**Supplementary Information**

**A Paradigm for Natural Eutectic Solvents Based on Fatty Acids: Molecular Interactions and Toxicological Considerations**

Sonia Martel-Martín,*a* Maria Enrica Di Pietro,*b* Alberto Gutiérrez,*c* Nuria Aguilar,*c* Alfredo Bol-Arreba,*a,d* Santiago Aparicio,*a,c\** Fatima Matroodi,e,f Barbara Rossi,e,g Andrea Mele*b\**

*a*International Research Centre in Critical Raw Materials-ICCRAM, University of Burgos, 09001 Burgos, Spain

*b*Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, 20133 Milano, Italy

*c* Department of Chemistry, University of Burgos, 09001 Burgos, Spain

*d*Department of Physics, University of Burgos, 09001 Burgos, Spain

e Elettra-Sincrotrone Trieste, S.S. 114 km 163.5, Basovizza, 34149 Trieste, Italy

f Department of Physics, Shahid Chamran University of Ahvaz, Ahvaz, Iran

g Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo (TN), Italy

\*Corresponding authors: [sapar@ubu.es](mailto:sapar@ubu.es) (S.A.) and [andrea.mele@polimi.it](mailto:andrea.mele@polimi.it) (A.M.)

**Table S1. Specifications of the chemicals used in this work for V-HDES.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| name | molar mass (g/mol) | purity (mass%) | supplier | CAS number | melting temperature / °C |
| MEN | 156.27 | ≥ 98% | Sigma Aldrich | 89-78-1 | 36 - 38 |
| C8 | 144.21 | ≥ 99% | Sigma Aldrich | 124-07-2 | 16.7 |
| C12 | 200.32 | ≥ 99% | Sigma Aldrich | 143-07-7 | 43.8 |

**Table S2. Force field parameterization used for MD simulations**



The general form of the applied force field is:



Graphene was maintained as rigid along the simulations, thus dihedrals (*Etor*) were null for all the molecules.

Improper dihedrals were described according to:

