Supporting Information

Development of a polarizable intermolecular potential function for liquid amides and alkanes

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Four tables containing results from vibrational force field analyses using the present PIPF-CHARMM potential, the CHARMM22 force field, and ab initio MP2/TZVP//HF/6-31G(p,d) method, plus the full list of the PIPF-CHARMM parameters for alkanes and amides (23 pages). Table S1 shows the results for N-methylacetamide, while the remainder three tables lists results for the C5, C7eq, and C7ax conformations of alanine dipeptide. Standard notations are used to describe contributing motions in the analyses. Additional information may be found from the vibran documentation at www.charmm.org. Table S5 contains the 2D grid correction data (CMAP) for alanine dipeptide potential energy surface. Table S6 contains a full list of the present PIPF-CHARMM force field internal (bonded) parameters.

Table S1. Vibrational Data for N-methylacetamide[a]

modes	exp./ab initio		CHARMM		PFF	
	freq.	assign.	freq.	assign.	freq.	assign.
1	VLF		64	τCCH3(101)	0	τ NCH3(97)
2	VLF		89	τNCH3(101)	69	τ CCH3(104)
3	171	ωN7H τ C5–N7	200	τC5–N7(107)	196	τ C5–N7(108)
4	279	βCNC βCCN	271	βCNC(62) βCCN(25)	273	βCNC(62) βCCN(25)
5	391	τ C5–N7 ωN7H	431	βCCN(50)	434	βCCN(50)
6	431	βCCN βC5=O	579	βC5=O(50) νC5–C4(29)	580	βC5=O(51) νC5–C4(28)
7	628	βC5=O νC5–C4	652	ωC5=O(67) ωN7H(30)	639	ωC5=O(57) ωN7H(44)
8	718	βC5=O rCH3	776	νC5–N7(34) νC5=O(20)	779	νC5–N7(33) νC5=O(21) νC4–C5(15)
9	812	νC5–N7 rCH3 νC5–C4	797	ωN7H(66) rCH3(15)	785	ωN7H(53) rCH3(24)
10	973	rCH3 νN7–C9 νC5–C4	949	rCH3(36) νN7–C9(34)	948	νN7–C9(40) rCH3(19)
11	1042	rCH3 βC5=O	996	rCH3(47) νN7–C9(26)	1002	rCH3(56) νN7–C9(19)
12	1092	νN7–C9 rCH3	1056	rCH3(83)	1055	rCH3(82)
13	1176	rCH3	1087	rCH3(72)	1085	rCH3(71)
14	1263	νN7–C9 βC5=O βN7H	1093	rCH3(67) ωC5=O(17)	1090	rCH3(67) ωC5=O(18)
15	1279	rCH3	1267	βN7H(44) νC5–C4(24)	1268	βN7H(43) νC5–C4(24)
16	1374	δCH3s	1384	δCH3s(94)	1395	δCH3s(96)
17	1410	δCH3s	1413	δCH3as(89)	1413	δCH3as(89)
18	1430	δCH3as	1416	δCH3as(88)	1415	δCH3as(89)
19	1430	δCH3as	1418	δCH3as(91)	1416	δCH3as(90)
20	1430	δCH3as	1426	δCH3as(87) rCH3(15)	1427	δCH3as(87) rCH3(15)
21	1430	δCH3as	1481	δCH3s(50) βN7H(21)	1479	δCH3s(53) βN7H(20)
22	1494	βN7H βN7–C9	1587	δCH3s(39) βN7H(20) νN7–C9(17)	1585	δCH3s(36) βN7H(21) νN7–C9(17)

						νC5–N7(15)
23	1723	νC5=O	1683	νC5=O(66)	1682	νC5=O(67)
24	2830	νCH3s	2852	νCH3s(100)	2852	νCH3s(100)
25	2830	νCH3s	2914	νCH3as(100)	2914	νCH3as(99)
26	2940	νCH3as	2915	νCH3as(100)	2915	νCH3as(100)
27	2940	νCH3as	2917	νCH3s(100)	2918	νCH3s(100)
28	2940	νCH3as	2975	νCH3as(100)	2975	νCH3as(100)
29	2940	νCH3as	2975	νCH3as(100)	2976	νCH3as(100)
30	3495	νN7H	3326	νN7H(99)	3326	νN7H(99)

[a]Frequencies in cm^{-1} . VLF indicates unobserved very low frequencies. ω indicates wagging modes, ν indicates stretching modes, τ indicates torsional rotations, r indicates rocking, δ indicates deformations, and β indicates bends. PFF denotes the polarizable force field.

Table S2. Alanine Dipeptide C5 Vibrational Spectra mode

Modes	PFF		CHARMM		MP2	
	Freq.	assign.	freq.	assign.	freq.	assign.
1	15.3	psi(78) phi(20)	33.2	psi(64) phi(33)	30.3	tCH3(67) psi(23)
2	47.2	tCH3(62) phi(28)	56.9	tCH3(69) phi(17)	34.3	psi(71) tCH3(39)
3	55.5	phi(48) tCH3(37)	69.5	phi(44) tCH3(35) psi(17)	46.8	tCH3(81)
4	93.6	tCH3(96)	90.7	tCH3(64) tC-N(21)	60.1	phi(90) tCH3(17)
5	103.8	tC-N(70)	96.0	dN-CT-C(26) tC-N(25) tCH3(24)	92.1	tC-N(78)
6	160.3	dC-N-CT(28) tC-N(23) dN-CT-C(21) dCT-C-N(19)	150.5	tC-N(40) dC-N-CT(16) dN-CT-C(16)	123.3	tC-N(83)
7	161.3	tC-N(82)	166.3	tC-N(83)	133.2	tC-N(31) dC-N-CT(29) dCT-C-N(17)
8	257.9	dC-N-CT(26) dC-CT-CT(24)	227.6	dC-N-CT(41)	221.7	dC-N-CT(26) dC-CT-CT(24) dCT-C-N(16)
9	269.6	tCH3(73)	253.0	tCH3(36) dCT-C-N(25) dC-N-CT(17)	238.2	tCH3(57) dC-CT-CT(16)
10	289.0	dCT-C-N(30)	265.3	tCH3(52)	272.8	tCH3(32) dCT-C-N(25) dC-N-CT(17)
11	314.6	dC-CT-CT(25) dC-N-CT(23) tCH3(15)	304.2	dC-CT-CT(31) dC-N-CT(21)	294.2	sC-CT(18) dC=O(16)
12	394.9	dC-N-CT(26) dCT-C-N(23) dC=O(20)	348.9	dCT-C-N(36) dC-N-CT(18) dC=O(16)	361.3	dC-N-CT(30) dCT-C-N(29) dC=O(22)
13	401.1	dN-CT-CT(46)	396.6	dN-CT-CT(43)	379.3	dN-CT-CT(47)
14	547.9	dCT-C-N(37) dC=O(21)	519.8	dCT-C-N(32) dC=O(29)	448.7	wN-H(91)
15	595.2	dC=O(54) sC-CT(23)	571.8	dC=O(44) sC-CT(21)	469.5	wN-H(83) wC=O(20)

