

SUPPLEMENTAL MATERIAL

Relevant radial distribution functions (RDF) for each MD simulation are reported in the figures below.

1) *Water extraction*

a) TODGA 0.2 mol/L

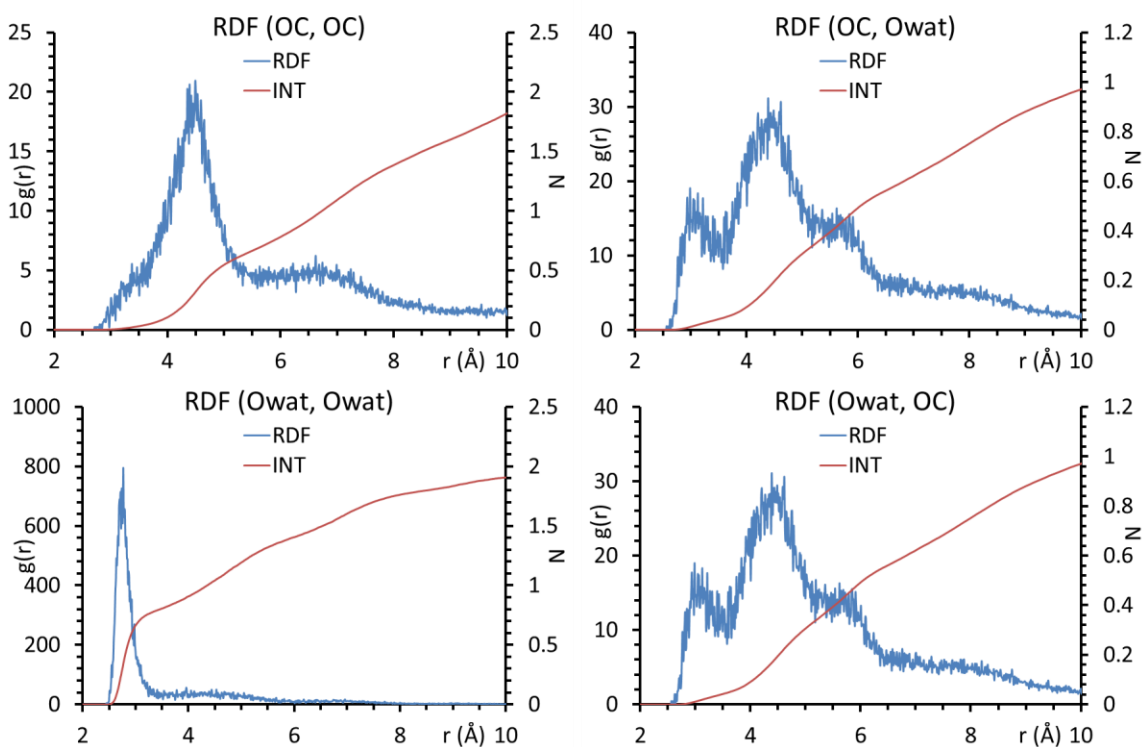


Figure S 1: RDF calculated from TODGA 0.2 mol/L simulation after extraction of water. OC: central oxygen atom of TODGA, Owat: oxygen atom of water. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