*Eimproper* = *kϕ*(*ϕ*-*ϕ0*)2



**MEN**

# Atoms

31

# X Y Z M Q sigma epsilon Type Number

# (A) (u) (e) (A) (kJ/M)

O 0.5271000 -1.2575000 -2.3567000 15.999400 -0.766381 3.120000 0.707880 O1 1

C -1.0774000 -0.3093000 -0.7803000 12.011000 -0.226594 3.500000 0.276100 C2 2

C 0.2098000 -1.1500000 -0.9658000 12.011000 0.514786 3.500000 0.276100 C3 3

C -0.7772000 1.1634000 -1.1431000 12.011000 -0.044956 3.500000 0.276100 C4 4

C 1.6633000 0.9082000 -0.5088000 12.011000 0.623659 3.500000 0.276100 C5 5

C 1.4106000 -0.5773000 -0.2040000 12.011000 -0.578877 3.500000 0.276100 C6 6

C 0.3869000 1.7417000 -0.3404000 12.011000 -0.256524 3.500000 0.276100 C7 7

C -1.7077000 -0.4698000 0.6422000 12.011000 0.561089 3.500000 0.276100 C8 8

C 2.7837000 1.4551000 0.3755000 12.011000 -0.562194 3.500000 0.276100 C9 9

C -2.9699000 0.3859000 0.8198000 12.011000 -0.558732 3.500000 0.276100 C10 10

C -2.0742000 -1.9293000 0.9483000 12.011000 -0.580991 3.500000 0.276100 C11 11

H -1.8171000 -0.6636000 -1.5124000 1.007947 0.047931 2.500000 0.125520 H12 12

H 0.0482000 -2.1805000 -0.6411000 1.007947 0.055556 2.500000 0.125520 H13 13

H -0.5366000 1.2317000 -2.2117000 1.007947 0.003270 2.500000 0.125520 H14 14

H -1.6629000 1.7931000 -1.0153000 1.007947 0.051211 2.500000 0.125520 H15 15

H 1.9960000 0.9989000 -1.5509000 1.007947 -0.090234 2.500000 0.125520 H16 16

H 2.3108000 -1.1469000 -0.4674000 1.007947 0.123039 2.500000 0.125520 H17 17

H 1.2518000 -0.7099000 0.8732000 1.007947 0.105524 2.500000 0.125520 H18 18

H 0.5741000 2.7699000 -0.6735000 1.007947 0.045753 2.500000 0.125520 H19 19

H 0.1123000 1.8049000 0.7193000 1.007947 0.056791 2.500000 0.125520 H20 20

H -0.9868000 -0.1490000 1.4033000 1.007947 -0.055466 2.500000 0.125520 H21 21

H 2.5174000 1.3999000 1.4364000 1.007947 0.123608 2.500000 0.125520 H22 22

H 3.7075000 0.8858000 0.2278000 1.007947 0.127753 2.500000 0.125520 H23 23

H 2.9932000 2.5023000 0.1331000 1.007947 0.108723 2.500000 0.125520 H24 24

H -2.7332000 1.4537000 0.8285000 1.007947 0.124415 2.500000 0.125520 H25 25

H -3.4600000 0.1688000 1.7755000 1.007947 0.118052 2.500000 0.125520 H26 26

H -3.6932000 0.1963000 0.0197000 1.007947 0.128750 2.500000 0.125520 H27 27

H -2.6195000 -2.0062000 1.8956000 1.007947 0.137725 2.500000 0.125520 H28 28

H -1.1839000 -2.5557000 1.0521000 1.007947 0.095688 2.500000 0.125520 H29 29

H -2.7065000 -2.3526000 0.1607000 1.007947 0.131844 2.500000 0.125520 H30 30

H2 0.7710000 -0.3811000 -2.6944000 1.007947 0.435780 0.400010 0.192464 H31 31

# Bonds

# N1 N2 R-eqv Force

0 1 3 1.418 1519.6875

0 1 31 0.972 2346.8265

0 2 3 1.508 1282.1115

0 2 4 1.508 1282.1115

0 2 8 1.508 1282.1115

0 2 12 1.093 1435.0745

0 3 6 1.508 1282.1115

0 3 13 1.093 1435.0745

0 4 7 1.508 1282.1115

0 4 14 1.093 1435.0745

0 4 15 1.093 1435.0745

0 5 6 1.508 1282.1115

0 5 7 1.508 1282.1115

0 5 9 1.508 1282.1115

0 5 16 1.093 1435.0745

0 6 17 1.093 1435.0745

0 6 18 1.093 1435.0745

0 7 19 1.093 1435.0745

0 7 20 1.093 1435.0745

0 8 10 1.508 1282.1115

0 8 11 1.508 1282.1115

0 8 21 1.093 1435.0745

0 9 22 1.093 1435.0745

0 9 23 1.093 1435.0745

0 9 24 1.093 1435.0745

0 10 25 1.093 1435.0745

0 10 26 1.093 1435.0745

0 10 27 1.093 1435.0745

0 11 28 1.093 1435.0745

0 11 29 1.093 1435.0745

0 11 30 1.093 1435.0745

# Angles

# N1 N2 N3 A-eqv Force

3 1 31 106.503 477.55

3 2 4 109.608 512.48

3 2 8 109.608 512.48

3 2 12 110.549 383

4 2 8 109.608 512.48

4 2 12 110.549 383

8 2 12 110.549 383

1 3 2 108.133 597.39

1 3 6 108.133 597.39

1 3 13 108.577 470.32

2 3 6 109.608 512.48

2 3 13 110.549 383

6 3 13 110.549 383

2 4 7 109.608 512.48

2 4 14 110.549 383

2 4 15 110.549 383

7 4 14 110.549 383

7 4 15 110.549 383

14 4 15 108.836 310.74

6 5 7 109.608 512.48

6 5 9 109.608 512.48

6 5 16 110.549 383

7 5 9 109.608 512.48

7 5 16 110.549 383

9 5 16 110.549 383

3 6 5 109.608 512.48

3 6 17 110.549 383

3 6 18 110.549 383

5 6 17 110.549 383

5 6 18 110.549 383

17 6 18 108.836 310.74

4 7 5 109.608 512.48

4 7 19 110.549 383

4 7 20 110.549 383

5 7 19 110.549 383

5 7 20 110.549 383

19 7 20 108.836 310.74

2 8 10 109.608 512.48

2 8 11 109.608 512.48

2 8 21 110.549 383

10 8 11 109.608 512.48

10 8 21 110.549 383

11 8 21 110.549 383

5 9 22 110.549 383

5 9 23 110.549 383

5 9 24 110.549 383

22 9 23 108.836 310.74

22 9 24 108.836 310.74

23 9 24 108.836 310.74

8 10 25 110.549 383

8 10 26 110.549 383

8 10 27 110.549 383

25 10 26 108.836 310.74

25 10 27 108.836 310.74

26 10 27 108.836 310.74

8 11 28 110.549 383

8 11 29 110.549 383

8 11 30 110.549 383

28 11 29 108.836 310.74

28 11 30 108.836 310.74

29 11 30 108.836 310.74

# Dihedrals

# N1 N2 N3 N4 A-eqv Force n Type

1 3 2 4 0 -1.4393 1

1 3 2 4 180 3.6777 2

1 3 2 4 0 0.9958 3

1 3 2 8 0 -1.4393 1

1 3 2 8 180 3.6777 2

1 3 2 8 0 0.9958 3

1 3 2 12 0 -1.3682 1

1 3 2 12 180 2.2426 2

1 3 2 12 0 0.5858 3

1 3 6 5 0 -1.4393 1

1 3 6 5 180 3.6777 2

1 3 6 5 0 0.9958 3

1 3 6 17 0 -1.3682 1

1 3 6 17 180 2.2426 2

1 3 6 17 0 0.5858 3

1 3 6 18 0 -1.3682 1

1 3 6 18 180 2.2426 2

1 3 6 18 0 0.5858 3

2 3 1 31 180 0.5648 2

2 3 1 31 0 0.4937 3

2 3 6 5 0 0.2134 1

2 3 6 5 180 1.4267 2

2 3 6 5 0 0.6945 3

2 3 6 17 0 1.3389 1

2 3 6 17 180 -1.318 2

2 3 6 17 0 0.5523 3

2 3 6 18 0 1.3389 1

2 3 6 18 180 -1.318 2

2 3 6 18 0 0.5523 3

2 4 7 5 0 0.2134 1

2 4 7 5 180 1.4267 2

2 4 7 5 0 0.6945 3

2 4 7 19 0 1.3389 1

2 4 7 19 180 -1.318 2

2 4 7 19 0 0.5523 3

2 4 7 20 0 1.3389 1

2 4 7 20 180 -1.318 2

2 4 7 20 0 0.5523 3

2 8 10 25 0 1.3389 1

2 8 10 25 180 -1.318 2

2 8 10 25 0 0.5523 3

2 8 10 26 0 1.3389 1

2 8 10 26 180 -1.318 2

2 8 10 26 0 0.5523 3

2 8 10 27 0 1.3389 1

2 8 10 27 180 -1.318 2

2 8 10 27 0 0.5523 3

2 8 11 28 0 1.3389 1

2 8 11 28 180 -1.318 2

2 8 11 28 0 0.5523 3

2 8 11 29 0 1.3389 1

2 8 11 29 180 -1.318 2

2 8 11 29 0 0.5523 3

2 8 11 30 0 1.3389 1

2 8 11 30 180 -1.318 2

2 8 11 30 0 0.5523 3

3 2 4 7 0 0.2134 1

3 2 4 7 180 1.4267 2

3 2 4 7 0 0.6945 3

3 2 4 14 0 1.3389 1

3 2 4 14 180 -1.318 2

3 2 4 14 0 0.5523 3

3 2 4 15 0 1.3389 1

3 2 4 15 180 -1.318 2

3 2 4 15 0 0.5523 3

3 2 8 10 0 0.2134 1

3 2 8 10 180 1.4267 2

3 2 8 10 0 0.6945 3

3 2 8 11 0 0.2134 1

3 2 8 11 180 1.4267 2

3 2 8 11 0 0.6945 3

3 2 8 21 0 1.3389 1

3 2 8 21 180 -1.318 2

3 2 8 21 0 0.5523 3

3 6 5 7 0 0.2134 1

3 6 5 7 180 1.4267 2

3 6 5 7 0 0.6945 3

3 6 5 9 0 0.2134 1

3 6 5 9 180 1.4267 2

3 6 5 9 0 0.6945 3

3 6 5 16 0 1.3389 1

3 6 5 16 180 -1.318 2

3 6 5 16 0 0.5523 3