16	661.8	dC=O(25) dC-N-CT(16) sC-CT(16)	639.6	dC=O(23) sC-CT(22) dC-N-CT(17)	494.9	dC=O(24) dCT-C-N(24) dN-CT-CT(16)
17	677.7	wC=O(71) wN-H(23)	668.8	wC=O(74) wN-H(18)	587.9	dC=O(36) sC-CT(18)
18	702.9	wN-H(49) wC=O(27)	704.6	wN-H(54) wC=O(29)	621.5	wC=O(55)
19	779.8	sC-CT(21) sC-N(21) sC=O(17)	766.1	sC-N(24) sC=O(17) sC-CT(17)	666.9	dC=O(25) sC-CT(22) wC=O(16)
20	833.8	wN-H(23) sCT-CT(20)	822.7	sC-N(24) sC=O(17)	714.8	wC=O(62)
21	847.0	wN-H(41)	832.7	wN-H(63)	833.3	dCH3(24)
22	878.6	wN-H(31) wC=O(31)	883.5	wN-H(28) wC=O(28) dCH3(16)	889.3	dCH3(28) sCT-CT(20)
23	908.4	sN-CT(29) dCH3(25)	908.1	dCH3(33) sN-CT(21)	952.7	sC-CT(36) dCH3(21)
24	958.9	sN-CT(41) dCH3(32)	953.5	sN-CT(48) dCH3(32)	981.7	dCH3(65)
25	997.6	dCH3(40) dCT-HA(25)	975.1	dCH3(78)	1023.2	sN-CT(48) dCH3(31)
26	1013.7	dCH3(81)	1002.9	dCH3(41) dCT-HA(21)	1028.0	dCH3(77) wC=O(18)
27	1042.7	dCH3(81)	1033.6	dCH3(71)	1043.4	dCH3(40) dCT-HA(24)
28	1062.9	dCH3(85)	1072.2	dCH3(89)	1089.3	sCT-CT(36)
29	1086.9	dCH3(74) wC=O(18)	1083.1	dCH3(72) wC=O(19)	1116.8	dCH3(96)
30	1102.5	dCH3(81)	1086.5	dCH3(83)	1130.8	dCH3(66)
31	1120.0	dCH3(32) sN-CT(23)	1121.0	dCH3(29) sN-CT(27)	1165.9	sN-CT(47) dCH3(17)
32	1237.9	dN-H(38) sC-CT(17)	1217.6	dN-H(33)	1191.6	dN-H(27) dCT-HA(26) sC-N(19)
33	1286.3	sC-CT(26) dN-H(25)	1272.8	dN-H(35) sC-CT(22)	1224.6	dN-H(45) sC-N(19)
34	1324.2	dCT-HA(44) sCT-CT(19)	1340.4	dCT-HA(48) sCT-CT(15)	1307.4	dCT-HA(48) dCH3(17)
35	1408.0	dCH3(96)	1383.8	dCH3(95)	1333.9	dCT-HA(65) dCH3(19)
36	1413.5	dCH3(99)	1406.0	dCH3(85)	1366.8	dCH3(96)
37	1418.1	dCH3(93)	1411.2	dCH3(86)	1373.6	dCH3(84)
38	1421.4	dCH3(100)	1415.1	dCH3(98)	1406.0	dCH3(98)
39	1426.4	dCH3(99)	1417.8	dCH3(100)	1444.2	dCH3(87)
40	1429.7	dCH3(99)	1422.7	dCH3(69)	1454.3	dCH3(92)

				dCT-HA(18)		
41	1431.5	dCH3(98)	1425.7	dCH3(100)	1460.8	dCH3(92)
42	1445.0	dCH3(100)	1432.8	dCH3(57)	1467.4	dCH3(84)
				dCT-HA(21)		
43	1461.9	dN-H(33)	1441.5	dCH3(98)	1474.4	dCH3(95)
		dCH3(30)				
		dCT-HA(21)				
44	1498.2	dCT-HA(23)	1479.9	dCH3(42)	1475.2	dCH3(97)
		dN-H(22)		dN-H(22)		
		dCH3(20)				
45	1577.6	dCH3(44)	1572.4	dCH3(37)	1489.7	dCH3(31)
		dN-H(19)		dN-H(20)		dN-H(28)
		sN-CT(17)		sN-CT(17)		sC-N(22)
46	1638.0	dCT-HA(27)	1608.5	dN-H(24)	1526.5	dN-H(38)
		dN-H(17)		dCT-HA(15)		dCH3(25)
		sC=O(16)				sC-N(22)
47	1682.5	sC=O(56)	1677.3	sC=O(63)	1674.9	sC=O(80)
		sC-N(16)				
48	1686.2	sC=O(62)	1683.9	sC=O(66)	1690.3	sC=O(75)
49	2851.3	sCH3(100)	2852.4	sCH3(100)	2928.9	sCT-HA(95)
50	2903.3	sCH3(71)	2901.8	sCH3(92)	2933.1	sCH3(96)
		sCT-HA(29)				