b) TODGA 0.2 mol/L + 5% octanol

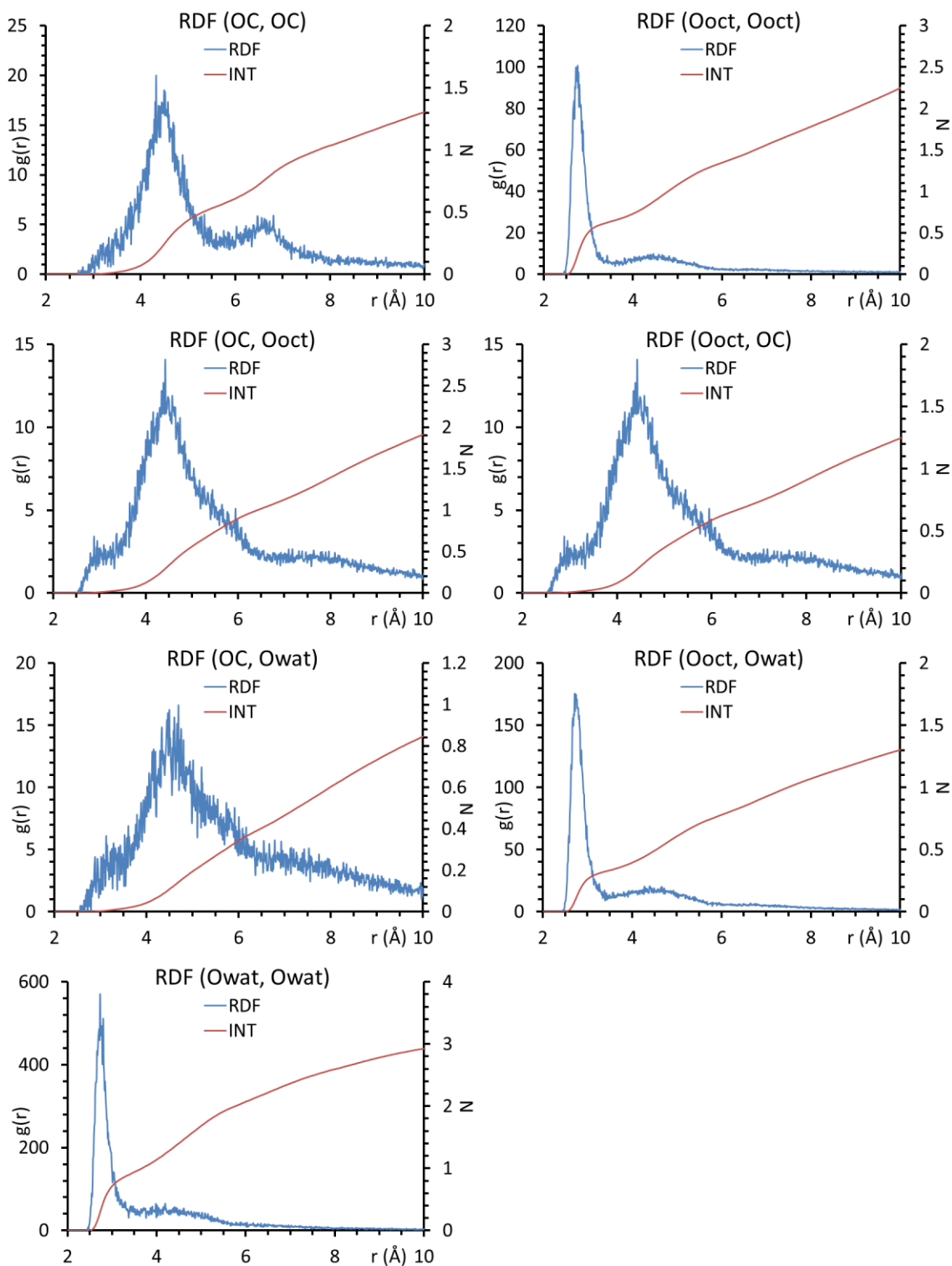


Figure S 2: RDF calculated from TODGA 0.2 mol/L + 5% octanol simulation after extraction of water. OC: central oxygen atom of TODGA, Owat: oxygen atom of water, Ooct: oxygen atom of

