Supplementary Material

for

"Experimental and predicted crystal structures of Pigment Red 168 and other dihalogenated anthanthrones"

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters (Å^2). U(eq) is defined as one third of the trace of the orthogonalised U_{ij} tensor.

Dichloro-anthanthrone (**1**)

Atom	x	y	z	U(eq)
C01	0.1611(13)	-0.4177(5)	-0.1222(5)	0.034(1)
C02	0.0342(14)	-0.4797(5)	-0.2518(5)	0.040(1)
C03	-0.1114(14)	-0.3947(5)	-0.3236(4)	0.036(1)
C04	-0.1422(12)	-0.2445(5)	-0.2644(4)	0.030(1)
C05	-0.0233(12)	-0.1824(4)	-0.1315(4)	0.027(1)
C06	-0.0598(11)	-0.0314(4)	-0.0684(4)	0.025(1)
C07	0.2934(13)	0.1530(5)	0.3335(4)	0.032(1)
C08	0.3311(13)	0.0092(5)	0.2740(4)	0.034(1)
C09	0.2136(12)	-0.0514(4)	0.1409(4)	0.028(1)
C10	0.2648(13)	-0.2075(5)	0.0785(4)	0.034(1)
C11	0.1315(12)	-0.2716(4)	-0.0601(4)	0.028(1)
O1	0.4278(10)	-0.2779(3)	0.1395(3)	0.047(1)
Cl1	0.4434(4)	0.2249(1)	0.4992(1)	0.047(1)
H01	0.270(13)	-0.470(5)	-0.076(4)	0.037(13)
H02	0.066(14)	-0.575(6)	-0.302(4)	0.049(14)
H03	-0.201(11)	-0.440(4)	-0.416(4)	0.024(11)
H08	0.427(14)	-0.055(6)	0.323(5)	0.054(15)

Dibromo-anthanthrone (**2**)

Atom	x	y	z	U(eq)
C01	0.2997(9)	-0.1936(2)	0.0111(4)	0.035(1)
C02	0.2213(10)	-0.2254(2)	0.1302(4)	0.041(1)
C03	0.0647(9)	-0.1887(2)	0.2269(4)	0.037(1)
C04	-0.0190(9)	-0.1185(2)	0.2087(3)	0.030(1)
C05	0.0539(8)	-0.0863(2)	0.0862(3)	0.028(1)
C06	-0.0361(7)	-0.0160(2)	0.0635(3)	0.027(1)
C07	0.1726(8)	0.0766(2)	-0.3070(3)	0.032(1)
C08	0.2574(9)	0.0098(2)	-0.2847(3)	0.034(1)
C09	0.1921(8)	-0.0212(2)	-0.1614(3)	0.029(1)
C10	0.3004(9)	-0.0934(2)	-0.1398(3)	0.032(1)
C11	0.2147(8)	-0.1256(2)	-0.0119(3)	0.030(1)
Br1	0.2671(1)	0.1147(1)	-0.4746(1)	0.044(1)
O1	0.4590(9)	-0.1252(1)	-0.2226(3)	0.047(1)
H01	0.429(11)	-0.220(2)	-0.055(4)	0.040(11)
H02	0.271(8)	-0.269(2)	0.159(3)	0.017(8)

H03	0.041(12)	-0.207(3)	0.308(5)	0.066(15)
H08	0.384(12)	-0.020(2)	-0.351(5)	0.054(13)

Table S1 (cont.)

Diiodo-anthanthrone (**3**)

Atom	x	y	z	U(eq)
C01	-0.6629(15)	-0.0254(3)	-0.3524(8)	0.043(2)
C02	-0.7531(16)	-0.0890(3)	-0.3743(8)	0.047(2)
C03	-0.6102(14)	-0.1339(3)	-0.2758(7)	0.043(2)
C04	-0.3734(13)	-0.1181(2)	-0.1537(7)	0.033(1)
C05	-0.2823(13)	-0.0522(3)	-0.1321(7)	0.033(1)
C06	-0.0459(13)	-0.0334(3)	-0.0101(7)	0.031(1)
C07	0.2127(14)	0.1636(3)	0.0507(7)	0.037(1)
C08	-0.0120(14)	0.1447(3)	-0.0650(7)	0.038(1)
C09	-0.0976(13)	0.0800(3)	-0.0872(6)	0.032(1)
C10	-0.3482(15)	0.0620(3)	-0.2160(7)	0.040(1)
C11	-0.4361(13)	-0.0067(2)	-0.2338(7)	0.036(1)
O1	-0.4752(12)	0.1020(2)	-0.3042(5)	0.061(2)
I1	0.3189(1)	0.2611(1)	0.0803(1)	0.049(1)
H01A	-0.7582	0.0052	-0.4195	0.051
H02A	-0.9084	-0.1009	-0.4547	0.057
H03A	-0.6725	-0.1763	-0.2904	0.051
H08A	-0.1121	0.1751	-0.1313	0.045

Table S2. Model potential parameters A, B, C_6, ρ_1, ρ_2 for all homoatomic atom-atom interactions (model 1 is shown for Br).

