.88	37.47	47.30
$\tau(\text{C15C19C22H24})$	165.76	155.48	166.43
$\tau(\text{C15C19C22C25})$	-77.49	-86.95	-75.59
$\tau(\text{H20C19C22H23})$	-74.95	-82.77	-74.06
$\tau(\text{H20C19C22H24})$	44.93	35.25	45.07
$\tau(\text{H20C19C22C25})$	161.68	152.81	163.05

$\tau(\text{H21C19C22H23})$	169.45	160.22	170.59
$\tau(\text{H21C19C22H24})$	-70.67	-81.76	-70.27
$\tau(\text{H21C19C22C25})$	46.08	35.80	47.71
$\tau(\text{C19C22C25O26})$	-72.29	-25.60	-59.58
$\tau(\text{C19C22C25O27})$	105.32	159.20	118.66
$\tau(\text{H23C22C25O26})$	163.89	-151.85	176.39
$\tau(\text{H23C22C25O27})$	-18.51	32.95	-5.38
$\tau(\text{H24C22C25O26})$	44.30	94.33	58.69
$\tau(\text{H24C22C25O27})$	-138.09	-80.86	-123.08
$\tau(\text{C22C25O27H31})$	-152.92	176.49	-153.40
$\tau(\text{O26C25O27H31})$	24.6706	1.1503	24.8176

Table S2

Definitions of internal coordinates adapted to local symmetry.

No.	Definition	Description
1	$v(\text{O11H30})$	$r(\text{O11H30})$
2	$v(\text{O27H31})$	$r(\text{O27H31})$
3	$v(\text{N13H14})$	$r(\text{N13H14})$
4	$v(\text{N1H2})$	$r(\text{N1H2})$
5	$v(\text{N1H29})$	$r(\text{N1H29})$
6	$v(\text{N1H32})$	$r(\text{N1H32})$
7	$v_s(\text{CH}_2)$	$1/\sqrt{2} [r(\text{C7H8})+r(\text{C7H9})]$
8	$v_{as}(\text{CH}_2)$	$1/\sqrt{2} [r(\text{C7H8})-r(\text{C7H9})]$
9	$v_s(\text{CH}_2')$	$1/\sqrt{2} [r(\text{C19H20})+r(\text{C19H21})]$
10	$v_{as}(\text{CH}_2')$	$1/\sqrt{2} [r(\text{C19H20})-r(\text{C19H21})]$
11	$v_s(\text{CH}_2'')$	$1/\sqrt{2} [r(\text{C22H23})+r(\text{C22H24})]$
12	$v_{as}(\text{CH}_2'')$	$1/\sqrt{2} [r(\text{C22H23})-r(\text{C22H24})]$
13	$v(\text{C3H4})$	$r(\text{C3H4})$
14	$v(\text{C15H16})$	$r(\text{C15H16})$
15	$v(\text{C5O6})$	$r(\text{C5O6})$
16	$v(\text{C10O12})$	$r(\text{C10O12})$
17	$v(\text{C25O26})$	$r(\text{C25O26})$
18	$v_s(\text{CO}_2)$	$1/\sqrt{2} [r(\text{C17O18})+r(\text{C17O28})]$
19	$v_{as}(\text{CO}_2)$	$1/\sqrt{2} [r(\text{C17O18})-r(\text{C17O28})]$
20	$v(\text{C10O11})$	$r(\text{C10O11})$
21	$v(\text{C25O27})$	$r(\text{C25O27})$
22	$v(\text{C3N1})$	$r(\text{C3N1})$
23	$v(\text{C5N13})$	$r(\text{C5N13})$
24	$v(\text{C15N13})$	$r(\text{C15N13})$
25	$v(\text{C3N1})$	$r(\text{C3N1})$
26	$v(\text{C7C10})$	$r(\text{C7C10})$
27	$v(\text{C3C7})$	$r(\text{C3C7})$
28	$v(\text{C3C5})$	$r(\text{C3C5})$
29	$v(\text{C15C17})$	$r(\text{C15C17})$
30	$v(\text{C15C19})$	$r(\text{C15C19})$
31	$v(\text{C19C22})$	$r(\text{C19C22})$
32	$v(\text{C22C25})$	$r(\text{C22C25})$
33	$\delta(\text{C10O11H30})$	$\theta(\text{C10O11H30})$
34	$\delta(\text{C25O27H31})$	$\theta(\text{C10O27H31})$
35	$\delta_{ip}(\text{NH})$	$\theta(\text{C5N13H14}) - \theta(\text{C15N13H14})$
36	$\delta_s(\text{NH}_3)$	$1/\sqrt{6}[\theta(\text{C3N1H2})+\theta(\text{C3N1H29})+\theta(\text{C3N1H32})$ $-\theta(\text{H29N1H32})-\theta(\text{C2N1H29})-\theta(\text{H2N1H32})]$
37	$\delta_{as}(\text{NH}_3)$	$1/\sqrt{6}[2\theta(\text{H29N1H32})-\theta(\text{C2N1H29})-\theta(\text{H2N1H32})]$
38	$\delta_{as'}(\text{NH}_3)$	$1/\sqrt{2}[\theta(\text{C2N1H29})-\theta(\text{H2N1H32})]$
39	$\rho_{ip}(\text{NH}_3)$	$1/\sqrt{6}[2\theta(\text{C3N1H2})-\theta(\text{C3N1H29})-\theta(\text{C3N1H32})]$
40	$\rho_{op}(\text{NH}_3)$	$1/\sqrt{2}[\theta(\text{C3N1H29})-\theta(\text{C3N1H32})]$