octanol. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

c) TODGA 0.2 mol/L + DMDOHEMA 0.5 mol/L

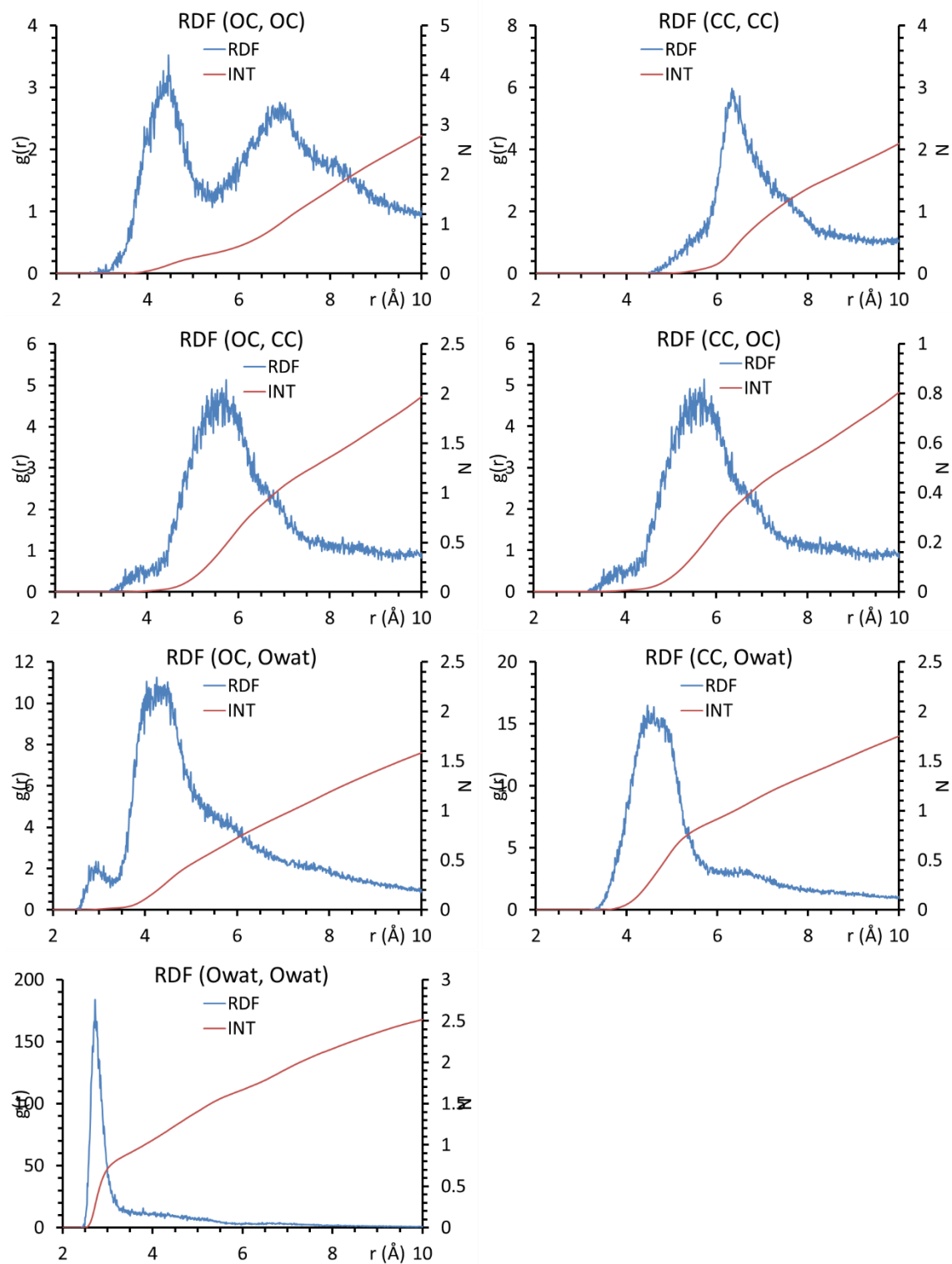


Figure S 3: RDF calculated from TODGA 0.2 mol/L + DMDOHEMA 0.5 mol/L simulation after extraction of water. OC: central oxygen atom of TODGA, CC central carbon atom of

DMDOHEMA, Owat: oxygen atom of water. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

