Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2013

Supporting Information for

Structural, spectroscopic and theoretical studies of diosmium(III,III) tetracarboxylates

Raquel Gracia and Nathan J. Patmore*

The University of Sheffield, Department of Chemistry, Sheffield, S3 7HF, UK

Email: n.patmore@sheffield.ac.uk

This journal is © The Royal Society of Chemistry 2013

Table S1. Calculated atomic coordinates for $Os_2(O_2CCH_3)_4Cl_2$ in vacuum.

Centre number	Atomic type	Atomic coordinates (Å)		
		x	y	z
1	C	-1.9262800	1.8212860	-0.0212370
2	O	-1.5330870	1.3376380	1.0788750
3	Os	-0.0010240	-0.0732050	1.1726650
4	Os	0.0010240	0.0732050	-1.1726650
5	O	1.5330870	-1.3376380	-1.0788750
6	O	1.4393950	-1.4835390	1.1554370
7	O	1.4985910	1.3726570	1.0823750
8	O	-1.4087100	-1.5156990	1.1522660
9	O	-1.4985910	-1.3726570	-1.0823750
10	O	1.4087100	1.5156990	-1.1522660
11	C	1.8908730	1.8579480	-0.0171690
12	C	-1.8908730	-1.8579480	0.0171690
13	C	1.9262800	-1.8212860	0.0212370
14	Cl	-0.0085510	0.5176660	3.4659390
15	O	-1.4393950	1.4835390	-1.1554370
16	Cl	0.0085510	-0.5176660	-3.4659390
17	C	-2.9919780	2.8681960	-0.0069480
18	H	-3.6429330	2.7299680	0.8578710
19	H	-2.5163670	3.8520750	0.0775140
20	H	-3.5620780	2.8416970	-0.9372360
21	C	-2.9896540	-2.8700200	0.0067340
22	H	-3.9498500	-2.3476700	0.0875720
23	H	-2.9799290	-3.4267480	-0.9316750
24	H	-2.8941220	-3.5400910	0.8630290
25	C	2.9896540	2.8700200	-0.0067340
26	H	3.9498500	2.3476700	-0.0875720
27	H	2.8941220	3.5400910	-0.8630290
28	H	2.9799290	3.4267480	0.9316750
29	C	2.9919780	-2.8681960	0.0069480
30	H	2.5163670	-3.8520750	-0.0775140
31	H	3.6429330	-2.7299680	-0.8578710
32	H	3.5620780	-2.8416970	0.9372360

This journal is © The Royal Society of Chemistry 2013

Table S2. Calculated atomic coordinates for $Os_2(O_2CCH_3)_4Cl_2$ in a CH_2Cl_2 solvent cavity using the polarizable continuum model.

Centre number	Atomic type	Atomic coordinates (Å)		
		x	x	z
1	C	-1.9227940	1.8316090	-0.0165540
2	O	-1.5125790	1.3542620	1.0841920
3	Os	-0.0004420	-0.0628190	1.1641370
4	Os	0.0004420	0.0628190	-1.1641370
5	O	1.5125790	-1.3542620	-1.0841920
6	O	1.4432420	-1.4651470	1.1473400
7	O	1.4749890	1.3926340	1.0866850
8	O	-1.4077490	-1.5013450	1.1451040
9	O	-1.4749890	-1.3926340	-1.0866850
10	O	1.4077490	1.5013450	-1.1451040
11	C	1.8833800	1.8717940	-0.0138510
12	C	-1.8833800	-1.8717940	0.0138510
13	C	1.9227940	-1.8316090	0.0165540
14	Cl	-0.0085490	0.4718740	3.5117350
15	O	-1.4432420	1.4651470	-1.1473400
16	Cl	0.0085490	-0.4718740	-3.5117350
17	C	-2.9783360	2.8817850	-0.0068210
18	H	-3.6215110	2.7629840	0.8662580
19	H	-2.4921480	3.8623660	0.0537520
20	H	-3.5608250	2.8430030	-0.9285680
21	C	-2.9756960	-2.8835760	0.0076720
22	H	-3.9358930	-2.3577930	0.0645780
23	H	-2.9530090	-3.4597620	-0.9183490
24	H	-2.8910620	-3.5380380	0.8765930
25	C	2.9756960	2.8835760	-0.0076720
26	H	3.9358930	2.3577930	-0.0645780
27	H	2.8910620	3.5380380	-0.8765930
28	H	2.9530090	3.4597620	0.9183490
29	C	2.9783360	-2.8817850	0.0068210
30	H	2.4921480	-3.8623660	-0.0537520
31	H	3.6215110	-2.7629840	-0.8662580
32	H	3.5608250	-2.8430030	0.9285680