Table S3. Alanine Dipeptide $C7_{eq}$ Vibrational Spectra mode

Modes	PFF		CHARMM		MP2	
	Freq.	assign.	freq.	assign.	Freq.	assign.
1	49.5	psi(83)	51.0	psi(95)	45.0	tCH3(79)
2	66.4	tCH3(83)	61.6	tCH3(94)	48.9	tCH3(72)
3	84.5	tCH3(44) tC-N(35)	83.6	tCH3(62) tC-N(29)	53.0	psi(57) tCH3(40)
4	93.6	tCH3(47) tC-N(39)	89.3	tC-N(42) tCH3(32) phi(17)	70.8	tC-N(67)
5	118.9	phi(84)	109.5	phi(82)	111.5	phi(75) tC-N(22)
6	180.2	tC-N(84)	179.2	tC-N(42) dC-N-CT(24)	145.8	tC-N(69) phi(26)
7	198.6	dC-N-CT(42) dCT-C-N(21) dN-CT-CT(18)	190.2	tC-N(57)	179.2	dC-N-CT(42) dCT-C-N(28)
8	254.1	dCT-C-N(38) dC-N-CT(32) dC-CT-CT(16)	229.7	dC-N-CT(40) dCT-C-N(33)	210.3	dCT-C-N(33) dC-N-CT(31) tCH3(19)
9	295.4	dN-CT-CT(23)	280.8	tCH3(76)	230.8	tCH3(71)
10	304.5	tCH3(73)	282.9	dN-CT-CT(25) dC-CT-CT(22)	275.8	dN-CT-C(20)
11	325.4	dN-CT-C(31) sC-CT(20) tC-N(17)	308.0	dN-CT-C(33) tC-N(19) sC-CT(18)	310.4	dN-CT-C(20) dC-CT-CT(19) dN-CT-CT(16)
12	382.4	dC-N-CT(34) dC=O(28) dC-CT-CT(21)	332.3	dC-N-CT(32) dC=O(31) dC-CT-CT(19)	325.0	dC-N-CT(37) dC=O(31)
13	440.3	dCT-C-N(24)	430.9	dCT-C-N(25)	387.9	wN-H(94)
14	493.0	dCT-C-N(49) dN-CT-CT(20)	466.2	dCT-C-N(50) dN-CT-CT(21)	414.0	dCT-C-N(40) dC=O(15)
15	592.0	dC=O(57) sC-CT(21)	569.4	dC=O(54) sC-CT(23)	478.7	dCT-C-N(32) dN-CT-CT(21)
16	645.3	dC=O(33) sC-CT(17)	636.1	dC=O(33) sC-CT(18)	566.7	dC=O(42) sC-CT(20)
17	670.8	wC=O(68) wN-H(27)	662.0	wC=O(70) wN-H(24)	589.6	wC=O(69)
18	745.2	wC=O(42) wN-H(41)	738.2	wC=O(41) wN-H(36)	625.5	wN-H(41) dC=O(19)

						wC=O(17)
19	783.5	sC=O(19)	774.9	sC=O(18)	680.0	wN-H(42)
		sC-N(16)		sC-N(15)		sC-CT(16)
		sC-CT(15)		wN-H(15)		
20	830.4	sC-N(30)	819.2	sC-N(32)	741.0	wC=O(60)
		sC=O(21)		sC=O(21)		dN-CT-C(20)
		sC-CT(20)		sC-CT(18)		
21	850.9	wN-H(61)	837.4	wN-H(64)	838.4	dCH3(25)
		dCH3(17)		dCH3(20)		sC-CT(15)
22	893.1	wN-H(42)	887.3	wN-H(41)	881.8	dCH3(39)
		wC=O(24)		wC=O(22)		sC-N(16)
23	913.7	sN-CT(35)	910.9	dCH3(28)	940.2	sC-CT(37)
		dCH3(23)		sN-CT(26)		sCT-CT(15)
		sCT-CT(19)		sCT-CT(20)		
24	957.6	dCH3(53)	946.2	dCH3(48)	986.7	dCH3(62)
		sN-CT(32)		sN-CT(37)		
25	1011.3	dCH3(88)	978.6	dCH3(84)	1021.9	dCH3(51)
						sN-CT(25)
26	1037.7	dCH3(60)	1022.0	dCH3(41)	1029.6	dCH3(46)
						sN-CT(26)
27	1050.1	dCH3(51)	1037.6	dCH3(60)	1033.0	dCH3(54)
		sCT-CT(23)		sCT-CT(18)		
28	1062.7	dCH3(79)	1073.1	dCH3(88)	1112.6	dCH3(70)
29	1089.0	dCH3(74)	1086.0	dCH3(77)	1114.3	dCH3(54)
		wC=O(20)				sCT-CT(18)
30	1118.9	dCH3(82)	1086.7	dCH3(77)	1146.9	dCH3(45)
						sN-CT(22)
31	1132.8	sN-CT(33)	1130.0	sN-CT(34)	1150.4	dCH3(53)
		dCH3(23)		dCH3(24)		
		dCT-HA(17)		dCT-HA(16)		
32	1199.5	dCT-HA(32)	1183.6	dCT-HA(33)	1217.3	sC-N(31)
		dN-H(22)		dN-H(23)		dN-H(25)
		sC-N(19)		sC-N(19)		dCT-HA(16)
33	1269.6	dN-H(44)	1264.8	dN-H(44)	1238.3	dN-H(33)
		sC-CT(22)		sC-CT(21)		dCH3(17)
						dCT-HA(16)
						sC-N(16)
34	1351.7	dCT-HA(41)	1349.7	dCT-HA(37)	1310.2	dCT-HA(69)
				dCH3(15)		
35	1407.1	dCH3(95)	1386.1	dCH3(94)	1337.1	dCT-HA(52)
36	1413.4	dCH3(90)	1405.9	dCH3(88)	1374.8	dCH3(93)
37	1415.1	dCH3(99)	1412.9	dCH3(92)	1381.3	dCH3(91)
38	1421.4	dCH3(100)	1415.9	dCH3(99)	1410.6	dCH3(98)
39	1426.2	dCH3(98)	1417.6	dCH3(100)	1443.4	dCH3(95)
40	1431.4	dCH3(83)	1425.3	dCH3(98)	1459.3	dCH3(92)
41	1435.3	dCH3(94)	1427.8	dCH3(68)	1460.1	dCH3(98)