2) Neodymium nitrate extraction

a) TODGA 0.2 mol/L + $\text{Nd}(\text{NO}_3)_3$ 0.02 mol/L

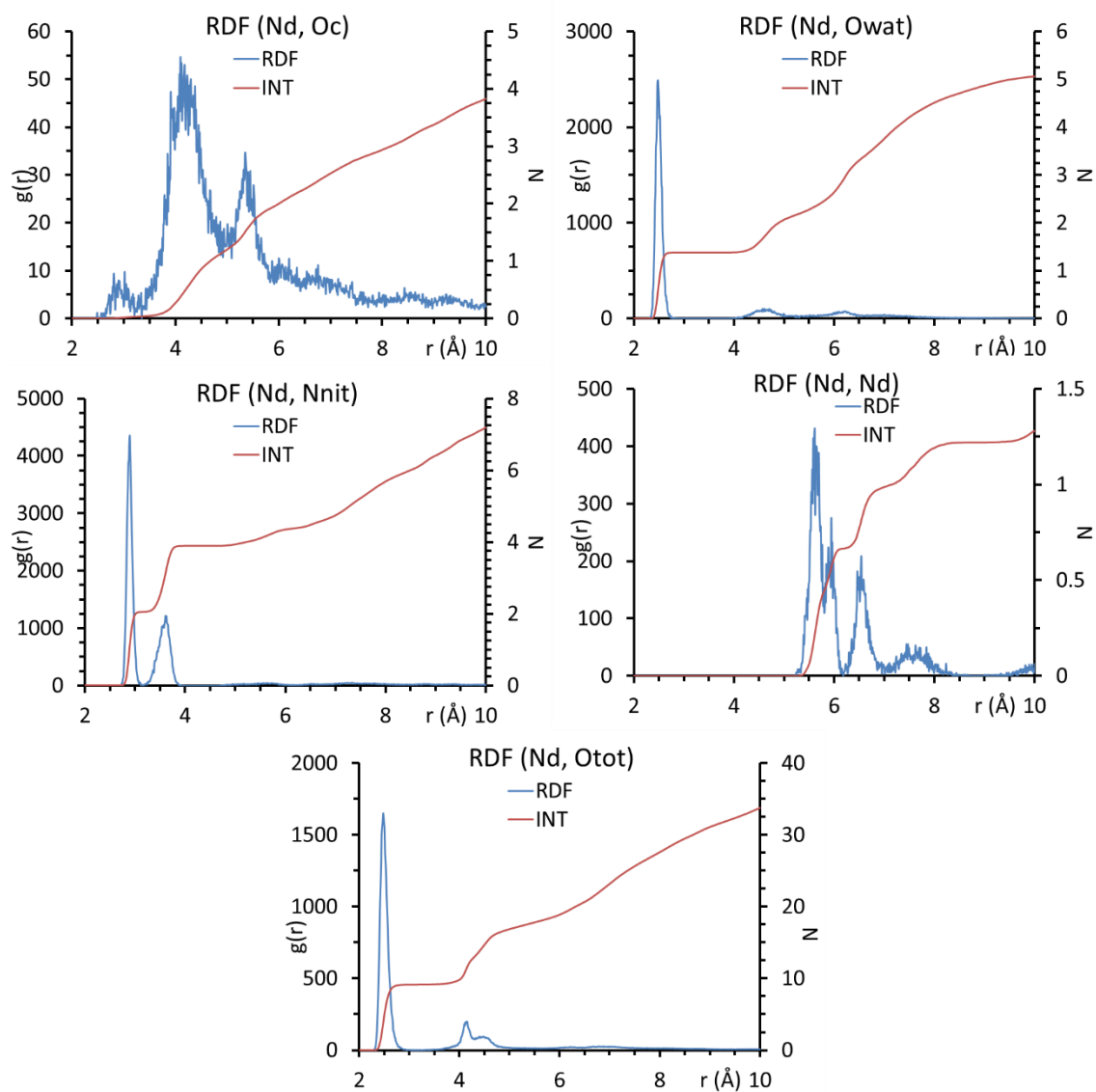


Figure S 4: RDF calculated from TODGA 0.2 mol/L + $\text{Nd}(\text{NO}_3)_3$ 0.02 mol/L simulation. Nd: neodymium atom, Oc: central oxygen atom of TODGA, Owat: oxygen atom of water, Otot: set of all oxygen atoms. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

