Supplementary Material (ESI) for Chemical Communications

Active peroxo titanium complexes: syntheses, characterization and their potential in the photooxidation of 2-propanol

Markus Rohe and Klaus Merz*

Anorganische Chemie I, Ruhr-Universität Bochum,

Universitätsstrasse 150, 44801 Bochum, Germany.

Fax: 49 234 32 14378;

Tel: 49 234 32 24187;

E-mail: Klaus.Merz@rub.de

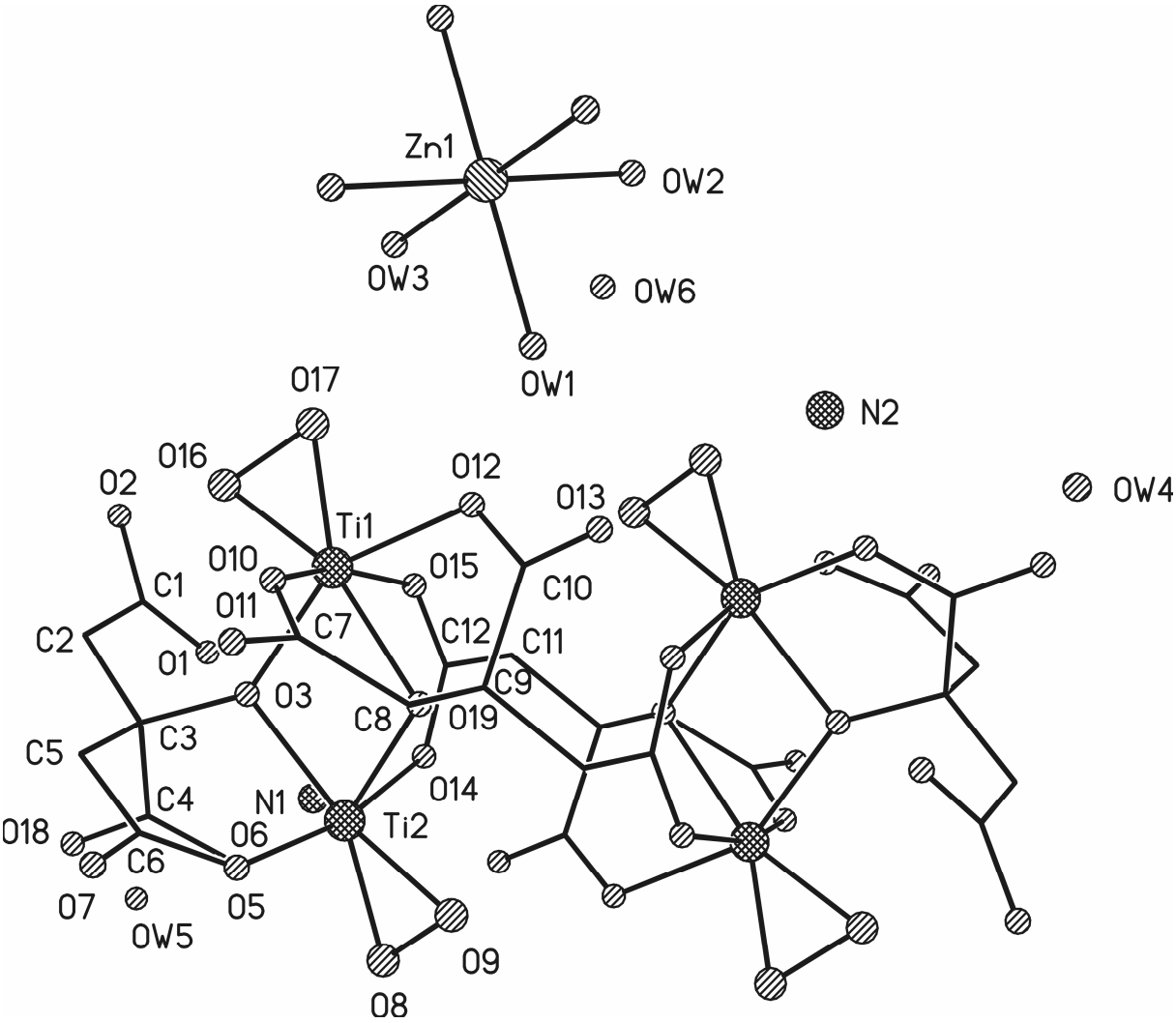

Fig. S1: Molecular structure of $Zn(NH_4)_4[Ti_4(O_2)_4(Hcit)_2(cit)_2]$ x ·12 $H_2O)_2$ **2**. Hydrogen are omitted for clarity. Selected distances [Å] and angles [°]:

Zn(1)-OW1 2.061(4), Zn(1)-OW1#1 2.061(4), Zn(1)-OW2#1 2.091(4), Zn(1)-OW2 2.091(4), Zn(1)-OW3#1 2.114(4), Zn(1)-OW3 2.114(4), Ti(1)-O(17) 1.841(4), Ti(1)-O(16) 1.871(4), Ti(1)-O(10) 1.997(4), Ti(1)-O(3) 2.020(4), Ti(1)-O(12) 2.057(4), Ti(1)-O(19) 