				dCT-HA(18)		
42	1444.7	dCH3(83)	1436.6	dCH3(80)	1460.8	dCH3(98)
43	1448.7	dCH3(51)	1440.6	dCH3(66)	1466.9	dCH3(96)
		dCT-HA(20)				
		dN-H(19)				
44	1503.6	dCH3(46)	1491.9	dCH3(50)	1479.9	dCH3(92)
		dN-H(15)				
45	1579.4	dN-H(26)	1573.8	dN-H(26)	1491.3	dN-H(39)
		dCH3(16)		sN-CT(15)		sC-N(27)
		sN-CT(15)				
46	1607.4	dCH3(24)	1597.7	dN-H(22)	1532.0	dN-H(54)
		dN-H(21)		dCH3(22)		sC-N(19)
		sC-N(17)		sC-N(18)		
		sN-CT(16)		sN-CT(16)		
47	1678.0	sC=O(64)	1679.9	sC=O(64)	1661.9	sC=O(77)
48	1684.7	sC=O(66)	1683.8	sC=O(65)	1692.7	sC=O(75)
49	2850.9	sCH3(100)	2852.1	sCH3(100)	2929.0	sCH3(100)
50	2903.2	sCH3(88)	2902.1	sCH3(92)	2941.7	sCH3(100)
51	2905.9	sCT-HA(87)	2904.8	sCT-HA(91)	2942.3	sCH3(100)
52	2912.6	sCH3(100)	2913.9	sCH3(100)	2956.5	sCT-HA(99)
53	2913.9	sCH3(100)	2914.5	sCH3(100)	3012.3	sCH3(100)
54	2922.0	sCH3(100)	2917.1	sCH3(100)	3025.8	sCH3(100)
55	2960.3	sCH3(100)	2959.2	sCH3(100)	3031.9	sCH3(100)
56	2961.2	sCH3(100)	2960.1	sCH3(100)	3036.5	sCH3(100)
57	2976.9	sCH3(100)	2974.9	sCH3(100)	3046.6	sCH3(100)
58	2977.5	sCH3(100)	2975.3	sCH3(100)	3053.2	sCH3(100)
59	3325.7	sN-H(99)	3318.5	sN-H(99)	3361.7	sN-H(100)
60	3327.5	sN-H(99)	3327.8	sN-H(100)	3440.1	sN-H(100)

Table S4. Alanine Dipeptide $C7_{ax}$ Vibrational Spectra

Modes	PFF		CHARMM		MP2	
	Freq.	assign.	freq.	assign.	Freq.	assign.
1	55.2	psi(74)	58.1	psi(83)	35.1	psi(69)
2	70.5	tCH3(79)	65.6	tCH3(90)	58.4	tCH3(91)
3	88.4	tC-N(45) tCH3(36)	82.4	tCH3(71) tC-N(22)	66.7	tCH3(55) tC-N(32)
4	94.1	tCH3(62) tC-N(28)	92.7	tC-N(62) tCH3(18) dN-CT-C(17)	74.4	tC-N(37) psi(33) tCH3(25)
5	135.0	phi(70) tC-N(30)	132.0	phi(101)	124.2	tC-N(99)
6	172.8	tC-N(52) phi(30)	174.3	tC-N(74)	143.4	phi(112)
7	219.4	dCT-C-N(33) dC-N-CT(28) dC-CT-CT(19)	197.9	dCT-C-N(31) dC-N-CT(23) dN-CT-C(18)	189.4	dCT-C-N(48) dC-N-CT(24)
8	252.4	dC-N-CT(51) dCT-C-N(21)	242.2	dC-N-CT(58) dCT-C-N(21)	206.8	dC-N-CT(59) dCT-C-N(17)
9	278.8	tCH3(81)	269.5	tCH3(81)	242.8	tCH3(81)
10	295.6	dC-CT-CT(27) dCT-C-N(15) tCH3(15)	284.7	dC-CT-CT(31) tCH3(16)	249.1	dC-CT-CT(35)
11	358.7	dC-N-CT(28) dN-CT-C(19) sC-CT(17) dN-CT-CT(16)	319.9	dC-N-CT(45)	302.2	dC-N-CT(42) dN-CT-C(18)
12	377.6	dN-CT-CT(38) dC=O(24) dC-N-CT(19)	356.6	dN-CT-CT(53) dC=O(19)	346.0	dN-CT-CT(48) dC=O(20)
13	419.9	dCT-C-N(29)	401.8	dCT-C-N(31)	381.9	dCT-C-N(42)
14	540.0	dC=O(52)	518.7	dC=O(53)	401.1	wN-H(100)
15	592.5	dCT-C-N(19) sC-CT(15)	576.9	dCT-C-N(19) sC-CT(16)	499.9	dC=O(58)
16	660.2	sC-CT(27) dC=O(25)	645.3	sC-CT(28) dC=O(20)	579.7	wC=O(48)
17	667.2	wC=O(69) wN-H(24)	656.2	wC=O(73) wN-H(23)	620.2	wC=O(34)
18	748.3	sC-N(19)	741.8	sC-N(21)	635.0	wN-H(90)
19	765.3	wN-H(38) wC=O(30)	754.7	wN-H(41) wC=O(33)	667.5	sC-CT(20)
20	815.2	sC-N(27) sC=O(20)	805.2	sC-N(28) sC=O(18)	748.6	wC=O(60)
21	846.0	wN-H(57)	833.0	wN-H(59) dCH3(15)	806.7	dC=O(19)

22	897.5	wN-H(48) wC=O(25)	892.6	wN-H(50) wC=O(26)	877.0	sC-N(25) dCH3(17)
23	917.7	dCH3(36) sN-CT(20)	908.5	dCH3(34) sN-CT(18) sCT-CT(15)	917.5	dCH3(33) sC-CT(21)
24	958.8	dCH3(42) sN-CT(41)	951.0	dCH3(46) sN-CT(38)	972.7	dCH3(48)
25	1005.9	dCH3(59)	976.2	dCH3(78)	1005.3	dCH3(67)
26	1019.6	dCH3(55)	1004.8	dCH3(32) dCT-HA(21) sN-CT(17)	1028.8	dCH3(81) wC=O(19)
27	1051.0	dCH3(79)	1044.1	dCH3(73)	1086.0	sN-CT(46)
28	1063.8	dCH3(79)	1072.4	dCH3(84)	1104.8	dCH3(40) sCT-CT(27)
29	1084.9	dCH3(51) dCT-HA(15)	1082.1	dCH3(53)	1119.3	dCH3(97)
30	1090.7	dCH3(56)	1085.7	dCH3(76)	1125.0	sN-CT(33) dCH3(32)
31	1119.2	dCH3(83)	1089.8	dCH3(58)	1152.6	dCH3(67)
32	1256.3	dN-H(29) sC-CT(21)	1243.7	dN-H(26) dCT-HA(22) sC-CT(15)	1254.8	dN-H(32) sC-N(28)
33	1273.5	dN-H(43) sC-CT(24)	1269.9	dN-H(43) sC-CT(23)	1273.5	dCT-HA(73)
34	1330.3	dCT-HA(46) sCT-CT(20)	1325.1	dCT-HA(41) sCT-CT(18)	1284.1	dN-H(30) sC-N(22) sC-CT(16)
35	1407.8	dCH3(96)	1385.9	dCH3(95)	1336.1	dCT-HA(79)
36	1415.0	dCH3(98)	1407.3	dCH3(81)	1372.8	dCH3(95)
37	1420.7	dCH3(89)	1412.7	dCH3(98)	1376.9	dCH3(92)
38	1421.8	dCH3(100)	1415.9	dCH3(99)	1417.1	dCH3(97)
39	1427.4	dCH3(97)	1417.9	dCH3(100)	1443.8	dCH3(96)
40	1431.2	dCH3(85)	1425.3	dCH3(98)	1454.9	dCH3(99)
41	1433.4	dCH3(98)	1428.9	dCH3(62) dCT-HA(22)	1460.0	dCH3(96)
42	1443.7	dCH3(97)	1437.8	dCH3(95)	1462.5	dCH3(98)
43	1450.9	dCT-HA(39) dCH3(30)	1442.4	dCH3(60) dCT-HA(20)	1480.3	dCH3(98)
44	1490.3	dCH3(49) dN-H(25)	1481.5	dCH3(53) dN-H(23)	1483.6	dCH3(97)
45	1556.0	dN-H(31) sC-N(22) sN-CT(17)	1552.0	dN-H(32) sC-N(22) sN-CT(17)	1503.8	dN-H(48) sC-N(25)
46	1597.3	dCH3(38) dN-H(23) sN-CT(16)	1589.7	dCH3(34) dN-H(25) sN-CT(17)	1536.8	dN-H(58) sC-N(20)