b) TODGA 0.2 mol/L + Nd(NO₃)₃ 0.06 mol/L

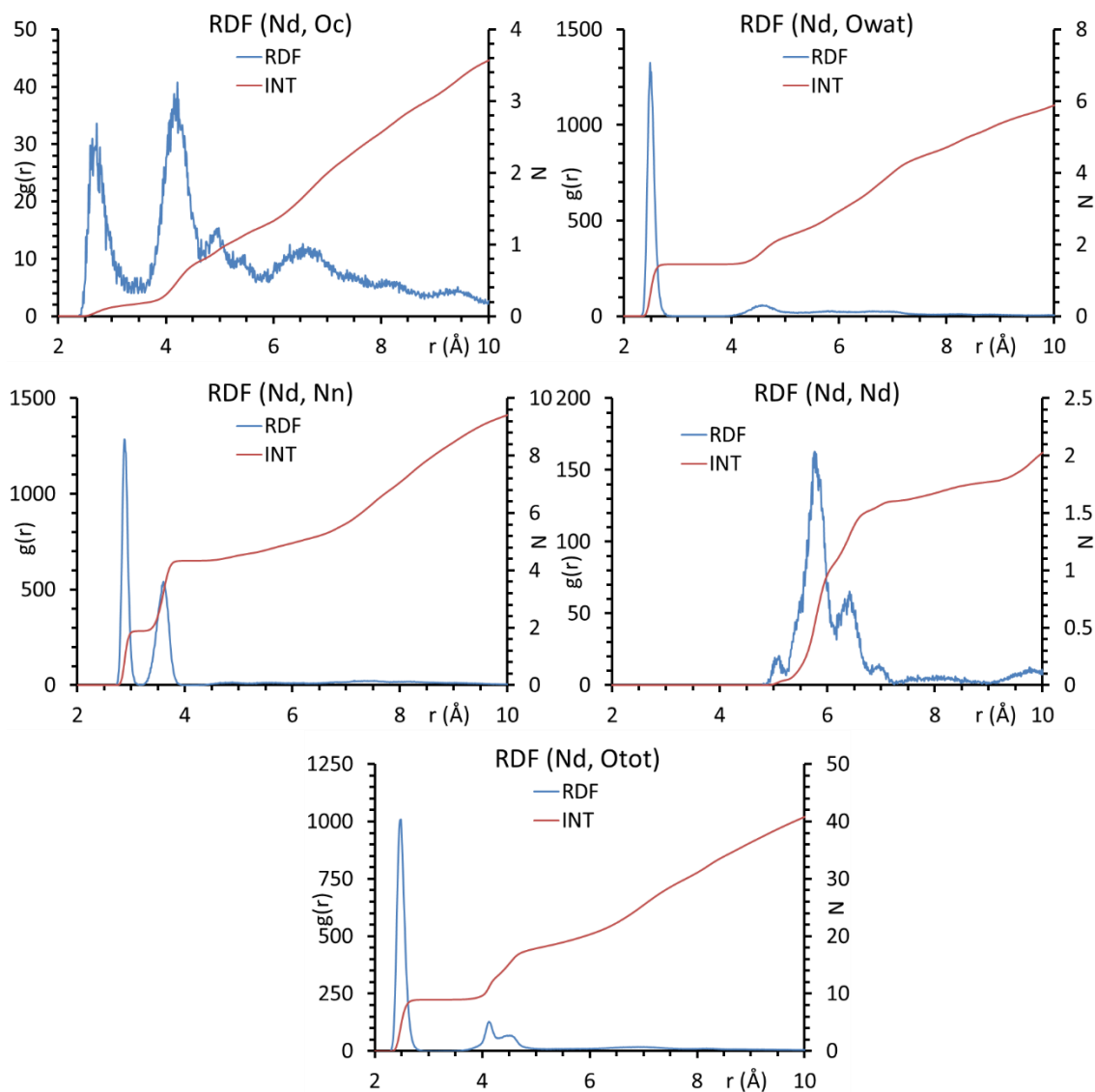


Figure S 5: RDF calculated from TODGA 0.2 mol/L + Nd(NO₃)₃ 0.06 mol/L simulation. Nd: neodymium atom, Oc: central oxygen atom of TODGA, Owat: oxygen atom of water, Otot: set of all oxygen atoms. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