41	$\delta(\text{CH}_2)$	$1/2\sqrt{6}[(2+\sqrt{6})\theta(\text{H8C7H9})+(2-\sqrt{6})\theta(\text{C3C7C10})-\theta(\text{C3C7H8})-\theta(\text{C3C7H9})-\theta(\text{C10C7H8})-\theta(\text{C10C7H9})]$
42	$\delta(\text{C3C7C10})$	$1/2\sqrt{6}[(2-\sqrt{6})\theta(\text{H8C7H9})+(2+\sqrt{6})\theta(\text{C3C7C10})-\theta(\text{C3C7H8})-\theta(\text{C3C7H9})-\theta(\text{C10C7H8})-\theta(\text{C10C7H9})]$
43	$\rho(\text{CH}_2)$	$1/2[\theta(\text{C3C7H8})-\theta(\text{C3C7H9})+\theta(\text{C10C7H8})-\theta(\text{C10C7H9})]$
44	$\omega(\text{CH}_2)$	$1/2[\theta(\text{C3C7H8})+\theta(\text{C3C7H9})-\theta(\text{C10C7H8})-\theta(\text{C10C7H9})]$
45	$\tau(\text{CH}_2)$	$1/2[\theta(\text{C3C7H8})-\theta(\text{C3C7H9})-\theta(\text{C10C7H8})+\theta(\text{C10C7H9})]$
46	$\delta(\text{CH}_2')$	$1/2\sqrt{6}[(2+\sqrt{6})\theta(\text{H20C19H21})+(2-\sqrt{6})\theta(\text{C15C19C22})-\theta(\text{C15C19H20})-\theta(\text{C15C19H21})-\theta(\text{C22C19H20})-\theta(\text{C22C19H21})]$
47	$\delta(\text{C15C19C22})$	$1/2\sqrt{6}[(2-\sqrt{6})\theta(\text{H20C19H21})+(2+\sqrt{6})\theta(\text{C15C19C22})-\theta(\text{C15C19H20})-\theta(\text{C15C19H21})-\theta(\text{C22C19H20})-\theta(\text{C22C19H21})]$
48	$\rho(\text{CH}_2')$	$1/2[\theta(\text{C15C19H20})-\theta(\text{C15C19H21})+\theta(\text{C22C19H20})-\theta(\text{C22C19H21})]$
49	$\omega(\text{CH}_2')$	$1/2[\theta(\text{C15C19H20})+\theta(\text{C15C19H21})-\theta(\text{C22C19H20})-\theta(\text{C22C19H21})]$
50	$\tau(\text{CH}_2')$	$1/2[\theta(\text{C15C19H20})-\theta(\text{C15C19H21})-\theta(\text{C22C19H20})+\theta(\text{C22C19H21})]$
51	$\delta(\text{CH}_2'')$	$1/2\sqrt{6}[(2+\sqrt{6})\theta(\text{H23C22H24})+(2-\sqrt{6})\theta(\text{C19C22C25})-\theta(\text{C19C22H23})-\theta(\text{C19C22H24})-\theta(\text{C25C22H23})-\theta(\text{C25C22H24})]$
52	$\delta(\text{C19C22C25})$	$1/2\sqrt{6}[(2-\sqrt{6})\theta(\text{H23C22H24})+(2+\sqrt{6})\theta(\text{C19C22C25})-\theta(\text{C19C22H23})-\theta(\text{C19C22H24})-\theta(\text{C25C22H23})-\theta(\text{C25C22H24})]$