4 2 3 6 0 0.2134 1

4 2 3 6 180 1.4267 2

4 2 3 6 0 0.6945 3

4 2 3 13 0 1.3389 1

4 2 3 13 180 -1.318 2

4 2 3 13 0 0.5523 3

4 2 8 10 0 0.2134 1

4 2 8 10 180 1.4267 2

4 2 8 10 0 0.6945 3

4 2 8 11 0 0.2134 1

4 2 8 11 180 1.4267 2

4 2 8 11 0 0.6945 3

4 2 8 21 0 1.3389 1

4 2 8 21 180 -1.318 2

4 2 8 21 0 0.5523 3

4 7 5 6 0 0.2134 1

4 7 5 6 180 1.4267 2

4 7 5 6 0 0.6945 3

4 7 5 9 0 0.2134 1

4 7 5 9 180 1.4267 2

4 7 5 9 0 0.6945 3

4 7 5 16 0 1.3389 1

4 7 5 16 180 -1.318 2

4 7 5 16 0 0.5523 3

5 6 3 13 0 1.3389 1

5 6 3 13 180 -1.318 2

5 6 3 13 0 0.5523 3

5 7 4 14 0 1.3389 1

5 7 4 14 180 -1.318 2

5 7 4 14 0 0.5523 3

5 7 4 15 0 1.3389 1

5 7 4 15 180 -1.318 2

5 7 4 15 0 0.5523 3

6 3 1 31 180 0.5648 2

6 3 1 31 0 0.4937 3

6 3 2 8 0 0.2134 1

6 3 2 8 180 1.4267 2

6 3 2 8 0 0.6945 3

6 3 2 12 0 1.3389 1

6 3 2 12 180 -1.318 2

6 3 2 12 0 0.5523 3

6 5 7 19 0 1.3389 1

6 5 7 19 180 -1.318 2

6 5 7 19 0 0.5523 3

6 5 7 20 0 1.3389 1

6 5 7 20 180 -1.318 2

6 5 7 20 0 0.5523 3

6 5 9 22 0 1.3389 1

6 5 9 22 180 -1.318 2

6 5 9 22 0 0.5523 3

6 5 9 23 0 1.3389 1

6 5 9 23 180 -1.318 2

6 5 9 23 0 0.5523 3

6 5 9 24 0 1.3389 1

6 5 9 24 180 -1.318 2

6 5 9 24 0 0.5523 3

7 4 2 8 0 0.2134 1

7 4 2 8 180 1.4267 2

7 4 2 8 0 0.6945 3

7 4 2 12 0 1.3389 1

7 4 2 12 180 -1.318 2

7 4 2 12 0 0.5523 3

7 5 6 17 0 1.3389 1

7 5 6 17 180 -1.318 2

7 5 6 17 0 0.5523 3

7 5 6 18 0 1.3389 1

7 5 6 18 180 -1.318 2

7 5 6 18 0 0.5523 3

7 5 9 22 0 1.3389 1

7 5 9 22 180 -1.318 2

7 5 9 22 0 0.5523 3

7 5 9 23 0 1.3389 1

7 5 9 23 180 -1.318 2

7 5 9 23 0 0.5523 3

7 5 9 24 0 1.3389 1

7 5 9 24 180 -1.318 2

7 5 9 24 0 0.5523 3

8 2 3 13 0 1.3389 1

8 2 3 13 180 -1.318 2

8 2 3 13 0 0.5523 3

8 2 4 14 0 1.3389 1

8 2 4 14 180 -1.318 2

8 2 4 14 0 0.5523 3

8 2 4 15 0 1.3389 1

8 2 4 15 180 -1.318 2

8 2 4 15 0 0.5523 3

9 5 6 17 0 1.3389 1

9 5 6 17 180 -1.318 2

9 5 6 17 0 0.5523 3

9 5 6 18 0 1.3389 1

9 5 6 18 180 -1.318 2

9 5 6 18 0 0.5523 3

9 5 7 19 0 1.3389 1

9 5 7 19 180 -1.318 2

9 5 7 19 0 0.5523 3

9 5 7 20 0 1.3389 1

9 5 7 20 180 -1.318 2

9 5 7 20 0 0.5523 3

10 8 2 12 0 1.3389 1

10 8 2 12 180 -1.318 2

10 8 2 12 0 0.5523 3

10 8 11 28 0 1.3389 1

10 8 11 28 180 -1.318 2

10 8 11 28 0 0.5523 3

10 8 11 29 0 1.3389 1

10 8 11 29 180 -1.318 2

10 8 11 29 0 0.5523 3

10 8 11 30 0 1.3389 1

10 8 11 30 180 -1.318 2

10 8 11 30 0 0.5523 3

11 8 2 12 0 1.3389 1

11 8 2 12 180 -1.318 2

11 8 2 12 0 0.5523 3

11 8 10 25 0 1.3389 1

11 8 10 25 180 -1.318 2

11 8 10 25 0 0.5523 3

11 8 10 26 0 1.3389 1

11 8 10 26 180 -1.318 2

11 8 10 26 0 0.5523 3

11 8 10 27 0 1.3389 1

11 8 10 27 180 -1.318 2

11 8 10 27 0 0.5523 3

12 2 3 13 0 0.5941 1

12 2 3 13 180 -2.8995 2

12 2 3 13 0 0.6569 3

12 2 4 14 0 0.5941 1

12 2 4 14 180 -2.8995 2

12 2 4 14 0 0.6569 3

12 2 4 15 0 0.5941 1

12 2 4 15 180 -2.8995 2

12 2 4 15 0 0.6569 3

12 2 8 21 0 0.5941 1

12 2 8 21 180 -2.8995 2

12 2 8 21 0 0.6569 3

13 3 1 31 0 1.2468 1

13 3 1 31 180 -0.5774 2

13 3 1 31 0 0.7238 3

13 3 6 17 0 0.5941 1

13 3 6 17 180 -2.8995 2

13 3 6 17 0 0.6569 3

13 3 6 18 0 0.5941 1

13 3 6 18 180 -2.8995 2

13 3 6 18 0 0.6569 3

14 4 7 19 0 0.5941 1

14 4 7 19 180 -2.8995 2

14 4 7 19 0 0.6569 3

14 4 7 20 0 0.5941 1

14 4 7 20 180 -2.8995 2

14 4 7 20 0 0.6569 3

15 4 7 19 0 0.5941 1

15 4 7 19 180 -2.8995 2

15 4 7 19 0 0.6569 3

15 4 7 20 0 0.5941 1

15 4 7 20 180 -2.8995 2

15 4 7 20 0 0.6569 3

16 5 6 17 0 0.5941 1

16 5 6 17 180 -2.8995 2

16 5 6 17 0 0.6569 3

16 5 6 18 0 0.5941 1

16 5 6 18 180 -2.8995 2

16 5 6 18 0 0.6569 3

16 5 7 19 0 0.5941 1

16 5 7 19 180 -2.8995 2

16 5 7 19 0 0.6569 3

16 5 7 20 0 0.5941 1

16 5 7 20 180 -2.8995 2

16 5 7 20 0 0.6569 3

16 5 9 22 0 0.5941 1

16 5 9 22 180 -2.8995 2

16 5 9 22 0 0.6569 3

16 5 9 23 0 0.5941 1

16 5 9 23 180 -2.8995 2

16 5 9 23 0 0.6569 3

16 5 9 24 0 0.5941 1

16 5 9 24 180 -2.8995 2

16 5 9 24 0 0.6569 3

21 8 10 25 0 0.5941 1

21 8 10 25 180 -2.8995 2

21 8 10 25 0 0.6569 3

21 8 10 26 0 0.5941 1

21 8 10 26 180 -2.8995 2

21 8 10 26 0 0.6569 3

21 8 10 27 0 0.5941 1

21 8 10 27 180 -2.8995 2

21 8 10 27 0 0.6569 3

21 8 11 28 0 0.5941 1

21 8 11 28 180 -2.8995 2

21 8 11 28 0 0.6569 3

21 8 11 29 0 0.5941 1

21 8 11 29 180 -2.8995 2

21 8 11 29 0 0.6569 3

21 8 11 30 0 0.5941 1

21 8 11 30 180 -2.8995 2

21 8 11 30 0 0.6569 3

**C8**

# Atoms

26

# X Y Z M Q sigma epsilon Type Number

# (A) (u) (e) (A) (kJ/M)

C 21.2641 -11.6771 0.0032 12.011 -0.419 3.87541 0.23012 C 1

C 20.0101 -12.5331 -0.0789 12.011 -0.276 3.87541 0.23012 C1 2

H 21.9583 -11.9194 -0.8078 1.007947 0.1462 2.35197 0.092048 H 3

H 21.7814 -11.8299 0.9558 1.007947 0.1462 2.35197 0.092048 H1 4

H 21.0053 -10.6167 -0.0765 1.007947 0.1462 2.35197 0.092048 H2 5

C 20.3413 -14.0214 0.0257 12.011 -0.277 3.87541 0.23012 C2 6

H 19.4983 -12.3312 -1.0271 1.007947 0.14682 2.35197 0.092048 H3 7

H 19.3252 -12.2458 0.7273 1.007947 0.1462 2.35197 0.092048 H4 8

C 19.0782 -14.8808 -0.0505 12.011 -0.277 3.87541 0.23012 C3 9

H 20.8612 -14.2165 0.9716 1.007947 0.1462 2.35197 0.092048 H5 10

H 21.0265 -14.3026 -0.7833 1.007947 0.14682 2.35197 0.092048 H6 11

C 19.4143 -16.3699 0.0449 12.011 -0.277 3.87541 0.23012 C4 12

H 18.5543 -14.6822 -0.9934 1.007947 0.14682 2.35197 0.092048 H7 13

H 18.3963 -14.6046 0.763 1.007947 0.1462 2.35197 0.092048 H8 14

C 18.1535 -17.2324 -0.0215 12.011 -0.277 3.87541 0.23012 C5 15

H 19.9445 -16.5675 0.9845 1.007947 0.1462 2.35197 0.092048 H9 16

H 20.0914 -16.6459 -0.7726 1.007947 0.1462 2.35197 0.092048 H10 17

C 18.4937 -18.7191 0.0636 12.011 -0.2777 3.87541 0.23012 C6 18

H 17.6145 -17.0303 -0.9556 1.007947 0.1462 2.35197 0.092048 H11 19

H 17.476 -16.9607 0.7978 1.007947 0.14682 2.35197 0.092048 H12 20

C 17.2598 -19.5778 0.0032 12.011 0.0928 3.56359 0.46024 C7 21

H 19.0106 -18.9299 1.0063 1.007947 0.1462 2.35197 0.092048 H13 22

H 19.1458 -18.9977 -0.7716 1.007947 0.1462 2.35197 0.092048 H14 23

O 16.0996 -19.2111 -0.0623 15.9994 -0.27231 3.02905 0.50208 O 24

O 17.5621 -20.8911 0.0345 15.9994 -0.20069 3.15378 0.636386 O1 25

H 16.6895 -21.3357 -0.0076 1.007947 0.26479 0.40001 0.192464 H15 26

# Bonds

# N1 N2 R-eqv Force Type

0 1 2 1.508 1282.11

0 1 3 1.093 1435.07

0 1 4 1.093 1435.07

0 1 5 1.093 1435.07

0 2 6 1.508 1282.11

0 2 7 1.093 1435.07

0 2 8 1.093 1435.07

0 6 9 1.508 1282.11

0 6 10 1.093 1435.07

0 6 11 1.093 1435.07

0 9 12 1.508 1282.11

0 9 13 1.093 1435.07

0 9 14 1.093 1435.07

0 12 15 1.508 1282.11