		sC-N(15)		sC-N(15)		
47	1685.8	sC=O(66)	1685.0	sC=O(66)	1664.2	sC=O(75)
48	1696.2	sC=O(58)	1692.2	sC=O(59)	1688.7	sC=O(73)
49	2850.9	sCH3(100)	2852.0	sCH3(100)	2933.3	sCH3(100)
50	2903.1	sCH3(59)	2902.1	sCH3(86)	2940.6	sCH3(100)
		sCT-HA(41)				
51	2904.1	sCT-HA(58)	2903.2	sCT-HA(86)	2941.2	sCH3(100)
		sCH3(41)				
52	2912.6	sCH3(100)	2913.9	sCH3(100)	2973.3	sCT-HA(99)
53	2913.9	sCH3(100)	2914.5	sCH3(100)	3011.6	sCH3(100)
54	2922.1	sCH3(100)	2917.1	sCH3(100)	3020.3	sCH3(100)
55	2959.3	sCH3(100)	2958.4	sCH3(100)	3023.1	sCH3(100)
56	2960.9	sCH3(100)	2960.4	sCH3(100)	3046.0	sCH3(100)
57	2977.0	sCH3(100)	2975.0	sCH3(100)	3049.9	sCH3(100)
58	2977.6	sCH3(100)	2975.2	sCH3(100)	3060.3	sCH3(100)
59	3326.6	sN-H(100)	3318.9	sN-H(99)	3349.6	sN-H(99)
60	3329.8	sN-H(99)	3325.4	sN-H(100)	3451.9	sN-H(100)

Table S5. Alanine Dipeptide 2D correction data (CMAP)

```
! alanine map

C    NH1  CT1  C    NH1  CT1  C    NH1   24

!-180
 -1.991190 -2.838498 -3.292723 -3.316014 -4.067712
 -4.109663 -2.939185 -1.794760  0.296445  2.817256
 -1.444433  4.018533  8.650390  8.087893  4.727155
  0.126906 -2.505183 -1.769400 -0.921656  0.415752
  1.245946  1.933839  2.228748  0.448227
!-165
  5.141626  3.514873  3.192162  3.427797  3.585139
  3.628710  3.767849  5.180332  8.101344  8.184321
  9.159416 15.396137 17.308164 14.461483  9.920818
  6.054986  4.069640  3.488313  3.974250  5.434570
  6.430730  7.184788  7.244171  6.576927
!-150
  8.947921  8.394265  7.870558  8.225470  8.408552
  8.489195  9.079360 10.282471 12.961215 10.934894
 17.453663 21.661768 21.117706 18.226618 14.274934
  9.979162  7.458806  7.006784  7.283248  8.606070
  9.271217 10.034624 10.340798  9.972061
!-135
 10.497635  9.758556  9.591401 10.191932 10.520130
 10.700704 11.367634 12.429717 13.626935 15.013251
```

```
 20.134843 22.492159 21.553273 18.604071 15.171186
 11.696844  9.190233  8.247898  9.015058  9.510543
 10.361080 10.788012 10.846450 10.756240
!-120
 10.095894  9.377368  9.130942  9.850154  9.506599
 10.348253 11.477740 12.253800 12.097096 16.021546
 19.624944 20.990294 19.930783 17.561833 14.286572
 10.980379  8.842599  8.877446  9.821192 10.081209
 10.086949 10.556240 10.661431 10.590922
!-105
  8.814977  7.858332  7.567569  8.352024  9.035904
  8.995379 10.046001 10.240146 11.091241 14.824734
 17.523491 17.914347 17.269278 14.696472 11.051835
  9.155562  8.377634  8.422422  9.266202  9.392427
  9.188354  9.555128  9.726713  9.662039
!-90
  6.903624  5.302303  5.662588  5.949908  6.391619
  6.632573  6.840227  5.640356  8.653626 12.281631
 14.186523 14.531222 13.103504 10.708229  8.954729
  7.872328  7.065330  6.708041  7.575349  7.575007
  7.793099  7.842965  8.080897  7.805844
!-75
  5.013864  3.962962  3.119843  2.844418  2.397943
  2.632701  2.485280  2.182209  5.781952  9.398223
 11.054098 10.857230  8.235789  7.636991  7.795643
  6.581490  5.499538  4.598800  4.074940  5.106975
  5.957088  5.621327  5.569397  6.131349
!-60
  4.664312  2.131688  0.921215 -0.533631 -1.218996
 -1.618152 -1.880376  0.177044  4.218557  7.367794
  8.141734  6.507307  6.528718  7.953282  7.572335
  6.561503  4.285700  2.363841  1.664554  3.385905
  4.751627  5.313013  5.584228  5.613190
!-45
  5.083360  1.390722 -2.202976 -4.300867 -5.226613
 -5.404384 -4.002234 -0.004906  3.937460  4.956668
  4.919116  5.157745  7.060248  8.722505  8.439620
  6.394306  3.235635 -0.385304 -0.717301  1.330164
  4.609150  6.172265  6.835887  6.119800
!-30
  2.966389 -1.761053 -7.060076-10.663672 -8.128619
 -5.862889 -2.443857  0.658281  2.063072  3.512254
  2.963877  6.519328  5.220281  6.846737  5.142298
  0.197410 -0.862795 -4.057895 -3.343791  0.654146
  4.266519  6.769356  7.164110  6.387329
!-15
```