c) TODGA 0.2 mol/L + 5% octanol + $\text{Nd}(\text{NO}_3)_3$ 0.06 mol/L

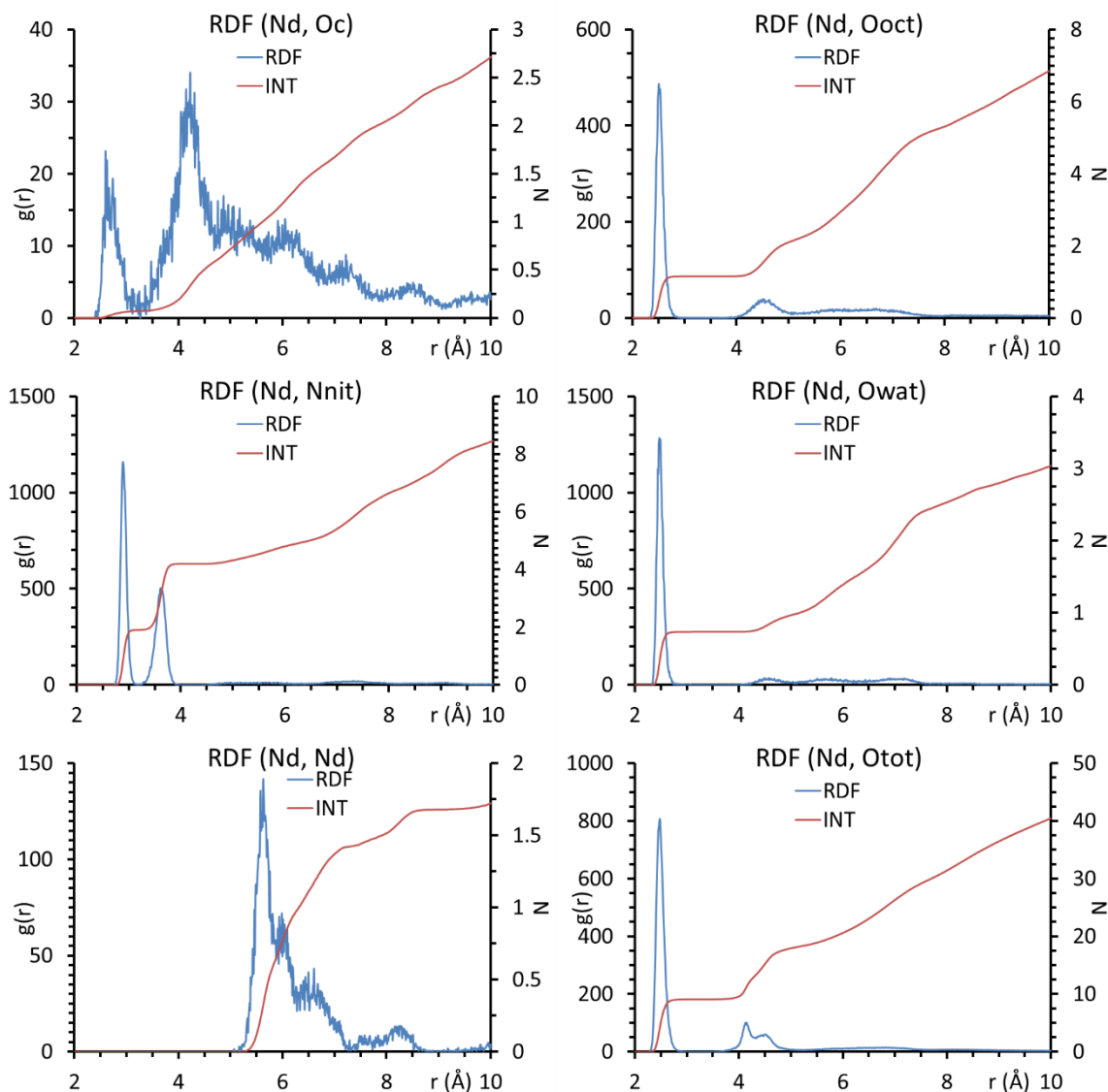


Figure S 6: RDF calculated from TODGA 0.2 mol/L + 5% octanol + $\text{Nd}(\text{NO}_3)_3$ 0.06 mol/L simulation. Nd: neodymium atom, Oc: central oxygen atom of TODGA, Ooct: oxygen atom of octanol, Owat: oxygen atom of water, Otot: set of all oxygen atoms. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

d) TODGA 0.2 mol/L + 5% octanol + $\text{Nd}(\text{NO}_3)_3$ 0.08 mol/L

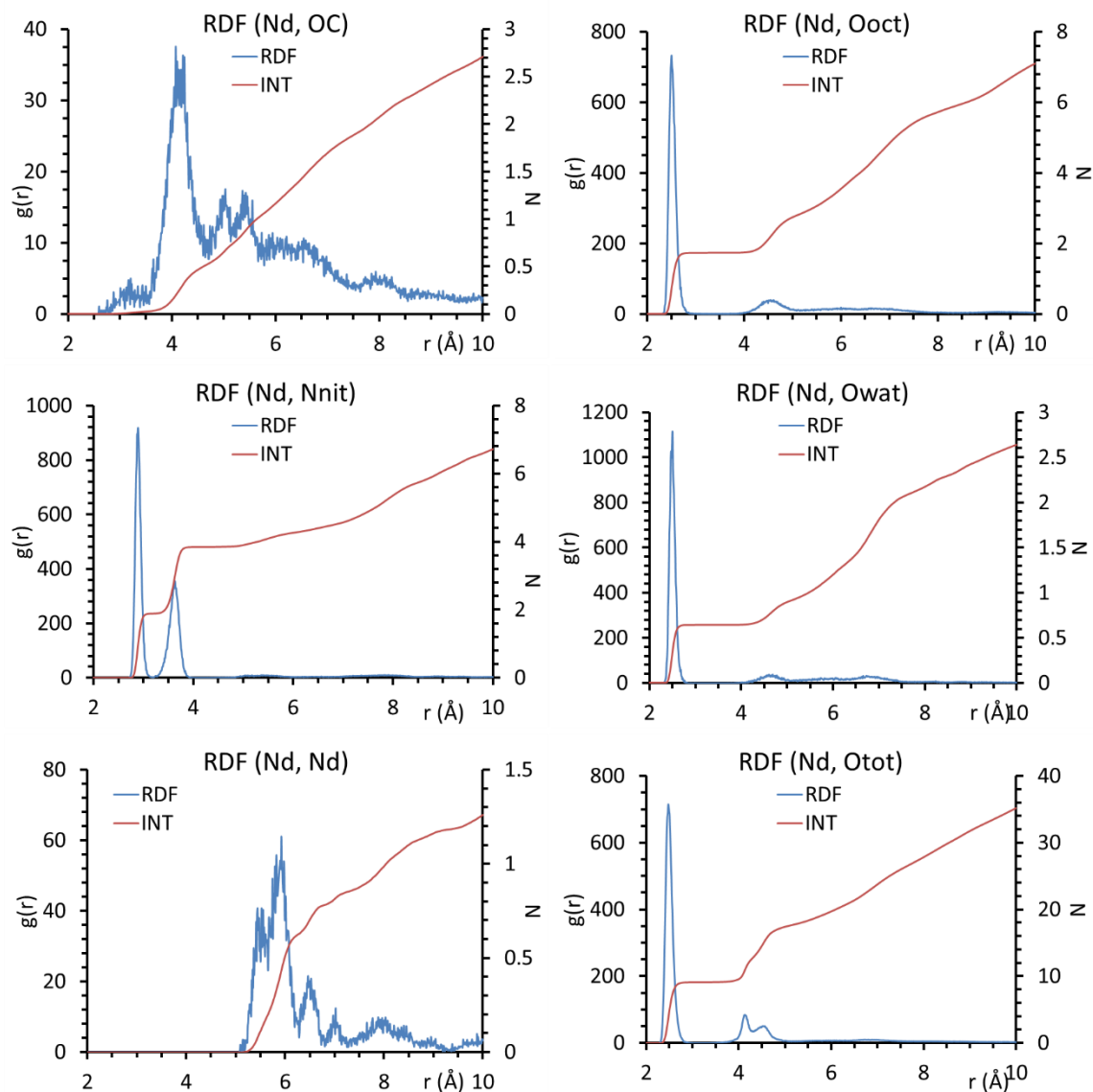


Figure S 7: RDF calculated from TODGA 0.2 mol/L + 5% octanol + $\text{Nd}(\text{NO}_3)_3$ 0.08 mol/L simulation. Nd: neodymium atom, OC: central oxygen atom of TODGA, Ooct: oxygen atom of octanol, Owat: oxygen atom of water, Otot: set of all oxygen atoms. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