53	$\rho(\text{CH}_2'')$	$1/2[\theta(\text{C19C22H23})-\theta(\text{C19C22H24})+\theta(\text{C25C22H23})-\theta(\text{C25C22H24})]$
54	$\omega(\text{CH}_2'')$	$1/2[\theta(\text{C19C22H23})+\theta(\text{C19C22H24})-\theta(\text{C25C22H23})-\theta(\text{C25C22H24})]$
55	$\tau(\text{CH}_2'')$	$1/2[\theta(\text{C19C22H23})-\theta(\text{C19C22H24})-\theta(\text{C25C22H23})+\theta(\text{C25C22H24})]$
56	$\delta(\text{C3H4})$	$1/\sqrt{6}[2\theta(\text{N1C3H4})-\theta(\text{C5C3H4})-\theta(\text{C7C3H4})]$
57	$\delta'(\text{C3H4})$	$1/\sqrt{2}[\theta(\text{C5C3H4})-\theta(\text{C7C3H4})]$
58	$\delta(\text{C5C3C7})$	$\theta(\text{C5C3C7})$
59	$\delta(\text{N1C3C5})$	$\theta(\text{N1C3C5})$
60	$\delta(\text{N1C3C7})$	$\theta(\text{N1C3C7})$
61	$\delta(\text{C15H16})$	$1/\sqrt{6}[2\theta(\text{N13C15H16})-\theta(\text{C17C15H16})-\theta(\text{C19C15H16})]$
62	$\delta'(\text{C15H16})$	$1/\sqrt{2}[\theta(\text{C17C15H16})-\theta(\text{C19C15H16})]$
63	$\delta(\text{C17C15C19})$	$\theta(\text{C17C15C19})$
64	$\delta(\text{C17C15N13})$	$\theta(\text{C17C15N13})$
65	$\delta(\text{C19C15N13})$	$\theta(\text{C19C15N13})$
66	$\delta(\text{C3C5N13})$	$1/\sqrt{6}[2\theta(\text{C3C5N13})-\theta(\text{C3C5O6})-\theta(\text{N13C5O6})]$
67	$\delta_{\text{ip}}(\text{C5O6})$	$1/\sqrt{2}[\theta(\text{C3C5O6})-\theta(\text{N13C5O6})]$
68	$\delta(\text{O11C10O12})$	$1/\sqrt{6}[2\theta(\text{O11C10O12})-\theta(\text{C7C10O11})-\theta(\text{C7C10O12})]$
69	$\rho(\text{O11C10O12})$	$1/\sqrt{2}[\theta(\text{C7C10O11})-\theta(\text{C7C10O12})]$
70	$\delta(\text{C5N13C15})$	$1/\sqrt{6}[2\theta(\text{C5N13C15})-\theta(\text{C5N13H14})-\theta(\text{C15N13H14})]$
71	$\delta(\text{O18C17O28})$	$1/\sqrt{6}[2\theta(\text{O18C17O28})-\theta(\text{C15C17O18})-\theta(\text{C15C17O28})]$
72	$\rho(\text{O18C17O28})$	$1/\sqrt{2}[\theta(\text{C15C17O18})-\theta(\text{C15C17O28})]$
73	$\delta(\text{O26C25O27})$	$1/\sqrt{6}[2\theta(\text{O26C25O27})-\theta(\text{C22C25O26})-\theta(\text{C22C25O26})]$
74	$\rho(\text{O26C25O27})$	$1/\sqrt{6}[\theta(\text{C22C25O26})-\theta(\text{C22C25O26})]$
75	$\omega(\text{O11C10O12})$	$\phi(\text{C7C10})$