0 12 16 1.093 1435.07

0 12 17 1.093 1435.07

0 15 18 1.508 1282.11

0 15 19 1.093 1435.07

0 15 20 1.093 1435.07

0 18 21 1.492 1261.64

0 18 22 1.093 1435.07

0 18 23 1.093 1435.07

0 21 24 1.222 3899.33

0 21 25 1.355 1746.72

0 25 26 0.981 2229.09

# Angles

# N1 N2 N3 A-eqv Force Type

2 1 3 110.55 383

2 1 4 110.55 383

2 1 5 110.55 383

3 1 4 108.84 310.74

3 1 5 108.84 310.74

4 1 5 108.84 310.74

1 2 6 109.61 512.48

1 2 7 110.55 383

1 2 8 110.55 383

6 2 7 110.55 383

6 2 8 110.55 383

7 2 8 108.84 310.74

2 6 9 109.61 512.48

2 6 10 110.55 383

2 6 11 110.55 383

9 6 10 110.55 383

9 6 11 110.55 383

10 6 11 108.84 310.74

6 9 12 109.61 512.48

6 9 13 110.55 383

6 9 14 110.55 383

12 9 13 110.55 383

12 9 14 110.55 383

13 9 14 108.84 310.74

9 12 15 109.61 512.48

9 12 16 110.55 383

9 12 17 110.55 383

15 12 16 110.55 383

15 12 17 110.55 383

16 12 17 108.84 310.74

12 15 18 109.61 512.48

12 15 19 110.55 383

12 15 20 110.55 383

18 15 19 110.55 383

18 15 20 110.55 383

19 15 20 108.84 310.74

15 18 21 107.52 467.91

15 18 22 110.55 383

15 18 23 110.55 383

21 18 22 108.39 391.44

21 18 23 108.39 391.44

22 18 23 108.84 310.74

18 21 24 124.41 564.87

18 21 25 109.72 628.1

24 21 25 124.43 695.55

21 25 26 111.95 351.09

# Dihedrals

# N1 N2 N3 N4 A-eqv Force n Type

1 2 6 9 0 0.2134 1

1 2 6 9 180 1.4267 2

1 2 6 9 0 0.6945 3

1 2 6 10 0 1.3389 1

1 2 6 10 180 -1.318 2

1 2 6 10 0 0.5523 3

1 2 6 11 0 1.3389 1

1 2 6 11 180 -1.318 2

1 2 6 11 0 0.5523 3

2 6 9 12 0 0.2134 1

2 6 9 12 180 1.4267 2

2 6 9 12 0 0.6945 3

2 6 9 13 0 1.3389 1

2 6 9 13 180 -1.318 2

2 6 9 13 0 0.5523 3

2 6 9 14 0 1.3389 1

2 6 9 14 180 -1.318 2

2 6 9 14 0 0.5523 3

3 1 2 6 0 1.3389 1

3 1 2 6 180 -1.318 2

3 1 2 6 0 0.5523 3

3 1 2 7 0 0.5941 1

3 1 2 7 180 -2.8995 2

3 1 2 7 0 0.6569 3

3 1 2 8 0 0.5941 1

3 1 2 8 180 -2.8995 2

3 1 2 8 0 0.6569 3

4 1 2 6 0 1.3389 1

4 1 2 6 180 -1.318 2

4 1 2 6 0 0.5523 3

4 1 2 7 0 0.5941 1

4 1 2 7 180 -2.8995 2

4 1 2 7 0 0.6569 3

4 1 2 8 0 0.5941 1

4 1 2 8 180 -2.8995 2

4 1 2 8 0 0.6569 3

5 1 2 6 0 1.3389 1

5 1 2 6 180 -1.318 2

5 1 2 6 0 0.5523 3

5 1 2 7 0 0.5941 1

5 1 2 7 180 -2.8995 2

5 1 2 7 0 0.6569 3

5 1 2 8 0 0.5941 1

5 1 2 8 180 -2.8995 2

5 1 2 8 0 0.6569 3

6 9 12 15 0 0.2134 1

6 9 12 15 180 1.4267 2

6 9 12 15 0 0.6945 3

6 9 12 16 0 1.3389 1

6 9 12 16 180 -1.318 2

6 9 12 16 0 0.5523 3

6 9 12 17 0 1.3389 1

6 9 12 17 180 -1.318 2

6 9 12 17 0 0.5523 3

7 2 6 9 0 1.3389 1

7 2 6 9 180 -1.318 2

7 2 6 9 0 0.5523 3

7 2 6 10 0 0.5941 1

7 2 6 10 180 -2.8995 2

7 2 6 10 0 0.6569 3

7 2 6 11 0 0.5941 1

7 2 6 11 180 -2.8995 2

7 2 6 11 0 0.6569 3

8 2 6 9 0 1.3389 1

8 2 6 9 180 -1.318 2

8 2 6 9 0 0.5523 3

8 2 6 10 0 0.5941 1

8 2 6 10 180 -2.8995 2

8 2 6 10 0 0.6569 3

8 2 6 11 0 0.5941 1

8 2 6 11 180 -2.8995 2

8 2 6 11 0 0.6569 3

9 12 15 18 0 0.2134 1

9 12 15 18 180 1.4267 2

9 12 15 18 0 0.6945 3

9 12 15 19 0 1.3389 1

9 12 15 19 180 -1.318 2

9 12 15 19 0 0.5523 3

9 12 15 20 0 1.3389 1

9 12 15 20 180 -1.318 2

9 12 15 20 0 0.5523 3

10 6 9 12 0 1.3389 1

10 6 9 12 180 -1.318 2

10 6 9 12 0 0.5523 3

10 6 9 13 0 0.5941 1

10 6 9 13 180 -2.8995 2

10 6 9 13 0 0.6569 3

10 6 9 14 0 0.5941 1

10 6 9 14 180 -2.8995 2

10 6 9 14 0 0.6569 3

11 6 9 12 0 1.3389 1

11 6 9 12 180 -1.318 2

11 6 9 12 0 0.5523 3

11 6 9 13 0 0.5941 1

11 6 9 13 180 -2.8995 2

11 6 9 13 0 0.6569 3

11 6 9 14 0 0.5941 1

11 6 9 14 180 -2.8995 2

11 6 9 14 0 0.6569 3

12 15 18 21 0 0.1381 1

12 15 18 21 180 -0.3264 2

12 15 18 21 0 0.2971 3

12 15 18 22 0 1.3389 1

12 15 18 22 180 -1.318 2

12 15 18 22 0 0.5523 3

12 15 18 23 0 1.3389 1

12 15 18 23 180 -1.318 2

12 15 18 23 0 0.5523 3

13 9 12 15 0 1.3389 1

13 9 12 15 180 -1.318 2

13 9 12 15 0 0.5523 3

13 9 12 16 0 0.5941 1

13 9 12 16 180 -2.8995 2

13 9 12 16 0 0.6569 3

13 9 12 17 0 0.5941 1

13 9 12 17 180 -2.8995 2

13 9 12 17 0 0.6569 3

14 9 12 15 0 1.3389 1

14 9 12 15 180 -1.318 2

14 9 12 15 0 0.5523 3

14 9 12 16 0 0.5941 1

14 9 12 16 180 -2.8995 2

14 9 12 16 0 0.6569 3

14 9 12 17 0 0.5941 1

14 9 12 17 180 -2.8995 2

14 9 12 17 0 0.6569 3

15 18 21 24 0 1.7238 1

15 18 21 24 180 0.2929 2

15 18 21 24 0 0.682 3

15 18 21 25 0 -0.2469 1

15 18 21 25 180 -0.6987 2

15 18 21 25 0 0.4226 3

16 12 15 18 0 1.3389 1

16 12 15 18 180 -1.318 2

16 12 15 18 0 0.5523 3

16 12 15 19 0 0.5941 1

16 12 15 19 180 -2.8995 2

16 12 15 19 0 0.6569 3

16 12 15 20 0 0.5941 1

16 12 15 20 180 -2.8995 2

16 12 15 20 0 0.6569 3

17 12 15 18 0 1.3389 1

17 12 15 18 180 -1.318 2

17 12 15 18 0 0.5523 3

17 12 15 19 0 0.5941 1

17 12 15 19 180 -2.8995 2

17 12 15 19 0 0.6569 3

17 12 15 20 0 0.5941 1

17 12 15 20 180 -2.8995 2

17 12 15 20 0 0.6569 3

18 21 25 26 0 -2.4393 1

18 21 25 26 180 10.6232 2

18 21 25 26 0 -1.1422 3

19 15 18 21 0 -0.5356 1

19 15 18 21 180 0.1213 2

19 15 18 22 0 0.5941 1

19 15 18 22 180 -2.8995 2

19 15 18 22 0 0.6569 3

19 15 18 23 0 0.5941 1

19 15 18 23 180 -2.8995 2

19 15 18 23 0 0.6569 3

20 15 18 21 0 -0.5356 1

20 15 18 21 180 0.1213 2

20 15 18 22 0 0.5941 1

20 15 18 22 180 -2.8995 2

20 15 18 22 0 0.6569 3

20 15 18 23 0 0.5941 1

20 15 18 23 180 -2.8995 2

20 15 18 23 0 0.6569 3

22 18 21 24 0 1.3807 1

22 18 21 24 180 -2.9455 2

22 18 21 24 0 0.6443 3

22 18 21 25 180 -1.3054 2

22 18 21 25 0 0.6904 3

23 18 21 24 0 1.3807 1

23 18 21 24 180 -2.9455 2

23 18 21 24 0 0.6443 3

23 18 21 25 180 -1.3054 2

23 18 21 25 0 0.6904 3

24 21 25 26 0 3.4769 1

24 21 25 26 180 12.87 2

24 21 25 26 0 -0.1213 3

improper

15

1 3 2 4 0 0

1 3 2 5 0 0

2 6 1 7 0 0

2 6 1 8 0 0

6 9 2 10 0 0

6 9 2 11 0 0

9 12 6 13 0 0

9 12 6 14 0 0

12 15 9 16 0 0

12 15 9 17 0 0

15 18 12 19 0 0

15 18 12 20 0 0

18 21 15 22 0 0

18 21 15 23 0 0

21 25 18 24 0 84.9101

**C12**

# Atoms

38

# X Y Z M Q sigma epsilon Type Number

# (A) (u) (e) (A) (kJ/M)

OH -8.0410000 0.7100000 0.0060000 15.999400 -0.20069 3.15378 0.636386 OH 1

O3 -7.1320000 -1.3640000 -0.0680000 15.999400 -0.27231 3.02905 0.502080 O3 2

C 0.6810000 -0.4850000 -0.0280000 12.011000 -0.27605 3.87541 0.230120 C 3

C -0.5780000 0.3880000 0.0130000 12.011000 -0.27587 3.87541 0.230120 C 4

C 1.9830000 0.3230000 0.0190000 12.011000 -0.27635 3.87541 0.230120 C 5

C -1.8850000 -0.4130000 -0.0290000 12.011000 -0.27471 3.87541 0.230120 C 6

C 3.2470000 -0.5440000 -0.0210000 12.011000 -0.27678 3.87541 0.230120 C 7

C -3.1360000 0.4710000 0.0090000 12.011000 -0.27312 3.87541 0.230120 C 8