e) TODGA 0.2 mol/L + DMDOHEMA 0.5 mol/L + Nd(NO₃)₃ 0.06 mol/L

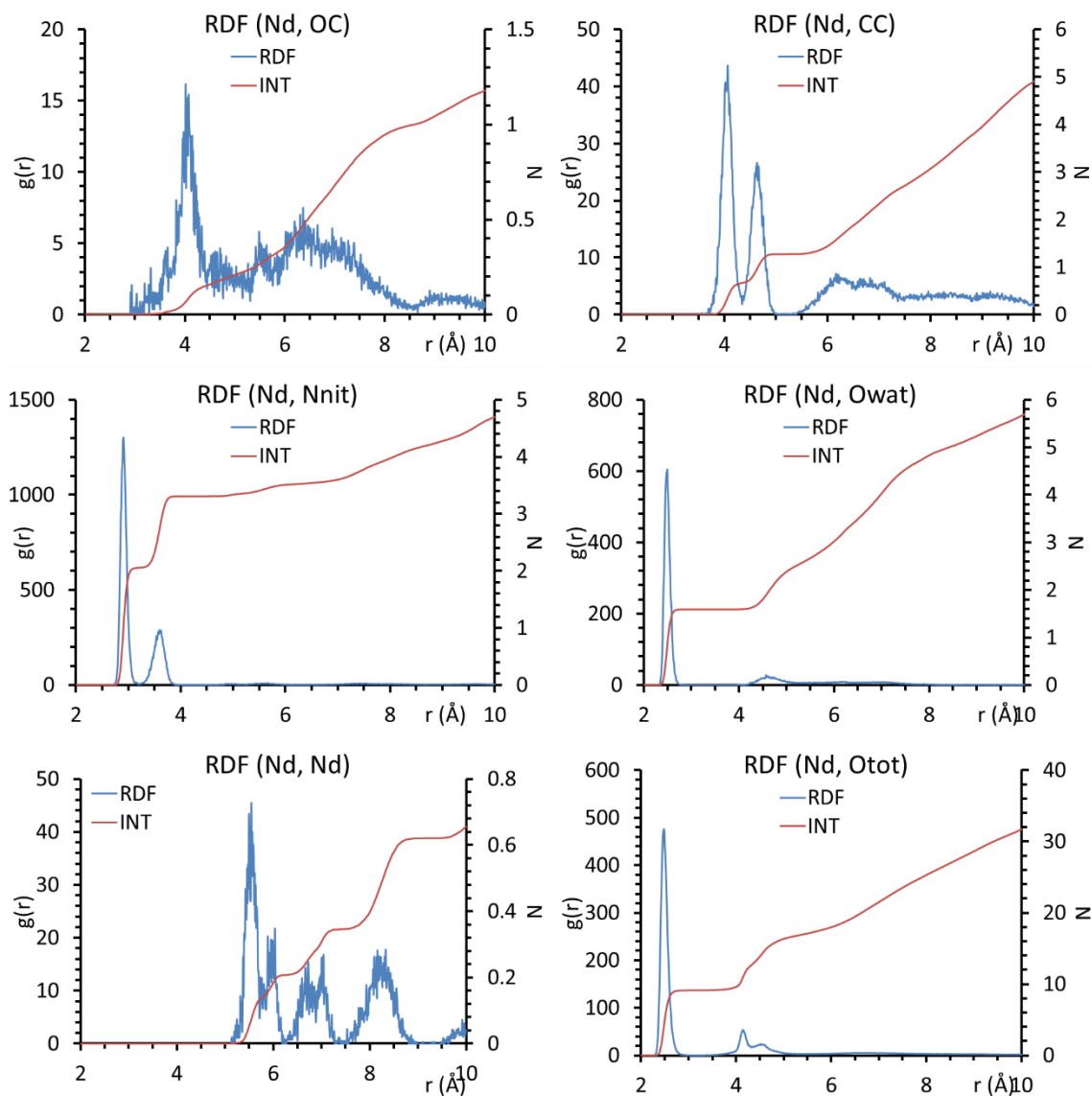


Figure S 8: RDF calculated from TODGA 0.2 mol/L + DMDOHEMA 0.5 mol/L + Nd(NO₃)₃ 0.06 mol/L simulation. Nd: neodymium atom, OC: central oxygen atom of TODGA, CC: central carbon atom of DMDOHEMA, Owat: oxygen atom of water, Otot: set of all oxygen atoms. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.