76	$\delta(\text{O26C25O27})$	$\phi(\text{C22C25})$
77	$\delta_{\text{op}}(\text{C5O6})$	$\phi(\text{C5O6})$
78	$\omega(\text{O18C17O28})$	$\phi(\text{C15C17})$
79	$\delta_{\text{op}}(\text{NH})$	$\phi(\text{N13H14})$
80	$\tau(\text{C10O11})$	$1/\sqrt{2}[\tau(\text{C7C10O11H30})+\tau(\text{O12C10O11H30})]$
81	$\tau(\text{C7C10})$	$1/\sqrt{6}[\tau(\text{C3C7C10O11})+\tau(\text{C3C7C10O12})+\tau(\text{C8C7C10O11})+\tau(\text{C8C7C10O12})+\tau(\text{C9C7C10O11})+\tau(\text{C9C7C10O12})]$
82	$\tau(\text{C3C7})$	$1/3[\tau(\text{C8C7C3N1})+\tau(\text{C8C7C3C4})+\tau(\text{C8C7C3C5})+\tau(\text{C9C7C3N1})+\tau(\text{C9C7C3C4})+\tau(\text{C9C7C3C5})+\tau(\text{C10C7C3N1})+\tau(\text{C10C7C3C4})+\tau(\text{C10C7C3C5})]$
83	$\tau(\text{N1C3})$	$1/3[\tau(\text{C4C3N1H2})+\tau(\text{C4C3N1H29})+\tau(\text{C4C3N1H32})+\tau(\text{C5C3N1H2})+\tau(\text{C5C3N1H29})+\tau(\text{C5C3N1H32})+\tau(\text{C7C3N1H2})+\tau(\text{C7C3N1H29})+\tau(\text{C7C3N1H32})]$
84	$\tau(\text{C3C5})$	$1/\sqrt{6}[\tau(\text{N1C3C5O6})+\tau(\text{N1C3C5N13})+\tau(\text{C4C3C5O6})+\tau(\text{C4C3C5N13})+\tau(\text{C7C3C5O6})+\tau(\text{C7C3C5N13})]$
85	$\tau(\text{C5N13})$	$1/2[\tau(\text{C3C5N13H14})+\tau(\text{C3C5N13C15})+\tau(\text{O6C5N13H14})+\tau(\text{O6C5N13C15})]$
86	$\tau(\text{N13C15})$	$1/\sqrt{6}[\tau(\text{C5N13C15H16})+\tau(\text{C5N13C15C17})+\tau(\text{C5N13C15C19})+\tau(\text{H14N13C15H16})+\tau(\text{H14N13C15C17})+\tau(\text{H14N13C15C19})]$
87	$\tau(\text{C15C19})$	$1/3[\tau(\text{N13C15C19H20})+\tau(\text{N13C15C19H21})+\tau(\text{N13C15C19C22})+\tau(\text{H16C15C19H20})+\tau(\text{H16C15C19H21})+\tau(\text{H16C15C19C22})+\tau(\text{C17C15C19H20})+\tau(\text{C17C15C19H21})+\tau(\text{C17C15C19C22})]$
88	$\tau(\text{C19C22})$	$1/3[\tau(\text{C15C19C22H23})+\tau(\text{C15C19C22H24})+\tau(\text{C15C19C22C25})+\tau(\text{H20C19C22H23})+\tau(\text{H20C19C22H24})+\tau(\text{H20C19C22C25})+\tau(\text{H21C19C22H23})+\tau(\text{H21C19C22H24})+\tau(\text{H21C19C22C25})]$
89	$\tau(\text{C22C25})$	$1/\sqrt{6}[\tau(\text{C19C22C25O26})+\tau(\text{C19C22C25O27})+\tau(\text{H23C22C25O26})+\tau(\text{H23C22C25O27})+\tau(\text{H24C22C25O26})+\tau(\text{H24C22C25O27})]$
90	$\tau(\text{C25O27})$	$1/\sqrt{2}[\tau(\text{C22C25O27H31})+\tau(\text{O26C25O27H31})]$

Defintions of out-of-plane angles:

$\phi(\text{C7C10})$ = angle between the bond C7C10 and the plane containing atoms C10, O11, O12
 $\phi(\text{C22C25})$ = angle between the bond C22C25 and the plane containing atoms C25, O26, O27
 $\phi(\text{C5O6})$ = angle between the bond C5O6 and the plane containing atoms C3, C5, N13
 $\phi(\text{C15C17})$ = angle between the bond C15C17 and the plane containing atoms C17, O18, O28
 $\phi(\text{N13H14})$ = angle between the bond N13H14 and the plane containing atoms C5, C15, N13

Abbreviations:

v = stretching, as = anti-symmetric, s = symmetric, δ = deformation,
 ω = wagging, τ = twisting, ρ = rocking, ip = in-plane, op = out-of-plane