C 4.5460000 0.2690000 0.0290000 12.011000 -0.27943 3.87541 0.230120 C 9

C -4.4440000 -0.3260000 -0.0290000 12.011000 -0.26802 3.87541 0.230120 C 10

C 5.8130000 -0.5950000 -0.0090000 12.011000 -0.27980 3.87541 0.230120 C 11

C -5.6700000 0.5850000 0.0090000 12.011000 -0.27520 3.87541 0.230120 C 12

C 7.1030000 0.2310000 0.0450000 12.011000 -0.41754 3.87541 0.230120 C 13

C3 -6.9870000 -0.1500000 -0.0230000 12.011000 0.09280 3.56359 0.460240 C3 14

H 0.6680000 -1.1020000 -0.9440000 1.007947 0.13881 2.35197 0.092048 H 15

H 0.6610000 -1.1930000 0.8210000 1.007947 0.13812 2.35197 0.092048 H 16

H -0.5610000 1.0070000 0.9270000 1.007947 0.13909 2.35197 0.092048 H 17

H -0.5580000 1.0950000 -0.8370000 1.007947 0.13846 2.35197 0.092048 H 18

H 1.9950000 0.9410000 0.9350000 1.007947 0.13867 2.35197 0.092048 H 19

H 2.0020000 1.0320000 -0.8290000 1.007947 0.13803 2.35197 0.092048 H 20

H -1.9090000 -1.1170000 0.8220000 1.007947 0.13926 2.35197 0.092048 H 21

H -1.9040000 -1.0330000 -0.9430000 1.007947 0.13990 2.35197 0.092048 H 22

H 3.2280000 -1.2540000 0.8260000 1.007947 0.13790 2.35197 0.092048 H 23

H 3.2370000 -1.1600000 -0.9390000 1.007947 0.13862 2.35197 0.092048 H 24

H -3.1110000 1.1740000 -0.8430000 1.007947 0.14109 2.35197 0.092048 H 25

H -3.1130000 1.0930000 0.9220000 1.007947 0.14168 2.35197 0.092048 H 26

H 4.5650000 0.9780000 -0.8180000 1.007947 0.13755 2.35197 0.092048 H 27

H 4.5550000 0.8850000 0.9460000 1.007947 0.13820 2.35197 0.092048 H 28

H -4.4810000 -1.0230000 0.8240000 1.007947 0.14577 2.35197 0.092048 H 29

H -4.4770000 -0.9460000 -0.9390000 1.007947 0.14639 2.35197 0.092048 H 30

H 5.7920000 -1.3040000 0.8370000 1.007947 0.13699 2.35197 0.092048 H 31

H 5.8040000 -1.2100000 -0.9250000 1.007947 0.13769 2.35197 0.092048 H 32

H -5.6680000 1.2150000 0.9140000 1.007947 0.17535 2.35197 0.092048 H 33

H -5.6670000 1.2900000 -0.8400000 1.007947 0.17469 2.35197 0.092048 H 34

H 7.1620000 0.9270000 -0.8080000 1.007947 0.14090 2.35197 0.092048 H 35

H 7.1490000 0.8310000 0.9670000 1.007947 0.14615 2.35197 0.092048 H 36

H 7.9970000 -0.4090000 0.0160000 1.007947 0.14420 2.35197 0.092048 H 37

H3 -8.8680000 0.1820000 -0.0130000 1.007947 0.26479 0.40001 0.192464 H3 38

# Bonds

# N1 N2 R-eqv Force Type

0 15 3 1.0930 1435.07

0 22 6 1.0930 1435.07

0 30 10 1.0930 1435.07

0 24 7 1.0930 1435.07

0 32 11 1.0930 1435.07

0 25 8 1.0930 1435.07

0 34 12 1.0930 1435.07

0 18 4 1.0930 1435.07

0 20 5 1.0930 1435.07

0 27 9 1.0930 1435.07

0 35 13 1.0930 1435.07

0 2 14 1.2220 3899.33

0 6 8 1.5080 1282.11

0 6 4 1.5080 1282.11

0 6 21 1.0930 1435.07

0 10 8 1.5080 1282.11

0 10 12 1.5080 1282.11

0 10 29 1.0930 1435.07

0 3 4 1.5080 1282.11

0 3 5 1.5080 1282.11

0 3 16 1.0930 1435.07

0 14 1 1.3550 1746.72

0 14 12 1.4920 1261.64

0 7 5 1.5080 1282.11

0 7 9 1.5080 1282.11

0 7 23 1.0930 1435.07

0 38 1 0.9810 2229.09

0 11 9 1.5080 1282.11

0 11 13 1.5080 1282.11

0 11 31 1.0930 1435.07

0 8 26 1.0930 1435.07

0 12 33 1.0930 1435.07

0 4 17 1.0930 1435.07

0 37 13 1.0930 1435.07

0 5 19 1.0930 1435.07

0 9 28 1.0930 1435.07

0 13 36 1.0930 1435.07

# Angles

# N1 N2 N3 A-eqv Force Type

14 1 38 111.95 351.09

4 3 5 109.61 512.48

4 3 15 110.55 383.00

4 3 16 110.55 383.00

5 3 15 110.55 383.00

5 3 16 110.55 383.00

15 3 16 108.84 310.74

3 4 6 109.61 512.48

3 4 17 110.55 383.00

3 4 18 110.55 383.00

6 4 17 110.55 383.00

6 4 18 110.55 383.00

17 4 18 108.84 310.74

3 5 7 109.61 512.48

3 5 19 110.55 383.00

3 5 20 110.55 383.00

7 5 19 110.55 383.00

7 5 20 110.55 383.00

19 5 20 108.84 310.74

4 6 8 109.61 512.48

4 6 21 110.55 383.00

4 6 22 110.55 383.00

8 6 21 110.55 383.00

8 6 22 110.55 383.00

21 6 22 108.84 310.74

5 7 9 109.61 512.48

5 7 23 110.55 383.00

5 7 24 110.55 383.00

9 7 23 110.55 383.00

9 7 24 110.55 383.00

23 7 24 108.84 310.74

6 8 10 109.61 512.48

6 8 25 110.55 383.00

6 8 26 110.55 383.00

10 8 25 110.55 383.00

10 8 26 110.55 383.00

25 8 26 108.84 310.74

7 9 11 109.61 512.48

7 9 27 110.55 383.00

7 9 28 110.55 383.00

11 9 27 110.55 383.00

11 9 28 110.55 383.00

27 9 28 108.84 310.74

8 10 12 109.61 512.48

8 10 29 110.55 383.00

8 10 30 110.55 383.00

12 10 29 110.55 383.00

12 10 30 110.55 383.00

29 10 30 108.84 310.74

9 11 13 109.61 512.48

9 11 31 110.55 383.00

9 11 32 110.55 383.00

13 11 31 110.55 383.00

13 11 32 110.55 383.00

31 11 32 108.84 310.74

10 12 14 107.52 467.91

10 12 33 110.55 383.00

10 12 34 110.55 383.00

14 12 33 108.39 391.44

14 12 34 108.39 391.44

33 12 34 108.84 310.74

11 13 35 110.55 383.00

11 13 36 110.55 383.00

11 13 37 110.55 383.00

35 13 36 108.84 310.74

35 13 37 108.84 310.74

36 13 37 108.84 310.74

1 14 2 124.43 695.55

1 14 12 109.72 628.10

2 14 12 124.41 564.87

# Dihedrals

# N1 N2 N3 N4 A-eqv Force n Type

1 14 12 10 0 -0.2469 1

1 14 12 10 180 -0.6987 2

1 14 12 10 0 0.4226 3

1 14 12 33 180 -1.3054 2

1 14 12 33 0 0.6904 3

1 14 12 34 180 -1.3054 2

1 14 12 34 0 0.6904 3

2 14 1 38 0 3.4769 1

2 14 1 38 180 12.8700 2

2 14 1 38 0 -0.1213 3

2 14 12 10 0 1.7238 1

2 14 12 10 180 0.2929 2

2 14 12 10 0 0.6820 3

2 14 12 33 0 1.3807 1

2 14 12 33 180 -2.9455 2

2 14 12 33 0 0.6443 3

2 14 12 34 0 1.3807 1

2 14 12 34 180 -2.9455 2

2 14 12 34 0 0.6443 3

3 4 6 8 0 0.2134 1

3 4 6 8 180 1.4267 2

3 4 6 8 0 0.6945 3

3 4 6 21 0 1.3389 1

3 4 6 21 180 -1.3180 2

3 4 6 21 0 0.5523 3

3 4 6 22 0 1.3389 1

3 4 6 22 180 -1.3180 2

3 4 6 22 0 0.5523 3

3 5 7 9 0 0.2134 1

3 5 7 9 180 1.4267 2

3 5 7 9 0 0.6945 3

3 5 7 23 0 1.3389 1

3 5 7 23 180 -1.3180 2

3 5 7 23 0 0.5523 3

3 5 7 24 0 1.3389 1

3 5 7 24 180 -1.3180 2

3 5 7 24 0 0.5523 3

4 3 5 7 0 0.2134 1

4 3 5 7 180 1.4267 2

4 3 5 7 0 0.6945 3

4 3 5 19 0 1.3389 1

4 3 5 19 180 -1.3180 2

4 3 5 19 0 0.5523 3

4 3 5 20 0 1.3389 1

4 3 5 20 180 -1.3180 2

4 3 5 20 0 0.5523 3

4 6 8 10 0 0.2134 1

4 6 8 10 180 1.4267 2

4 6 8 10 0 0.6945 3

4 6 8 25 0 1.3389 1

4 6 8 25 180 -1.3180 2

4 6 8 25 0 0.5523 3

4 6 8 26 0 1.3389 1

4 6 8 26 180 -1.3180 2

4 6 8 26 0 0.5523 3

5 3 4 6 0 0.2134 1

5 3 4 6 180 1.4267 2

5 3 4 6 0 0.6945 3

5 3 4 17 0 1.3389 1

5 3 4 17 180 -1.3180 2

5 3 4 17 0 0.5523 3

5 3 4 18 0 1.3389 1

5 3 4 18 180 -1.3180 2

5 3 4 18 0 0.5523 3

5 7 9 11 0 0.2134 1

5 7 9 11 180 1.4267 2

5 7 9 11 0 0.6945 3

5 7 9 27 0 1.3389 1

5 7 9 27 180 -1.3180 2

5 7 9 27 0 0.5523 3

5 7 9 28 0 1.3389 1

5 7 9 28 180 -1.3180 2

5 7 9 28 0 0.5523 3

6 4 3 15 0 1.3389 1

6 4 3 15 180 -1.3180 2

6 4 3 15 0 0.5523 3

6 4 3 16 0 1.3389 1

6 4 3 16 180 -1.3180 2

