Supplementary material with the data for “Structure of Gel Phase DPPC Determined by X-ray Diffraction” by John F Nagle, Pierre Cognet, Fernando Dupuy and Stephanie Tristram-Nagle.

There are 28 separate data sets with different samplist numbers (e). The values for the |F(q)| data have already been scaled by experimental scaling factors Ke to best fit the VHDC model in the text. New Ke should be chosen for each of the 28 data sets to minimize differences with simulations or other models.

In addition to the first and second columns, the fifth column of assigned uncertainties is important for working with these data. Other non-essential columns give the fitted value of |F(q)| for the VHDC model, the difference deltaF, and finally the contribution of each order to the total chi^2 for each order of diffraction.

q |F(q)| |F(q)| deltaF Assigned chi^2

data fit uncertainty

D=60.8 rotations (samplist 1)

0.104 2.132 2.101 -0.03141 0.3506 0.008026

0.207 1.244 1.393 0.1493 0.05387 7.68

0.311 0.9857 1.002 0.01654 0.01381 1.435

0.415 1.304 1.328 0.0232 0.01573 2.174

0.519 0.4787 0.4011 -0.07763 0.01724 20.27

0.622 0.1891 0.2865 0.09742 0.04348 5.02

0.726 0.4512 0.3751 -0.07614 0.0201 14.34

0.83 0 0.01843 0.01843 0.1553 0.01409

0.934 0.6114 0.4978 -0.1136 0.02276 24.91

1.037 0.1093 0.02747 -0.08181 0.09516 0.739

1.141 0.1144 0.0212 -0.09324 0.09966 0.8753

1.245 0.3651 0.2688 -0.09625 0.04592 4.394

average 6.8

D=62.6 rotations (2)

0.1004 1.825 1.979 0.1536 0.658 0.05446

0.2007 1.509 1.637 0.128 0.07742 2.735

0.3011 1.063 1.069 0.006387 0.03657 0.0305

0.4015 1.047 1.122 0.07529 0.02074 13.18

0.5019 0.7215 0.6842 -0.03728 0.01233 9.138

0.6022 0.1101 0.1253 0.01513 0.07265 0.04336

0.7026 0.5435 0.5244 -0.01906 0.02219 0.7374

0.803 0 0.04229 0.04229 0.1672 0.06398

0.9033 0.4646 0.4374 -0.0272 0.03253 0.6995

1.004 0.4403 0.2204 -0.2198 0.0377 34.01

1.104 0.1509 0.1148 -0.03609 0.09552 0.1428

1.204 0.2874 0.2215 -0.06585 0.06458 1.04

1.305 0.1494 0.09984 -0.04953 0.1093 0.2052

average 4.3

Fixed angle, h=1,2 (3)

0.1033 2.388 2.079 -0.3081 0.527 0.3417

0.2067 1.377 1.406 0.02836 0.1315 0.04653

Fixed angle, h=2,3 (4)

0.207 1.395 1.393 -0.001857 0.01875 0.00981

0.311 0.9725 1.002 0.02968 0.06357 0.218

Fixed angle, h=3,4 (6)

0.311 1.002 1.002 0.0002835 0.09013 9.895e-06

0.414 1.316 1.316 -0.0001616 0.07795 4.296e-06

Fixed angle, h=4,5 (7)

0.414 1.316 1.316 8.144e-05 0.007813 0.0001086

0.518 0.4468 0.4164 -0.03036 0.08487 0.128

Fixed angle, h=5,6 (8)

0.516 0.4488 0.4476 -0.001237 0.01674 0.005462

0.62 0.1658 0.2695 0.1036 0.1189 0.7598

Fixed angle, h=5,7 (9)

0.515 0.4649 0.4634 -0.001473 0.006377 0.05332

0.721 0.4047 0.412 0.007247 0.01334 0.2952

Fixed angle, h=7,9 (10)

0.721 0.4262 0.412 -0.01417 0.007812 3.292

0.927 0.4805 0.4955 0.01498 0.008808 2.893

Fixed angle, h=5,6 (11)

0.921 0.488 0.488 -6.739e-06 0.003145 4.592e-06

1.023 0.07473 0.1039 0.0292 0.09554 0.09342

Fixed angle, h=10,11 (12)

1.027 0.07954 0.08108 0.00154 0.002287 0.4535

1.129 0.06687 0.06168 -0.005196 0.003664 2.011

Fixed angle, h=9,12 (13)

0.924 0.4923 0.4924 8.82e-05 0.0006061 0.02118

1.232 0.2731 0.2692 -0.003884 0.002974 1.706

Fixed angle, h=1,2 (14)

0.1012 2.107 2.007 -0.09996 0.3123 0.1025

0.2024 1.546 1.575 0.02845 0.1476 0.03716

Fixed angle, h=2,3 (16)

0.199 1.877 1.702 -0.1751 0.2632 0.4426

0.298 0.9976 1.076 0.07823 0.1398 0.3129

Fixed angle, h=3,4 (17)