Atom types		$A^{\iota\kappa}$	$B^{\iota\kappa}$	$C_6^{\iota\kappa}$	ρ_1^{ι}	ρ_1^{κ}	ρ_2^{ι}	ρ_2^{κ}
ι	κ	kJ/mol	$Å^{-1}$	$Å^6$ kJ/mol	Å	Å	Å	Å
I	I	1261494	3.1422	16632.3	0	0	–0.1216	–0.1216
Br	Br	1160965	3.3000	16420.3	0	0	–0.1064	–0.1064
Cl	Cl	569746	3.3427	8366.9	+0.0156	+0.0156	–0.0939	–0.0939
C_X	C_X	28957	3.2131	2146.4	–0.2054	–0.2054	–0.3109	–0.3109
C	C	107333	3.1936	2146.4	–0.0026	–0.0026	+0.0419	+0.0419
O	O	205074	3.9600	833.5	0	0	0	0
H	H	2220	3.2575	200.0	–0.0449	–0.0449	+0.0036	+0.0036

C_X is a carbon bonded to a halogen, C is any other carbon atom. Atomic **z**-axes are defined along the bonds pointing out from the aromatic ring. Heteroatomic interaction parameters are determined from combining rules.

Table S3. Observed and lattice energy minimised unit cells of the crystal structures of anthanthrone, 4,10-dichloro-, 4,10-dibromo- and 4,10-diiodo-anthanthrone, using atom-atom model potentials.

	a (Å)	**b (Å)**	**c (Å)**	**α (deg.)**	**β (deg.)**	**γ (deg.)**	**RMS error (a,b,c)**	**ρ (g/cm^3)**
chloro								
expt	3.795	9.527	10.662	105.78	93.27	95.26		1.693
calculated	3.932	9.684	10.198	106.53	92.54	89.98		1.675
error	*+3.62%*	*+1.65%*	*-4.35%*	*+0.71%*	*-0.78%*	*-5.54%*	*3.40%*	*-1.04%*
bromo								
expt	3.865	19.424	10.113	90	92.56	90		2.032
calculated (model 1[a])	3.888	19.767	10.048	90	92.54	90		1.998
error	*+0.59%*	*+1.76%*	*-0.64%*	*0*	*-0.02%*	*0*	*1.13%*	*-1.68%*
calculated (model 2 [b])	4.016	19.477	10.304	90	93.85	90		1.917
error	*+3.90%*	*+0.27%*	*+1.89%*	*0*	*+1.40%*	*0*	*2.51%*	*-5.67%*
calculated (model 3 [c])	4.009	19.590	10.313	90	92.46	90		1.905
error	*+3.74%*	*+0.86%*	*+1.98%*	*0*	*-0.10%*	*0*	*2.49%*	*-6.28%*
iodo								
expt	4.202	20.956	9.276	90	100.63	90		2.309
calculated [d]	4.225	21.159	9.254	90	101.49	90		2.286
error	*+0.55%*	*+0.97%*	*-0.24%*	*0*	*+0.86%*	*0*	*0.66%*	*-0.97%*
unsubstituted								
expt	20.900	3.860	33.200	90	92.00	90		1.520
calculated	21.832	3.865	31.846	90	89.77	90		1.535
error	*+3.03%*	*+0.12*	*-4.08%*	*0*	*-2.42%*	*0*	*2.93%*	*+1.00%*

[a] model 1 is the model potential with Br and O parameters fitted specifically for this work.

[b] model 2 is the model potential with Br···Br and Br···X (X = C, H, O) parameters taken from Price's contribution to Motherwell et al., 2002.

[c] model 3 uses all parameters from this work, except Br···Br parameters from Price's contribution to Motherwell et al., 2002 and geometric combining rules for all Br···X interactions.

[d] The results are slightly different from those reported in reference Day et al., 2005, because an MP2 molecular structure and electrostatics were used, to be consistent with the other compounds and the SCDS-Pixel calculations.

Table S4. Observed and lattice energy minimised unit cells of the crystal structures of anthanthrone, 4,10-dichloro-, 4,10-dibromo- and 4,10-diiodo-anthanthrone, using the SCDS-Pixel energy model.

	a (Å)	**b (Å)**	**c (Å)**	**α (deg.)**	**β (deg.)**	**γ (deg.)**	**RMS error (a,b,c)**	**ρ (g/cm^3)**
chloro								
expt	3.795	9.527	10.662	105.78	93.27	95.26		1.693
calculated	3.937	9.660	10.236	106.44	91.73	90.58		1.673
error	*+3.74%*	*+1.40%*	*-4.00%*	*+0.62%*	*-1.65%*	*-4.91%*	*3.26%*	*-1.18%*
bromo								
expt	3.865	19.424	10.113	90	92.56	90		2.032
calculated	4.042	20.416	9.527	90	102.15	90		2.005
error	*+4.04%*	*+5.11%*	*-5.79%*	*0*	*10.36%*	*0*	*5.18%*	*-1.32%*
iodo								
expt	4.202	20.956	9.276	90	100.63	90		2.309
calculated	4.236	21.401	9.133	90	101.43	90		2.284
error	*+0.81%*	*+2.12%*	*-1.54%*	*0*	*+0.79%*	*0*	*1.59%*	*-1.08%*