6 4 3 16 0 0.5523 3

6 8 10 12 0 0.2134 1

6 8 10 12 180 1.4267 2

6 8 10 12 0 0.6945 3

6 8 10 29 0 1.3389 1

6 8 10 29 180 -1.3180 2

6 8 10 29 0 0.5523 3

6 8 10 30 0 1.3389 1

6 8 10 30 180 -1.3180 2

6 8 10 30 0 0.5523 3

7 5 3 15 0 1.3389 1

7 5 3 15 180 -1.3180 2

7 5 3 15 0 0.5523 3

7 5 3 16 0 1.3389 1

7 5 3 16 180 -1.3180 2

7 5 3 16 0 0.5523 3

7 9 11 13 0 0.2134 1

7 9 11 13 180 1.4267 2

7 9 11 13 0 0.6945 3

7 9 11 31 0 1.3389 1

7 9 11 31 180 -1.3180 2

7 9 11 31 0 0.5523 3

7 9 11 32 0 1.3389 1

7 9 11 32 180 -1.3180 2

7 9 11 32 0 0.5523 3

8 6 4 17 0 1.3389 1

8 6 4 17 180 -1.3180 2

8 6 4 17 0 0.5523 3

8 6 4 18 0 1.3389 1

8 6 4 18 180 -1.3180 2

8 6 4 18 0 0.5523 3

8 10 12 14 0 0.1381 1

8 10 12 14 180 -0.3264 2

8 10 12 14 0 0.2971 3

8 10 12 33 0 1.3389 1

8 10 12 33 180 -1.3180 2

8 10 12 33 0 0.5523 3

8 10 12 34 0 1.3389 1

8 10 12 34 180 -1.3180 2

8 10 12 34 0 0.5523 3

9 7 5 19 0 1.3389 1

9 7 5 19 180 -1.3180 2

9 7 5 19 0 0.5523 3

9 7 5 20 0 1.3389 1

9 7 5 20 180 -1.3180 2

9 7 5 20 0 0.5523 3

9 11 13 35 0 1.3389 1

9 11 13 35 180 -1.3180 2

9 11 13 35 0 0.5523 3

9 11 13 36 0 1.3389 1

9 11 13 36 180 -1.3180 2

9 11 13 36 0 0.5523 3

9 11 13 37 0 1.3389 1

9 11 13 37 180 -1.3180 2

9 11 13 37 0 0.5523 3

10 8 6 21 0 1.3389 1

10 8 6 21 180 -1.3180 2

10 8 6 21 0 0.5523 3

10 8 6 22 0 1.3389 1

10 8 6 22 180 -1.3180 2

10 8 6 22 0 0.5523 3

11 9 7 23 0 1.3389 1

11 9 7 23 180 -1.3180 2

11 9 7 23 0 0.5523 3

11 9 7 24 0 1.3389 1

11 9 7 24 180 -1.3180 2

11 9 7 24 0 0.5523 3

12 10 8 25 0 1.3389 1

12 10 8 25 180 -1.3180 2

12 10 8 25 0 0.5523 3

12 10 8 26 0 1.3389 1

12 10 8 26 180 -1.3180 2

12 10 8 26 0 0.5523 3

12 14 1 38 0 -2.4393 1

12 14 1 38 180 10.6232 2

12 14 1 38 0 -1.1422 3

13 11 9 27 0 1.3389 1

13 11 9 27 180 -1.3180 2

13 11 9 27 0 0.5523 3

13 11 9 28 0 1.3389 1

13 11 9 28 180 -1.3180 2

13 11 9 28 0 0.5523 3

14 12 10 29 0 -0.5356 1

14 12 10 29 180 0.1213 2

14 12 10 30 0 -0.5356 1

14 12 10 30 180 0.1213 2

15 3 4 17 0 0.5941 1

15 3 4 17 180 -2.8995 2

15 3 4 17 0 0.6569 3

15 3 4 18 0 0.5941 1

15 3 4 18 180 -2.8995 2

15 3 4 18 0 0.6569 3

15 3 5 19 0 0.5941 1

15 3 5 19 180 -2.8995 2

15 3 5 19 0 0.6569 3

15 3 5 20 0 0.5941 1

15 3 5 20 180 -2.8995 2

15 3 5 20 0 0.6569 3

16 3 4 17 0 0.5941 1

16 3 4 17 180 -2.8995 2

16 3 4 17 0 0.6569 3

16 3 4 18 0 0.5941 1

16 3 4 18 180 -2.8995 2

16 3 4 18 0 0.6569 3

16 3 5 19 0 0.5941 1

16 3 5 19 180 -2.8995 2

16 3 5 19 0 0.6569 3

16 3 5 20 0 0.5941 1

16 3 5 20 180 -2.8995 2

16 3 5 20 0 0.6569 3

17 4 6 21 0 0.5941 1

17 4 6 21 180 -2.8995 2

17 4 6 21 0 0.6569 3

17 4 6 22 0 0.5941 1

17 4 6 22 180 -2.8995 2

17 4 6 22 0 0.6569 3

18 4 6 21 0 0.5941 1

18 4 6 21 180 -2.8995 2

18 4 6 21 0 0.6569 3

18 4 6 22 0 0.5941 1

18 4 6 22 180 -2.8995 2

18 4 6 22 0 0.6569 3

19 5 7 23 0 0.5941 1

19 5 7 23 180 -2.8995 2

19 5 7 23 0 0.6569 3

19 5 7 24 0 0.5941 1

19 5 7 24 180 -2.8995 2

19 5 7 24 0 0.6569 3

20 5 7 23 0 0.5941 1

20 5 7 23 180 -2.8995 2

20 5 7 23 0 0.6569 3

20 5 7 24 0 0.5941 1

20 5 7 24 180 -2.8995 2

20 5 7 24 0 0.6569 3

21 6 8 25 0 0.5941 1

21 6 8 25 180 -2.8995 2

21 6 8 25 0 0.6569 3

21 6 8 26 0 0.5941 1

21 6 8 26 180 -2.8995 2

21 6 8 26 0 0.6569 3

22 6 8 25 0 0.5941 1

22 6 8 25 180 -2.8995 2

22 6 8 25 0 0.6569 3

22 6 8 26 0 0.5941 1

22 6 8 26 180 -2.8995 2

22 6 8 26 0 0.6569 3

23 7 9 27 0 0.5941 1

23 7 9 27 180 -2.8995 2

23 7 9 27 0 0.6569 3

23 7 9 28 0 0.5941 1

23 7 9 28 180 -2.8995 2

23 7 9 28 0 0.6569 3

24 7 9 27 0 0.5941 1

24 7 9 27 180 -2.8995 2

24 7 9 27 0 0.6569 3

24 7 9 28 0 0.5941 1

24 7 9 28 180 -2.8995 2

24 7 9 28 0 0.6569 3

25 8 10 29 0 0.5941 1

25 8 10 29 180 -2.8995 2

25 8 10 29 0 0.6569 3

25 8 10 30 0 0.5941 1

25 8 10 30 180 -2.8995 2

25 8 10 30 0 0.6569 3

26 8 10 29 0 0.5941 1

26 8 10 29 180 -2.8995 2

26 8 10 29 0 0.6569 3

26 8 10 30 0 0.5941 1

26 8 10 30 180 -2.8995 2

26 8 10 30 0 0.6569 3

27 9 11 31 0 0.5941 1

27 9 11 31 180 -2.8995 2

27 9 11 31 0 0.6569 3

27 9 11 32 0 0.5941 1

27 9 11 32 180 -2.8995 2

27 9 11 32 0 0.6569 3

28 9 11 31 0 0.5941 1

28 9 11 31 180 -2.8995 2

28 9 11 31 0 0.6569 3

28 9 11 32 0 0.5941 1

28 9 11 32 180 -2.8995 2

28 9 11 32 0 0.6569 3

29 10 12 33 0 0.5941 1

29 10 12 33 180 -2.8995 2

29 10 12 33 0 0.6569 3

29 10 12 34 0 0.5941 1

29 10 12 34 180 -2.8995 2

29 10 12 34 0 0.6569 3

30 10 12 33 0 0.5941 1

30 10 12 33 180 -2.8995 2

30 10 12 33 0 0.6569 3

30 10 12 34 0 0.5941 1

30 10 12 34 180 -2.8995 2

30 10 12 34 0 0.6569 3

31 11 13 35 0 0.5941 1

31 11 13 35 180 -2.8995 2

31 11 13 35 0 0.6569 3

31 11 13 36 0 0.5941 1

31 11 13 36 180 -2.8995 2

31 11 13 36 0 0.6569 3

31 11 13 37 0 0.5941 1

31 11 13 37 180 -2.8995 2

31 11 13 37 0 0.6569 3

32 11 13 35 0 0.5941 1

32 11 13 35 180 -2.8995 2

32 11 13 35 0 0.6569 3

32 11 13 36 0 0.5941 1

32 11 13 36 180 -2.8995 2

32 11 13 36 0 0.6569 3

32 11 13 37 0 0.5941 1

32 11 13 37 180 -2.8995 2

32 11 13 37 0 0.6569 3

improper

23

14 12 1 2 0 84.9101

12 10 14 34 0 0

12 34 14 33 0 0

10 8 12 30 0 0

10 30 12 29 0 0

8 6 10 25 0 0

8 25 10 26 0 0

6 4 8 22 0 0

6 22 8 21 0 0

4 3 6 18 0 0

4 18 6 17 0 0

3 5 4 15 0 0

3 15 4 16 0 0

5 7 3 20 0 0

5 20 3 19 0 0

7 9 5 24 0 0

7 24 5 23 0 0

9 11 7 27 0 0

9 27 7 28 0 0

11 13 9 32 0 0

11 32 9 31 0 0

13 35 11 37 0 0

13 35 11 36 0 0

**Table S3. Systems considered for molecular dynamics simulations of for the studied V-HDES. *N* stands for the number of molecules of each type, *Natoms* for the total number of atoms used in each system, and *L* for the initial dimensions of the cubic simulation boxes in the studied temperature range.**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound A aAa a | Compound B a | | *N*(A) ()(HBA) | *N*(B) ([HBD]) | *Natoms* | *p* / bar | *T* / K | *L* / Å | |
| MEN | C8 | | 250 | 250 | 14000 | 1 | 288, 298, 308, 318 |  | |
| C8 | C12 | | 300 | 100 | 14000 | 1 | 288, 298, 308, 318 |  | |
|  |  |  | |  |  |  |  | |  |

**Table S4. System used for Coarse Grained MD simulations of V-HNADES in aqueous solutions at different concentrations in contact with a DPPC lipid bilayer. *N*(*i*) stands for the number of molecules of each type per leaflet considered in the simulations. For water, the reported number indicates the number of water beads, each one corresponding to 4 water molecules, i.e. total number of water molecules parenthesized. For the number of DPPC molecules, values are reported for each leaflet.**