f) TODGA 0.2 mol/L + DMDOHEMA 0.5 mol/L + $\text{Nd}(\text{NO}_3)_3$ 0.09 mol/L

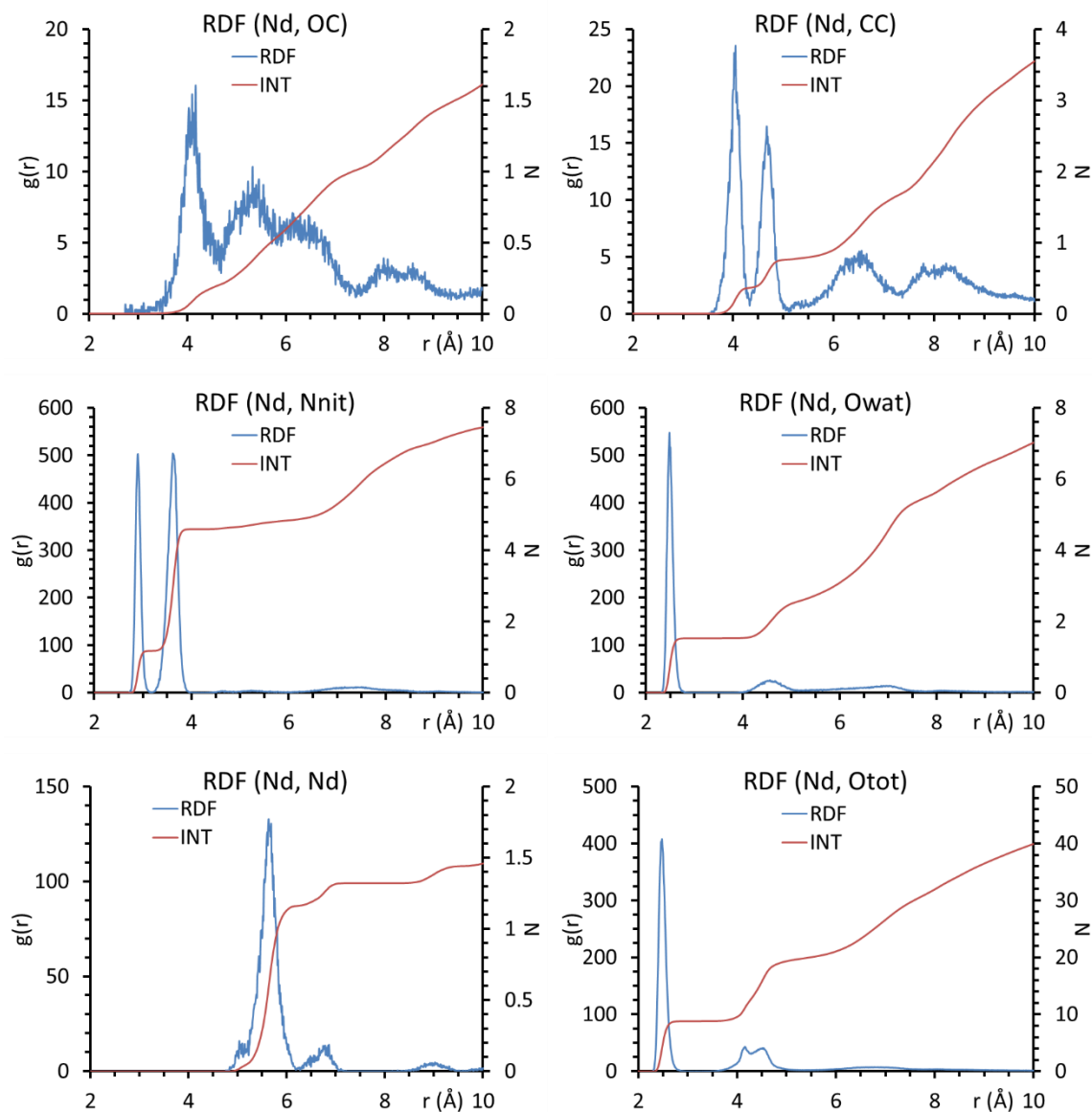


Figure S 9: RDF calculated from TODGA 0.2 mol/L + DMDOHEMA 0.5 mol/L + $\text{Nd}(\text{NO}_3)_3$ 0.09 mol/L simulation. Nd: neodymium atom, OC: central oxygen atom of TODGA, CC: central carbon atom of DMDOHEMA, Owat: oxygen atom of water, Otot: set of all oxygen atoms. RDF(XX, YY): radial distribution functions of YY centered on XX. The blue curve corresponds to the normalized $g(r)$, and the red curve to the integral of the RDF.