2.076(4), Ti(1)-O(15) 2.087(4), Ti(2)-O(8) 1.873(4), Ti(2)-O(9) 1.891(4), Ti(2)-O(6) 1.986(4), Ti(2)-O(19) 2.014(4), Ti(2)-O(14) 2.020(4), Ti(2)-O(3) 2.030(4), Ti(2)-O(5) 2.091(4), O(8)-O(9) 1.475(5) O(16)-O(17) 1.453(5), OW1-Zn(1)-OW2 89.83(18), OW1-Zn(1)-OW1#1 180.0(3), OW2-Zn(1)-OW3 90.86(16), OW1-Zn(1)-OW3 92.17(19), O(17)-Ti(1)-O(16) 46.08(17), O(10)-Ti(1)-O(3) 91.79(16), O(10)-Ti(1)-O(12) 86.61(16), O(3)-Ti(1)-O(12) 149.70(16), O(10)-Ti(1)-O(19) 82.07(15), O(3)-Ti(1)-O(19) 73.59(14), O(12)-Ti(1)-O(19) 76.23(15), O(10)-Ti(1)-O(15) 165.52(16), O(3)-Ti(1)-O(15) 85.88(14), O(12)-Ti(1)-O(15) 88.21(15), O(19)-Ti(1)-O(15) 83.57(15), O(10)-Ti(1)-Ti(2) 93.10(12), O(3)-Ti(1)-Ti(2) 37.39(10), O(12)-Ti(1)-Ti(2) 112.43(12), O(19)-Ti(1)-Ti(2) 37.33(10), O(15)-Ti(1)-Ti(2) 76.42(11).
Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y+2,-z+1