-1.073688-12.273120 -7.922918 -5.591341 -4.577737
-3.253223 -1.907919 -1.200609 0.081744 1.022458
 0.892927 5.769867 9.358557 8.709712 3.385075
-3.854257 -4.737375 -6.751529 -3.935862 0.448790
 4.264907 5.786316 5.846162 3.711505
!0
-8.957538 -5.705067 -4.161799 -3.249921 -2.385835
-2.196744 -3.109122 -3.458648 -2.658285 -2.507104
 3.046643 8.423265 10.369945 5.534518 -1.254088
-3.591673 -7.256830 -5.578201 -3.098800 0.272543
 2.145462 3.256839 2.867646 -0.251315
!15
-4.927369 -3.299180 -2.382209 -1.531317 -1.857647
-3.323959 -5.558661 -5.752960 -2.128161 -0.528418
 5.656757 8.761139 6.464012 0.242824 -5.633144
-6.766172 -6.149434 -4.302900 -3.288714 -2.598849
-1.684880 -1.059066 -8.595755 -5.757188
!30
-2.713238 -2.042189 -1.167329 -1.336490 -2.577584
-4.967080 -6.191009 -4.493955 -0.264876 0.862502
 5.102184 4.751050 0.706640 -3.717257 -4.216692
-5.614017 -4.999786 -5.178333 -6.295073 -6.424311
-6.554758 -6.467557 -4.220468 -2.700510
!45
-2.680312 -2.847784 -2.510328 -3.009381 -4.474131
-5.697400 -5.371584 -2.743755 1.426146 1.411502
 3.311508 1.551441 1.387561 -2.591205 -3.832283
-4.129073 -5.012763 -7.339441 -9.476633 -9.033050
-6.349864 -3.637186 -2.165442 -1.904414
!60
-5.935958 -5.822959 -4.957218 -4.688312 -4.636134
-4.687906 -3.039911 0.126425 -0.922669 1.651315
 7.038586 5.069381 1.706019 -0.135677 -1.076966
-1.546558 -3.573270 -6.455935 -7.648062 -5.620660
-3.667620 -2.565035 -1.764205 -1.947310
!75
-7.301228 -6.560700 -5.911579 -5.576845 -5.286263
-4.475069 -2.337014 0.833991 3.311135 4.911913
 4.844435 3.621894 2.325826 1.800546 0.388336
-1.249432 -4.169398 -6.140534 -6.317218 -4.228207
-2.922060 -2.608673 -1.850101 -3.861929
!90
-7.713929 -7.470273 -7.107224 -6.845365 -6.530855
-5.609114 -4.263935 -1.608541 0.024329 1.519696
 1.869509 1.578234 1.719110 1.930153 0.201477
-3.378791 -5.552791 -8.480507 -6.801288 -5.100959

-4.811054 -4.305823 -4.715821 -5.387890
!105
-8.155380 -8.144686 -7.836671 -7.373635 -7.759438
-6.539407 -5.119268 -3.357236 -2.101271 -1.067868
0.309793 1.358489 2.168256 1.182888 -1.290457
-5.391446 -9.798419 -7.704346 -6.239189 -5.615016
-4.530444 -4.363496 -5.133683 -6.485147
!120
-7.256670 -8.084349 -7.915530 -7.208537 -7.705643
-7.240570 -5.992147 -4.797221 -3.768270 -1.509277
0.170793 1.667929 1.564783 0.669352 -2.456579
-10.161664 -9.076768 -7.234832 -5.788159 -5.490927
-4.923607 -4.548135 -4.810981 -5.721299
!135
-5.062802 -6.486505 -7.257770 -6.682012 -6.114757
-6.639078 -5.633968 -4.704957 -3.387730 -0.923400
1.040650 2.184110 2.048322 -9.202443 -7.256186
-6.511234 -6.837291 -6.644965 -5.487007 -5.331993
-3.526973 -2.291717 -1.794933 -3.174318
!150
-2.182993 -4.754667 -5.163601 -5.019816 -4.521160
-4.771945 -4.206636 -3.012886 -1.149330 0.891229
2.964836 -8.869774 -4.269220 -0.324675 -0.431565
-2.107297 -3.854484 -4.673172 -3.810335 -2.629616
-1.012968 0.195661 1.382825 -0.048682
!165
1.268721 -0.395333 -1.217615 -1.011856 -1.558241
-1.250156 -0.518994 0.310700 2.036344 4.846306
6.985198 1.161857 6.455697 8.647095 6.296187
3.269040 0.591887 -0.134140 1.269145 2.604475
4.081689 4.979598 4.927819 4.079106

