## Crystal Packing and Melting Temperatures of Small Oxalate Esters: The Role of C–H···O Hydrogen Bonding

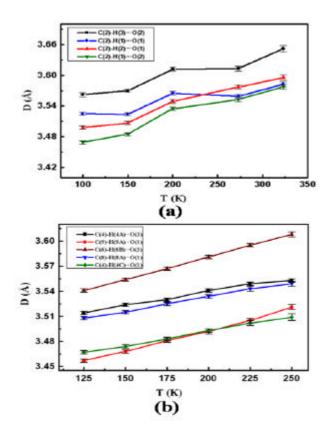
Sumy Joseph, Ranganathan Sathishkumar, Sudarshan Mahapatra and Gautam R. Desiraju\*

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India.

Fax: (+91) 80 23602306; Tel: (+91) 80 22933311; E-mail: desiraju@sscu.iisc.ernet.in

## **Supplementary Information**

**Figure S1** C···O distance (D) vs temperature for (a) DMO and (b) DtBO showing increased attractive interaction with decreasing temperature.



## **ORTEP diagrams**

Figure S2 ORTEP diagrams of dimethyl oxalate with ellipsoids drawn at 50% probability

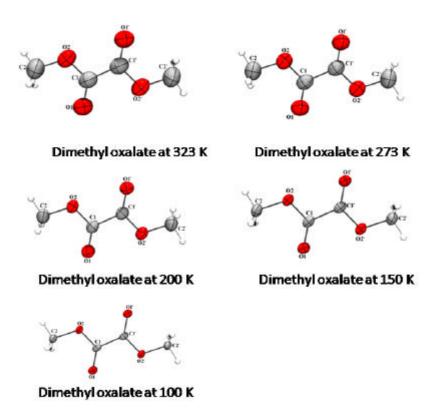
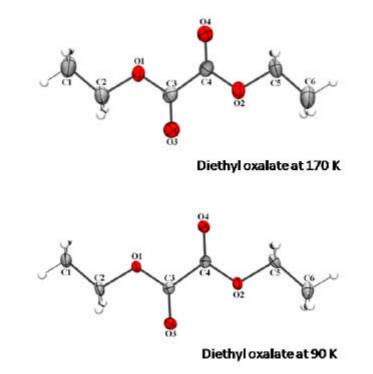
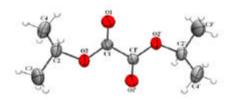


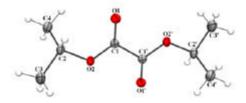
Figure S3 ORTEP diagrams of diethyl oxalate with ellipsoids drawn at 50% probability



**Figure S4** ORTEP diagrams of di-*iso*-propyl oxalate with ellipsoids drawn at 50% probability

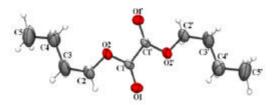


Di-iso-propyl oxalate at 210 K

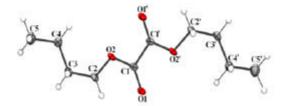


Di-iso-propyl oxalate at 90 K

**Figure S5** ORTEP diagrams of di-*n*-butyl oxalate with ellipsoids drawn at 50% probability



Di-n-butyl oxalate at 210 K



Di-n-butyl oxalate at 90 K.

Figure S6 ORTEP diagrams of di-tert-butyl oxalate with ellipsoids drawn at 50% probability

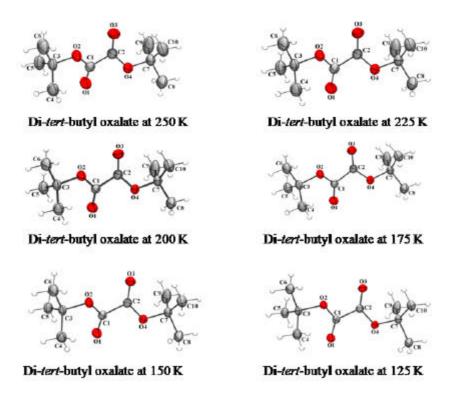
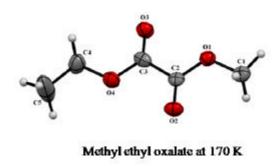
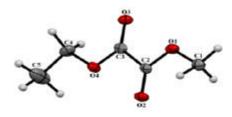


Figure S7 ORTEP diagrams of methyl ethyl oxalate with ellipsoids drawn at 50% probability





Methyl ethyl oxalate at 90 K