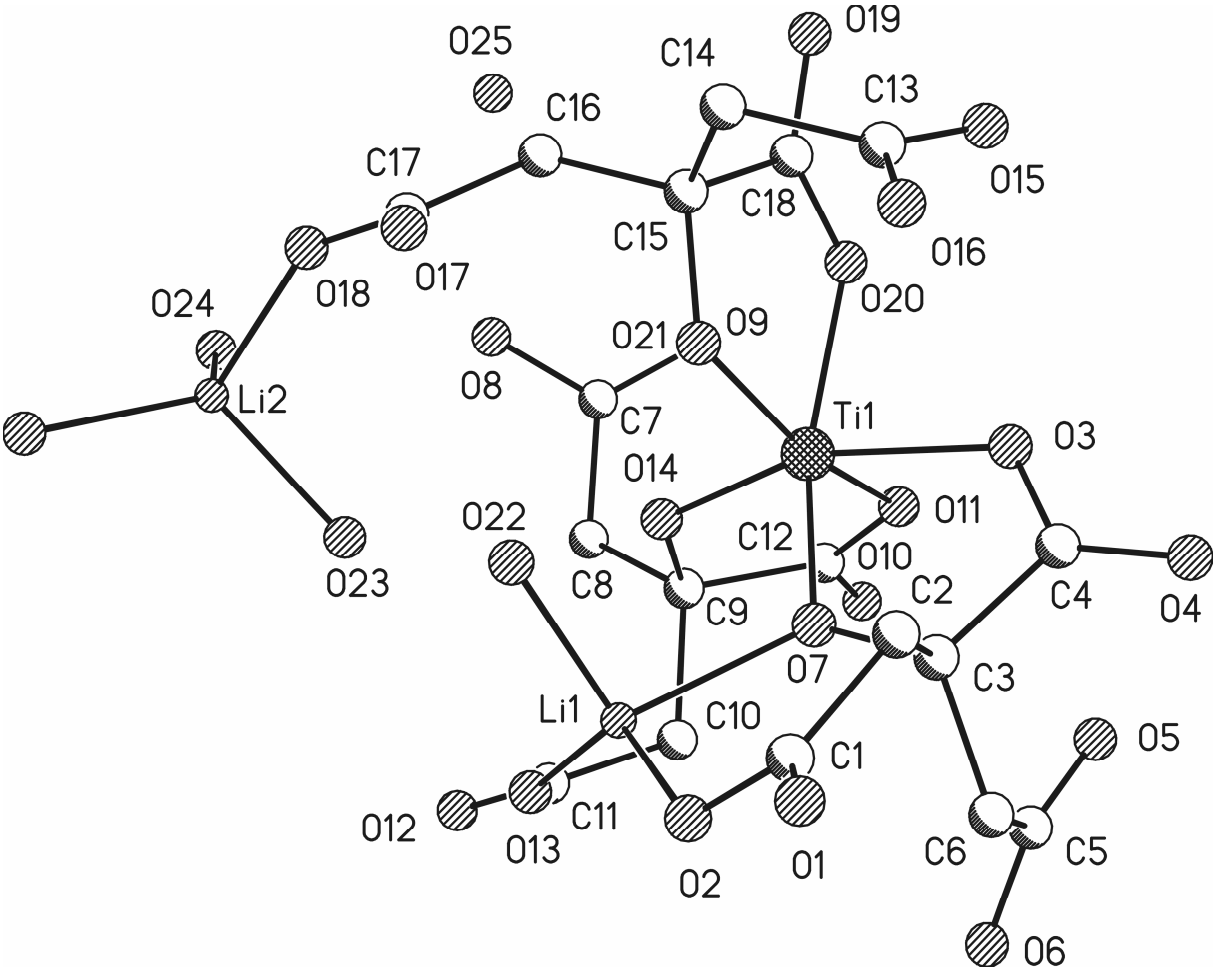

Fig. S2: Molecular structure of $Li_2Ti(H_2cit)_3 \cdot 4\ H_2O$ **3**. Hydrogen are omitted for clarity. Selected distances [Å] and angles [°]:
Ti(1)-O(14) 1.850(3), Ti(1)-O(21) 1.861(3), Ti(1)-O(7), 1.915(3), Ti(1)-O(3) 2.010(3), Ti(1)-O(20) 2.028(3), Ti(1)-O(11) 2.070(3), Ti(1)-Li(1) 3.356(7) O(7)-Li(1) 2.030(8), O(13)-Li(1) 1.930(7), O(2)-Li(1) 2.033(7), O(18)-Li(2) 1.923(8), O(9)-Li(2)#1 1.955(8), O(22)-Li(1) 1.869(8), O(23)-Li(2) 1.889(8), O(24)-Li(2) 1.949(8), Li(2)-O(9)#2 1.955(8),
O(14)-Ti(1)-O(21) 96.25(12), O(14)-Ti(1)-O(7) 91.88(11), O(21)-Ti(1)-O(7) 96.44(10), O(14)-Ti(1)-O(3) 157.37(11), O(21)-Ti(1)-O(3) 105.10(11), O(7)-Ti(1)-O(3) 78.54(11), O(14)-Ti(1)-O(20) 106.44(11), O(21)-Ti(1)-O(20) 78.89(11), O(7)-Ti(1)-O(20) 161.43(11), O(3)-Ti(1)-O(20) 85.30(11), O(14)-Ti(1)-O(11) 78.33(11), O(21)-Ti(1)-O(11) 157.93(10), O(7)-Ti(1)-O(11) 105.05(11), O(3)-Ti(1)-O(11) 84.38(11), O(20)-Ti(1)-O(11) 82.16(10).
Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z-1/2 #2 x,-y+1/2,z+1/2.