Table S6. Internal (bonded) parameter file for the PIPF-CHARMM force field for alkanes and amides.

```
*>>>> CHARMM22 All-Hydrogen Parameter File for Proteins <<<<<<<<<<
*>>>>>>>>>>>>>>>>>>>>> August 1999 <<<<<<<<<<<<<<<<<<<<<<<<<<<<
*>>>>>>> Direct comments to Alexander D. MacKerell Jr. <<<<<<<<<
*>>>>>> 410-706-7442 or email: alex,mmiris.ab.umd.edu  <<<<<<<<<
*

! references
!
!PROTEINS
!
!MacKerell, Jr., A. D.; Bashford, D.; Bellott, M.; Dunbrack Jr., R.L.;
!Evanseck, J.D.; Field, M.J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.;
!Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F.T.K.; Mattos,
!C.; Michnick, S.; Ngo, T.; Nguyen, D.T.; Prodhom, B.; Reiher, III,
!W.E.; Roux, B.; Schlenkrich, M.; Smith, J.C.; Stote, R.; Straub, J.;
!Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M.  All-atom
!empirical potential for molecular modeling and dynamics Studies of
!proteins.  Journal of Physical Chemistry B, 1998, 102, 3586-3616.
!
!PHOSPHOTYROSINE
!
!Feng, M.-H., Philippopoulos, M., MacKerell, Jr., A.D. and Lim, C.
!Structural Characterization of the Phosphotyrosine Binding Region of a
!High-Affinity aSH2 Domain-Phosphopeptide Complex by Molecular Dynamics
!Simulation and Chemical Shift Calculations. Journal of the American
!Chemical Society, 1996, 118: 11265-11277.
!
!IONS (see lipid and nucleic acid topology and parameter files for
!additional ions
!
!ZINC
!
!Roland H. Stote and Martin Karplus, Zinc Binding in Proteins and
!Solution: A Simple but Accurate Nonbonded Representation, PROTEINS:
!Structure, Function, and Genetics 23:12-31 (1995)
```

```
!

BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
!
C    C     600.000     1.3350 ! ALLOW ARO HEM
               ! Heme vinyl substituent (KK, from propene (JCS))
CT1  C     250.000     1.4900 ! ALLOW   ALI PEP POL ARO
               ! Ala Dipeptide ab initio calc's (LK) fixed from 10/90 (5/91)
CT2  CT1   222.500     1.5380 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
CT2  CT2   222.500     1.5300 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
CT3  C     250.000     1.4900 ! ALLOW   ALI PEP POL ARO
               ! Ala Dipeptide ab initio calc's (LK) fixed from 10/90 (5/91)
CT3  CT1   222.500     1.5380 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
CT3  CT2   222.500     1.5280 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
CT3  CT3   222.500     1.5300 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
HA   C     330.000     1.1000 ! ALLOW ARO HEM
               ! Heme vinyl substituent (KK, from propene (JCS))
HA   CT1   309.000     1.1110 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
HA   CT2   309.000     1.1110 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
HA   CT3   322.000     1.1110 ! ALLOW   ALI
               ! alkane update, adm jr., 3/2/92
HB   CT1   330.000     1.0800 ! ALLOW   PEP
               ! Alanine Dipeptide ab initio calc's (LK)
NH1  C     370.000     1.3450 ! ALLOW   PEP POL ARO
```

```
                ! Alanine Dipeptide ab initio calc's (LK)
NH1  CT1   320.000     1.4300 ! ALLOW   ALI PEP POL ARO
                ! NMA Gas & Liquid Phase IR Spectra (LK)
NH1  CT3   320.000     1.4300 ! ALLOW   ALI PEP POL ARO
                ! NMA Gas & Liquid Phase IR Spectra (LK)
NH1  H     440.000     0.9970 ! ALLOW   PEP POL ARO
                ! Alanine Dipeptide ab initio calc's (LK)
O    C     620.000     1.2300 ! ALLOW   PEP POL ARO
                ! Peptide geometry, condensed phase (LK)

ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
!
CT1  NH1  C      50.000   120.0000 ! ALLOW   ALI PEP POL ARO
                ! NMA Vib Modes (LK)
CT3  CT1  C      52.000   108.0000 ! ALLOW   ALI PEP POL ARO
                ! Alanine Dipeptide ab initio calc's (LK)
CT3  CT2  CT2   58.000    115.00    8.00   2.56100 ! ALLOW   ALI
                ! alkane update, adm jr., 3/2/92
CT3  CT2  CT3   53.350    114.00    8.00   2.56100 ! ALLOW   ALI
                ! alkane update, adm jr., 3/2/92
CT3  NH1  C      50.000   120.0000 ! ALLOW   ALI PEP POL ARO
CT3  NH1  CT3    50.000   120.0000 !
                ! NMA Vib Modes (LK)
H    NH1  C      34.000   123.0000 ! ALLOW   PEP POL ARO
                ! NMA Vib Modes (LK)
H    NH1  CT1    35.000   117.0000 ! ALLOW   PEP POL ARO ALI
                ! NMA Vibrational Modes (LK)
```

```
H    NH1  CT3    35.000   117.0000 ! ALLOW   PEP POL ARO ALI
                 ! NMA Vibrational Modes (LK)
HA   CT1  C     33.000    109.50   30.00   2.16300 ! ALLOW   ALI PEP POL ARO
                 ! alanine dipeptide, LK, replaced, adm jr., 5/09/91
HA   CT1  CT3   34.500    110.10   22.53   2.17900 ! ALLOW   ALI
                 ! alkane update, adm jr., 3/2/92
HA   CT2  CT3   34.600    110.10   22.53   2.17900 ! ALLOW   ALI
                 ! alkane update, adm jr., 3/2/92
HA   CT2  HA    35.500    109.00    5.40   1.80200 ! ALLOW   ALI
                 ! alkane update, adm jr., 3/2/92
HA   CT3  C     33.000    109.50   30.00   2.16300 ! ALLOW   ALI PEP POL ARO
                 ! alanine dipeptide, LK, replaced, adm jr., 5/09/91
HA   CT3  CT1   33.430    110.10   22.53   2.17900 ! ALLOW   ALI
                 ! alkane frequencies (MJF), alkane geometries (SF)
HA   CT3  CT2   34.600    110.10   22.53   2.17900 ! ALLOW   ALI
                 ! alkane update, adm jr., 3/2/92
HA   CT3  CT3   37.500    110.10   22.53   2.17900 ! ALLOW   ALI
                 ! alkane update, adm jr., 3/2/92
HA   CT3  HA    35.500    108.40    5.40   1.80200 ! ALLOW   ALI
                 ! alkane update, adm jr., 3/2/92
HB   CT1  C      50.000   109.5000 ! ALLOW  PEP
                 ! Alanine Dipeptide ab initio calc's (LK)
NH1  C    HA    44.000    116.00   50.00   1.98000  !
NH1  C    CT1    80.000   116.5000 ! ALLOW   ALI PEP POL ARO
                 ! NMA Vib Modes (LK)
NH1  C    CT3    80.000   116.5000 ! ALLOW   ALI PEP POL ARO
                 ! NMA Vib Modes (LK)
NH1  CT1  C      50.000   107.0000 ! ALLOW   PEP POL ARO ALI
                 ! Alanine Dipeptide ab initio calc's (LK)
NH1  CT1  CT3    70.000   113.5000 ! ALLOW   ALI PEP POL ARO
                 ! Alanine Dipeptide ab initio calc's (LK)
NH1  CT1  HB     48.000   108.0000 ! ALLOW PEP
                 ! Alanine Dipeptide ab initio calc's (LK)
NH1  CT3  HA     51.500   109.5000 ! ALLOW   ALI PEP POL ARO
                 ! NMA crystal (JCS)
O    C    CT1    80.000   121.0000 ! ALLOW   ALI PEP POL ARO
                 ! Alanine Dipeptide ab initio calc's (LK)