0.298 1.191 1.076 -0.1149 0.1553 0.5477

0.398 1.01 1.055 0.04518 0.09643 0.2195

Fixed angle, h=4,5 (18)

0.398 1.061 1.055 -0.005467 0.003677 2.21

0.497 0.6947 0.769 0.07426 0.01157 41.21

Fixed angle, h=5,7 (20)

0.500 0.7183 0.7165 -0.001786 0.001992 0.8043

0.700 0.5128 0.5363 0.02345 0.006244 14.11

Fixed angle, h=7,9 (21)

0.702 0.5275 0.5272 -0.0003138 0.00175 0.03216

0.902 0.4302 0.432 0.001765 0.003756 0.2209

Fixed angle, h=9,10 (22)

0.902 0.4321 0.432 -0.0001796 0.0006734 0.07115

1.003 0.2175 0.2247 0.007209 0.003077 5.488

Fixed angle, h=10,11 (23)

1.00 2.204 0.2431 -1.961 0.006582 8.872e+04

1.10 1.067 0.1185 -0.9481 0.006911 1.882e+04

Fixed angle, h=11,12 (24)

1.101 0.1289 0.1178 -0.01117 0.004007 7.776

1.201 0.1921 0.2115 0.01939 0.007074 7.513

Fixed angle, h=10,13 (26)

1.001 0.2376 0.237 -0.0006076 0.002401 0.06403

1.301 0.1112 0.1157 0.004482 0.004557 0.9672

Torbet & Wilkins (27)

0.09817 1.914 1.901 -0.01287 0.01538 0.7006

0.1963 1.853 1.8 -0.05241 0.01537 11.62

0.2945 1.019 1.075 0.05574 0.01532 13.23

0.3927 0.8645 0.9435 0.07901 0.0153 26.66

0.4909 0.8645 0.8759 0.01141 0.0153 0.5558

0.589 0.03088 0.04236 0.01149 0.01279 0.8065

0.6872 0.6175 0.5763 -0.04123 0.01525 7.309

0.7854 0.09263 0.01431 -0.07832 0.02695 8.443

0.8836 0.3705 0.3382 -0.03229 0.02969 1.183

0.9817 0.6484 0.3493 -0.2991 0.5438 0.3026

Wiener & Nagle (28)

0.09864 1.901 1.918 0.01686 0.01552 1.18

0.1973 1.776 1.766 -0.01008 0.01551 0.4219

0.2959 1.122 1.076 -0.04573 0.01548 8.73

0.3945 1.028 0.9839 -0.04455 0.01547 8.297

0.4932 0.748 0.8357 0.08776 0.01542 32.38

0.5918 0.03117 0.0572 0.02604 0.01291 4.068

0.6905 0.5298 0.5692 0.0394 0.04485 0.7718

Older CMU MLV data (29)

0.09879 1.89 1.923 0.03324 0.009041 13.51

0.1976 1.773 1.755 -0.01819 0.007713 5.561

0.2964 1.108 1.076 -0.0314 0.01383 5.155

0.3952 1.047 0.9971 -0.04995 0.05111 0.9554

0.494 0.878 0.8222 -0.05582 0.09267 0.3629

0.5928 0.01571 0.06253 0.04682 0.1421 0.1085

0.6915 0.6077 0.5663 -0.04139 0.02702 2.345

0.7903 0 0.02775 0.02775 0.2094 0.01755

0.8891 0.4081 0.3697 -0.03832 0.06313 0.3685

0.9879 0.4534 0.3149 -0.1385 0.07014 3.90230

Older CMU MLV data (30)

0.1032 2.107 2.074 -0.03312 0.01017 10.61

0.2063 1.299 1.419 0.1201 0.01642 53.5

0.3095 0.983 1.017 0.03364 0.02427 1.92

0.4127 1.311 1.299 -0.01153 0.06397 0.03247

0.5159 0.4241 0.4498 0.0257 0.03055 0.708

0.619 0.4029 0.2613 -0.1416 0.0454 9.731

0.7222 0.4587 0.4033 -0.05544 0.05414 1.049

0.8254 0.008289 9.827e-05 -0.008191 0.254 0.00104

0.9285 0.5824 0.4966 -0.08577 0.0704 1.484

1.032 0.1036 0.05507 -0.04855 0.24 0.04091

Older CMU MLV data (31)

0.09942 1.974 1.945 -0.02891 0.0541 0.2855

0.1988 1.639 1.708 0.06975 0.07746 0.8109

0.2983 1.168 1.076 -0.0925 0.3613 0.06554

0.3977 1.002 1.049 0.0464 0.6521 0.005064

2018 CMU MLV data (32)

0.09864 1.943 1.918 -0.02544 0.01934 1.731

0.1973 1.755 1.766 0.01083 0.02138 0.2566

0.2959 1.023 1.076 0.05304 0.0327 2.631

0.3945 0.8153 0.9839 0.1686 0.07102 5.636

0.4932 0.8013 0.8357 0.03445 0.1102 0.09765

The samplist numbers (e) have gaps due to software considerations.