Fig. S3: Acetone formation during the photochemical oxidation of 2-propanol in presence of the zinc peroxo titanium aggregates **2.**

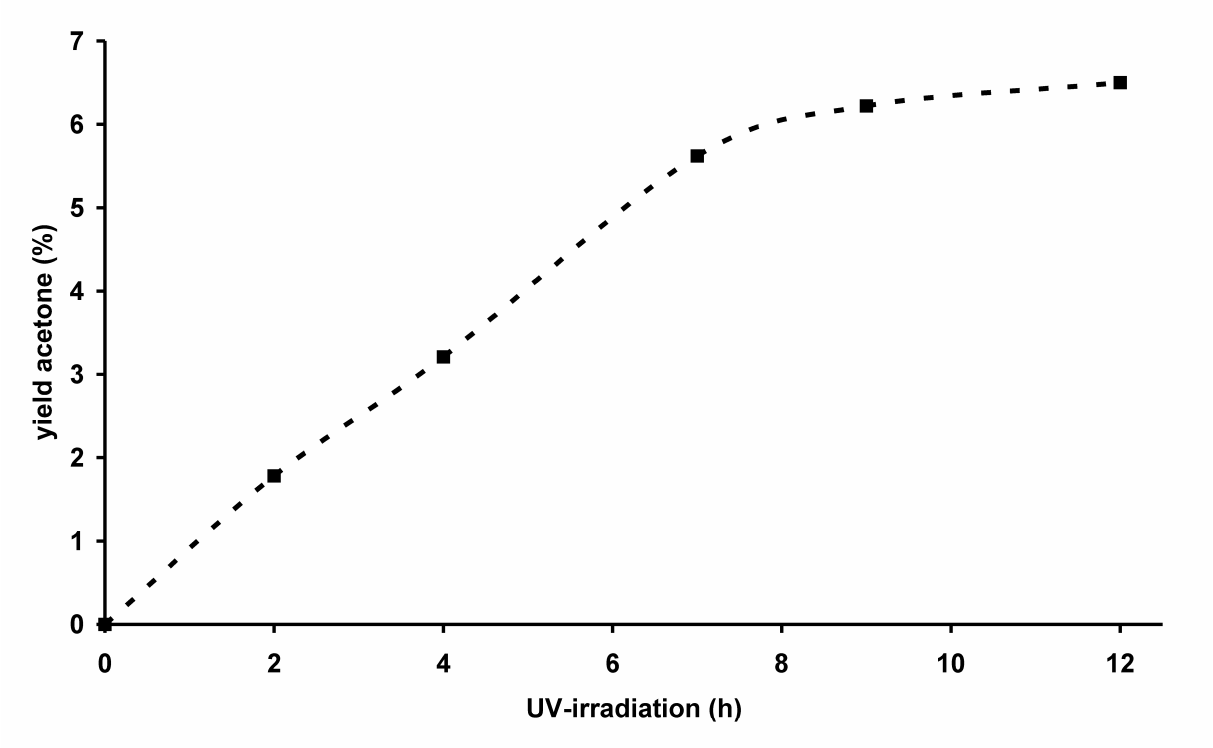

Fig. S4: Formation of CO_2 during the UV-irradiation of **1**