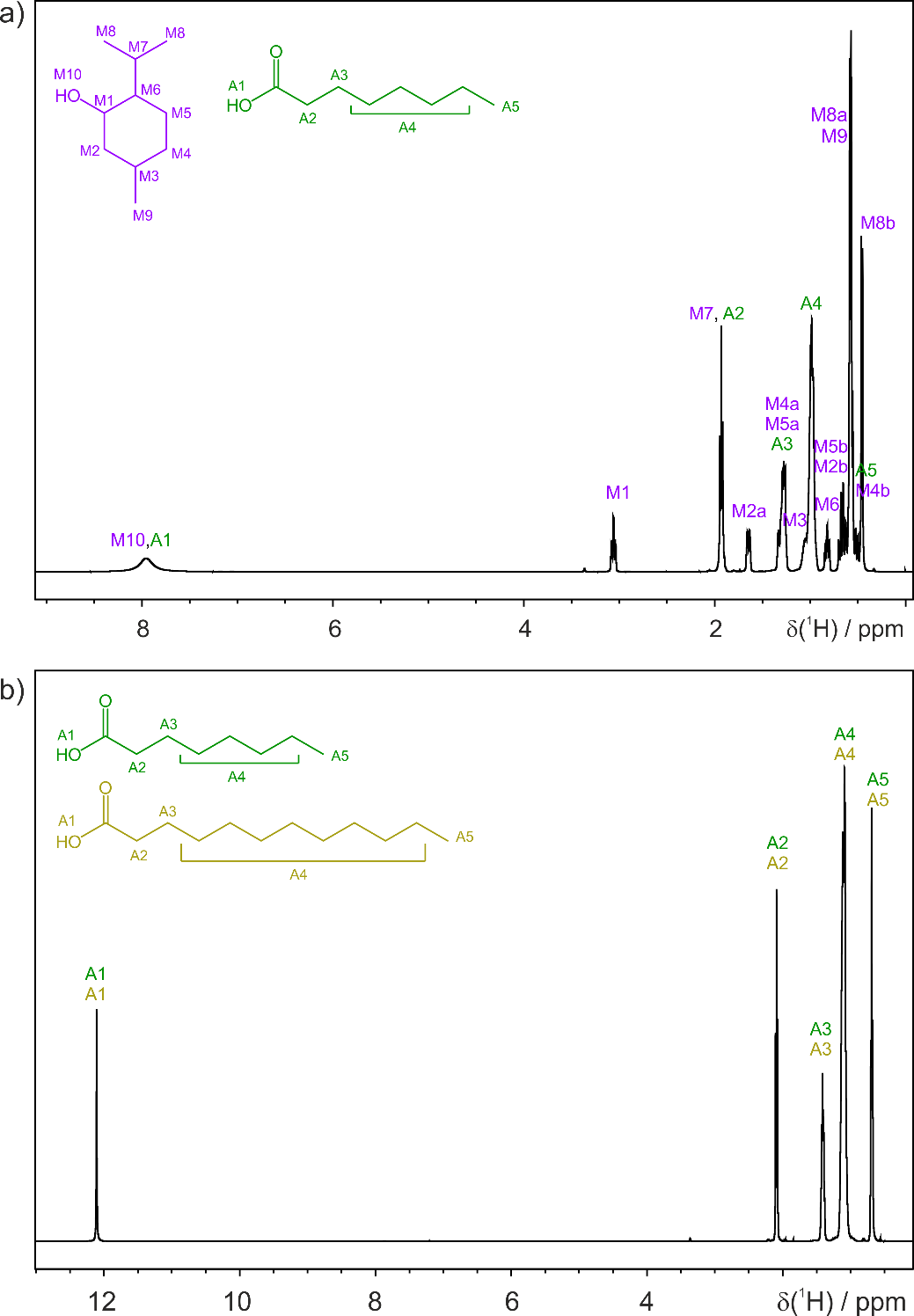
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| total V-HDES concentration / wt % | *N*(V-HDES) | *N*(V-HDES) | *N*(water) | *N*(DPPC) | water / lipid ratio |
| MEN : C8 (1 : 1) | | | | | |
| 20 | 127 (MEN) | 127 (C8) | 1640(6560) | 63 | 52 |
| C8 : C12 (3 : 1) | | | | | |
| 20 | 142 (C8) | 48 (C12) | 1640(6560) | 63 | 52 |



**Figure S1.** Beading of molecules considered in this work for CG-MD simulations of V-HDES interacting with DPPC lipid bilayers. For each type of bead, the assigned Martini3 type is reported.



**Figure S2.** Solvation numbers in the first shell as obtained from the integration of Radial Distribution Functions reported in Figures 9 and 10 for the first peak corresponding to the for the reported V-HDES from MD simulations as a function of temperature.

****

**Figure S3.** Experimental1H NMR spectra acquired at 298 K on the two samples (MEN : C8 1 : 1 and C8 : C12 3 : 1).



**Figure S4.** (center-of-mass) Self – diffusion coefficient, *D*, for the reported molecules in MEN : C8 (1 : 1) and C8 C12 (1 : 1) V-HDES as obtained from MD simulations.