O    C    CT3    80.000   121.0000 ! ALLOW   ALI PEP POL ARO
```

```
                ! Alanine Dipeptide ab initio calc's (LK)
O    C    NH1    80.000   122.5000 ! ALLOW   PEP POL ARO
                ! NMA Vib Modes (LK)
O    C    HA     44.000   122.0000 !
                ! adm jr. 5/02/91, acetic acid pure solvent

DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!
C    CT1  NH1  C        0.2000  1   180.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
C    CT2  NH1  C        0.2000  1   180.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
CT1  C    NH1  CT1      1.6000  1     0.00 !  ALLOW PEP
                ! Revised to adjust NMA cis/trans energy difference. (LK)
CT1  C    NH1  CT1      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
CT1  CT1  NH1  C        1.8000  1     0.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
CT3  C    NH1  CT1      1.6000  1     0.00 !  ALLOW PEP
                ! Revised to adjust NMA cis/trans energy difference. (LK)
CT3  C    NH1  CT1      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
CT3  C    NH1  CT3      1.2000  1     0.00 !  ALLOW PEP
                ! Revised to adjust NMA cis/trans energy difference. (LK)
CT3  C    NH1  CT3      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
CT3  CT1  NH1  C        1.8000  1     0.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
CT3  NH1  C    CT1      1.6000  1     0.00 !  ALLOW PEP
                ! Revised to adjust NMA cis/trans energy difference. (LK)
```

```
CT3  NH1  C    CT1      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
H    NH1  C    CT1      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
H    NH1  C    CT3      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
H    NH1  CT1  C        0.0000  1     0.00 ! ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
H    NH1  CT1  CT3      0.0000  1     0.00 ! ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
HA   C    NH1  H        1.4000  2   180.00 !
HA   C    NH1  CT3      2.5000  2   180.00 !
HA   CT3  NH1  C        0.0000  3     0.00 ! ALLOW PEP
                ! LK for autogenerate dihe, sp2-methyl, no dihedral potential
HA   CT3  NH1  CT3      0.0000  3     0.00 !
HA   CT3  NH1  H        0.1100  3     0.00 ! ALLOW PEP
HB   CT1  NH1  C        0.0000  1     0.00 ! ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
HB   CT1  NH1  H        0.0000  1     0.00 ! ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
HB   CT3  NH1  C        0.0000  1     0.00 ! ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
HB   CT3  NH1  H        0.0000  1     0.00 ! ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
NH1  C    CT1  CT3      0.0000  1     0.00 !   ALLOW PEP
                ! ala dipeptide corrxn for new C VDW Rmin, 4/10/93 (LK)
NH1  C    CT1  HB       0.0000  1     0.00 !   ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
NH1  C    CT3  HA       0.0000  3     0.00 ! ALLOW PEP
                ! his, adm jr., 6/27/90
O    C    CT1  CT3      1.4000  1     0.00 !   ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr., 3/3/93c
O    C    CT1  HB       0.0000  1     0.00 !   ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
O    C    CT1  NH1      0.0000  1     0.00 !   ALLOW PEP
                ! Alanine Dipeptide ab initio calc's (LK)
O    C    CT3  HA       0.0400  3   180.00 ! ALLOW POL
                ! adm jr., 8/13/90 acetamide geometry and vibrations
```

```
O    C    NH1  CT1      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
O    C    NH1  CT3      2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
O    C    NH1  H        2.5000  2   180.00 !  ALLOW PEP
                ! Gives appropriate NMA cis/trans barrier. (LK)
X    CT1  CT3  X        0.2000  3     0.00 ! ALLOW   ALI
                ! alkane update, adm jr., 3/2/92
X    CT2  CT2  X        0.1950  3     0.00 ! ALLOW   ALI
                ! alkane update, adm jr., 3/2/92
X    CT2  CT3  X        0.1600  3     0.00 ! ALLOW   ALI
                ! rotation barrier in Ethane (SF)
X    CT3  CT3  X        0.1550  3     0.00 ! ALLOW   ALI
                ! alkane update, adm jr., 3/2/92

IMPROPER
!
!V(improper) = Kpsi(psi - psi0)**2
!
!Kpsi: kcal/mole/rad**2
!psi0: degrees
!note that the second column of numbers (0) is ignored
!
!atom types           Kpsi                   psi0
!
NH1  X    X    H      20.0000         0      0.0000 ! ALLOW   PEP POL ARO
                ! NMA Vibrational Modes (LK)
NH1  C    CT3  CT3    20.0000         0      0.0000 !
O    X    X    C     120.0000         0      0.0000 ! ALLOW   PEP POL ARO
                ! NMA Vibrational Modes (LK)

NONBONDED nbxmod  5 atom cdiel shift vatom vdistance vswitch -
cutnb 14.0 ctofnb 12.0 ctonnb 10.0 eps 1.0 e14fac 1.0 wmin 1.5
                !adm jr., 5/08/91, suggested cutoff scheme
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
```

```
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!
!atom  ignored    epsilon      Rmin/2   ignored   eps,1-4       Rmin/2,1-4
!
C      1.334000  -0.110000     1.960000 ! ALLOW   PEP POL ARO
               ! NMA pure solvent, adm jr., 3/3/93
CC     1.334     -0.110000     1.960000 ! ALLOW   PEP POL ARO
               ! adm jr. 3/3/92, acetic acid heat of solvation
CT1    1.334000  -0.035000     2.200000   0.000000  -0.010000     1.900000 ! ALLOW   ALI
               ! isobutane pure solvent properties, adm jr, 2/3/92
CT2    1.334000  -0.060000     2.120000   0.000000  -0.010000     1.900000 ! ALLOW   ALI
               ! propane pure solvent properties, adm jr, 2/3/92
CT3    1.334000  -0.080000     2.020000   0.000000  -0.010000     1.900000 ! ALLOW   ALI
               !  methane/ethane a.i. and ethane pure solvent, adm jr, 2/3/92
H      0.496     -0.015000     0.757700 ! ALLOW PEP POL SUL ARO ALC
               ! same as TIP3P hydrogen, adm jr., 7/20/89
HA     0.496     -0.025000     1.340000 ! ALLOW PEP ALI POL SUL ARO PRO ALC
               ! methane/ethane a.i. and ethane pure solvent, adm jr, 2/3/92
HB     0.496     -0.025000     1.340000 ! ALLOW PEP ALI POL SUL ARO PRO ALC
               ! methane/ethane a.i. and ethane pure solvent, adm jr, 2/3/92
NH1    1.073000  -0.200000     1.850000   0.000000  -0.200000     1.550000 ! ALLOW   PEP POL ARO
               ! This 1,4 vdW allows the C5 dipeptide minimum to exist.(LK)
O      0.837     -0.120000     1.730000   0.000000  -0.120000     1.400000 ! ALLOW   PEP POL
               ! This 1,4 vdW allows the C5 dipeptide minimum to exist.(LK)

END
```