**Table S5. Results of cluster – protein docking showing average binding energy (*Ebinding*), as obtained from the 9-largest binding poses for each protein, as well as the standard deviation between the binding energy for these 9-poses, σ(*Ebinding*).**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| PDB #ID | description | *Ebinding* / kJ mol-1 | σ(*Ebinding)* / kJ mol-1 | *Ebinding* / kJ mol-1 | σ(*Ebinding)* / kJ mol-1 | *Ebinding* / kJ mol-1 | σ(*Ebinding)* / kJ mol-1 |
| MEN : C8 (1 :1) | | C8 : C12 (1 : 1) | | C8 : C12 (1 : 3) | |
| **1fzv** | HORMONE | -26.70 | 1.06 | -29.93 | 1.02 | -39.93 | 1.20 |
| **6pxw** | HORMONE | -31.68 | 0.93 | -35.11 | 1.08 | -49.39 | 3.03 |
| **6gnq** | HORMONE | -35.28 | 2.23 | -38.81 | 2.26 | -42.67 | 1.66 |
| **2kax** | METAL BINDING | -27.57 | 1.23 | -27.93 | 1.02 | -34.84 | 1.96 |
| **4fl5** | SIGNALING | -27.51 | 0.87 | -30.15 | 0.75 | -43.38 | 1.01 |
| **2mgs** | SIGNALING | -27.87 | 1.30 | -26.77 | 0.85 | -35.44 | 1.65 |
| **4g5q** | SIGNALING | -25.00 | 1.19 | -28.04 | 2.13 | -40.04 | 3.02 |
| **1ro5** | SIGNALING | -28.96 | 2.13 | -29.47 | 1.03 | -35.98 | 0.78 |
| **4glr** | IMMUNE SYSTEM | -29.46 | 1.23 | -33.23 | 1.68 | -45.18 | 3.22 |
| **4tqe** | IMMUNE SYSTEM | -29.72 | 1.31 | -31.96 | 1.71 | -47.14 | 2.04 |
| **5d14** | IMMUNE SYSTEM | -24.60 | 0.73 | -24.89 | 0.69 | -33.29 | 1.56 |
| **3oxs** | IMMUNE SYSTEM | -33.32 | 2.28 | -35.69 | 2.34 | -41.69 | 2.41 |
| **4mhe** | IMMUNE SYSTEM | -29.31 | 1.64 | -29.79 | 1.39 | -37.28 | 2.23 |
| **1p0p** | HYDROLASE | -34.47 | 1.25 | -33.06 | 1.06 | -41.62 | 0.87 |
| **1owe** | HYDROLASE | -28.84 | 1.13 | -31.21 | 0.75 | -39.16 | 1.47 |
| **4gwc** | HYDROLASE | -30.30 | 1.83 | -32.87 | 0.76 | -40.02 | 2.00 |
| **4c6i** | HYDROLASE | -27.26 | 0.89 | -28.43 | 0.92 | -38.79 | 1.20 |
| **3lii** | HYDROLASE | -32.31 | 2.46 | -36.53 | 4.15 | -44.13 | 3.70 |
| **2c2m** | HYDROLASE | -27.93 | 1.11 | -28.59 | 0.57 | -39.01 | 0.95 |
| **2pm8** | HYDROLASE | -34.41 | 1.36 | -33.01 | 1.25 | -41.51 | 1.70 |
| **4zcg** | HYDROLASE | -28.66 | 0.82 | -30.87 | 1.38 | -40.05 | 1.31 |
| **2glq** | HYDROLASE | -29.71 | 1.95 | -33.19 | 1.04 | -45.20 | 2.05 |
| **1m6d** | HYDROLASE | -28.69 | 0.88 | -33.33 | 1.29 | -41.65 | 1.68 |
| **1yk8** | HYDROLASE | -26.72 | 0.52 | -28.14 | 0.80 | -39.25 | 1.51 |
| **1r6h** | HYDROLASE | -31.70 | 2.78 | -32.19 | 1.05 | -36.89 | 1.62 |
| **3kme** | HYDROLASE | -30.31 | 0.43 | -35.26 | 1.89 | -41.43 | 2.00 |
| **4gqq** | HYDROLASE | -35.03 | 2.79 | -32.96 | 1.19 | -42.26 | 1.38 |
| **1l6j** | HYDROLASE | -29.82 | 2.36 | -34.50 | 4.48 | -41.84 | 1.63 |
| **1gqs** | HYDROLASE | -31.89 | 1.63 | -33.52 | 1.89 | -42.02 | 1.56 |
| **2ac0** | APOPTOSIS/DNA | -27.62 | 0.83 | -31.10 | 1.51 | -42.14 | 1.83 |
| **1E31** | APOPTOSIS INHIBITOR | -28.44 | 1.82 | -33.01 | 2.04 | -36.42 | 2.16 |
| **4fm9** | ISOMERASE | -30.59 | 1.94 | -33.39 | 1.15 | -44.87 | 3.05 |
| **1ek5** | ISOMERASE | -31.46 | 2.41 | -29.83 | 2.85 | -37.29 | 1.85 |
| **4zvj** | ISOMERASE | -28.00 | 0.83 | -29.66 | 0.59 | -37.17 | 1.73 |
| **1svc** | TRANSCRIPTION/DNA | -26.34 | 1.20 | -29.03 | 0.64 | -39.40 | 1.54 |
| **1ubq** | CHROMOSOMAL | -22.40 | 0.77 | -23.37 | 0.54 | -29.79 | 0.83 |
| **1m8a** | CYTOKINE | -29.71 | 1.64 | -34.37 | 2.90 | -34.44 | 2.74 |
| **1l1b** | CYTOKINE | -26.15 | 0.62 | -32.99 | 1.18 | -36.68 | 1.52 |
| **5m2m** | CYTOKINE | -25.47 | 0.38 | -28.46 | 0.98 | -39.29 | 0.80 |
| **1il8** | CYTOKINE | -27.59 | 0.58 | -27.58 | 1.23 | -35.55 | 1.60 |
| **1msg** | CYTOKINE | -27.73 | 1.22 | -29.12 | 1.35 | -37.99 | 2.97 |
| **4oeo** | CELL ADHESION | -29.71 | 1.72 | -31.81 | 1.01 | -42.10 | 1.20 |
| **1p53** | CELL ADHESION | -29.91 | 1.17 | -33.10 | 0.60 | -59.39 | 4.72 |
| **1r9o** | OXIDOREDUCTASE | -33.66 | 3.33 | -37.15 | 2.08 | -39.69 | 1.07 |
| **4gqs** | OXIDOREDUCTASE | -33.34 | 2.65 | -32.90 | 1.11 | -41.98 | 1.37 |
| **4xrz** | OXIDOREDUCTASE | -33.84 | 1.28 | -38.80 | 1.76 | -44.38 | 0.54 |
| **2hi4** | OXIDOREDUCTASE | -30.61 | 2.51 | -31.10 | 1.73 | -39.40 | 1.38 |
| **3gph** | OXIDOREDUCTASE | -30.91 | 0.90 | -32.06 | 0.76 | -43.10 | 1.84 |
| **3gzo** | OXIDOREDUCTASE | -32.74 | 0.83 | -35.36 | 0.64 | -44.02 | 1.64 |
| **1dgf** | OXIDOREDUCTASE | -33.34 | 1.87 | -42.57 | 1.01 | -46.24 | 1.84 |
| **1d7w** | OXIDOREDUCTASE | -34.41 | 3.00 | -37.51 | 1.38 | -47.51 | 3.14 |
| **3b96** | OXIDOREDUCTASE | -30.82 | 2.54 | -38.39 | 1.86 | -43.02 | 3.92 |
| **1u3u** | OXIDOREDUCTASE | -34.14 | 1.59 | -38.10 | 3.13 | -39.35 | 0.44 |
| **6dqg** | OXIDOREDUCTASE | -33.08 | 0.82 | -35.45 | 0.33 | -47.89 | 1.62 |
| **5l01** | OXIDOREDUCTASE | -35.12 | 1.79 | -32.62 | 1.57 | -39.61 | 1.75 |
| **4fr8** | OXIDOREDUCTASE | -34.36 | 2.63 | -35.51 | 1.18 | -51.45 | 2.01 |
| **2z5y** | OXIDOREDUCTASE | -29.08 | 0.88 | -32.72 | 1.04 | -44.14 | 2.50 |
| **1ba9** | OXIDOREDUCTASE | -25.13 | 1.30 | -26.06 | 1.15 | -35.11 | 1.12 |
| **5te8** | OXIDOREDUCTASE | -35.35 | 1.63 | -33.25 | 1.22 | -43.05 | 1.59 |
| **6agf** | MEMBRANE | -34.73 | 1.35 | -39.83 | 0.70 | -64.17 | 1.89 |
| **7e1z** | MEMBRANE | -31.13 | 0.74 | -33.47 | 1.53 | -43.54 | 1.32 |
| **6irg** | MEMBRANE | -34.86 | 1.92 | -39.94 | 5.43 | -50.92 | 1.85 |
| **2znt** | MEMBRANE | -29.08 | 1.69 | -29.63 | 1.15 | -36.33 | 1.15 |
| **1g5w** | LIPID BINDING | -23.36 | 0.73 | -26.12 | 0.67 | -33.05 | 1.34 |
| **5z62** | ELECTRON TRANSPORT | -35.36 | 1.40 | -39.91 | 1.34 | -53.68 | 1.38 |
| **2h35** | OXYGEN STORAGE | -34.10 | 0.34 | -35.82 | 1.11 | -46.63 | 1.56 |
| **2jk4** | TRANSPORT | -32.23 | 1.49 | -33.91 | 1.97 | -43.52 | 1.26 |
| **6pzt** | TRANSPORT | -34.58 | 1.62 | -37.76 | 0.73 | -45.49 | 1.97 |
| **5eqg** | TRANSPORT | -34.53 | 2.87 | -40.48 | 1.77 | -51.86 | 2.67 |
| **6c0v** | TRANSPORT | -32.80 | 1.69 | -35.53 | 2.06 | -41.84 | 1.53 |
| **4act** | TRANSPORT | -25.28 | 0.83 | -27.00 | 0.50 | -38.69 | 0.92 |
| **1ao6** | CARRIER | -35.69 | 3.36 | -35.17 | 1.07 | -40.88 | 1.68 |
| **3w8q** | TRANSFERASE | -30.34 | 0.97 | -32.46 | 1.52 | -41.53 | 0.89 |
| **2e9n** | TRANSFERASE | -30.86 | 1.18 | -30.84 | 1.15 | -38.98 | 1.31 |
| **2nzt** | TRANSFERASE | -30.08 | 2.37 | -31.37 | 1.37 | -44.57 | 1.66 |
| **4fsm** | TRANSFERASE | -29.41 | 1.84 | -31.95 | 1.19 | -39.25 | 1.83 |
| **3i5z** | TRANSFERASE | -29.04 | 0.94 | -32.39 | 1.55 | -43.53 | 2.45 |
| **4dm4** | TRANSFERASE | -31.20 | 1.59 | -30.95 | 1.41 | -39.02 | 1.50 |
| **2wzb** | TRANSFERASE | -29.80 | 1.85 | -31.17 | 1.06 | -41.17 | 1.60 |
| **4g1n** | TRANSFERASE | -29.56 | 0.89 | -30.98 | 2.06 | -41.48 | 3.39 |
| **5ikp** | TRANSFERASE | -31.77 | 0.86 | -34.07 | 1.23 | -43.82 | 1.62 |
| **1oth** | TRANSFERASE | -27.10 | 1.37 | -29.93 | 0.59 | -38.58 | 0.90 |
| **4ijq** | TRANSFERASE | -31.50 | 1.73 | -38.34 | 1.15 | -45.38 | 1.80 |
| **3ie3** | TRANSFERASE | -29.18 | 0.75 | -33.32 | 0.77 | -41.43 | 3.17 |
| **2avd** | TRANSFERASE | -30.93 | 1.28 | -31.48 | 0.48 | -39.81 | 1.04 |
| **4ic8** | TRANSFERASE | -31.12 | 1.00 | -33.08 | 1.34 | -44.22 | 1.51 |
| **4x90** | TRANSFERASE | -37.12 | 1.24 | -37.66 | 0.74 | -48.73 | 1.97 |
| **4ez3** | TRANSFERASE | -32.81 | 2.74 | -34.43 | 1.69 | -39.58 | 1.72 |
| **2xir** | TRANSFERASE | -31.95 | 2.43 | -38.81 | 2.96 | -39.01 | 2.00 |
| **2zb2** | TRANSFERASE | -31.41 | 0.50 | -35.89 | 0.95 | -45.57 | 2.25 |
| **2b3x** | LYASE | -31.08 | 1.95 | -32.35 | 0.88 | -41.81 | 1.36 |
| **5d6b** | LYASE | -28.40 | 1.60 | -31.34 | 1.85 | -38.51 | 1.64 |
| **4fpt** | LYASE | -28.23 | 0.81 | -30.94 | 1.02 | -38.74 | 2.03 |
| **5pah** | MONOOXYGENASE | -35.26 | 2.52 | -36.10 | 1.42 | -43.84 | 4.36 |
| **1gkg** | COMPLEMENT | -24.05 | 1.03 | -25.35 | 0.70 | -32.74 | 1.01 |
| **2hgs** | AMINE LIGASE | -29.08 | 1.28 | -31.62 | 1.77 | -38.23 | 1.04 |
| **1o9k** | APOPTOSIS | -32.30 | 0.95 | -34.76 | 1.08 | -45.51 | 1.95 |
| **2o2m** | APOPTOSIS | -28.97 | 2.06 | -28.66 | 1.23 | -34.00 | 1.59 |
| **2rmn** | ANTITUMOR | -29.33 | 2.74 | -28.96 | 0.83 | -38.10 | 1.49 |
| **6v5v** | STUCTURAL | -26.86 | 1.04 | -28.17 | 0.92 | -36.63 | 0.49 |

**Table S6. Self-diffusion coefficients (in m²∙s-1) measured by PFG-NMR for the type V HES studied here.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| T (K) | MEN : C8 1 1 | | | C8 : C12 3 : 1 | |
|  | exchangeable H | MEN | C8 | exchangeable H | C8, C12 |
| 288 | 4.50E-11 | 4.30E-11 | 4.48E-11 | 1.01E-10 | 9.82E-11 |
| 298 | 7.27E-11 | 6.96E-11 | 7.17E-11 | 1.41E-10 | 1.36E-10 |
| 308 | n.d. | 1.07E-10 | 1.09E-10 | 1.88E-10 | 1.815E-10 |
| 318 | 1.67E-10 | 1.69E-10 | 1.61E-10 | 2.47E-10 | 2.38E-10 |
| 328 | 2.37E-10 | 2.41E-10 | 2.25E-10 | 3.25E-10 | 3.15E-10 |

**Table S7. Best-fit parameters obtained from the linear fit of the Arrhenius plot of the diffusion data in the whole temperature range.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sample | Species |  |  |  |
| MEN : C8 1 : 1 | exchangeable H | -10.178 | 32.6 | 0.9997 |
|  | MEN | -9.646 | 34.0 | 0.9995 |
|  | C8 | -10.555 | 31.7 | 0.9994 |
| C8 : C12 3 : 1 | exchangeable H | -13.488 | 22.8 | 0.9998 |
|  | C8.C12 | -13.565 | 22.7 | 0.9997 |