Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for jeff.
U(eq) is defined as

$$U_{eq}=1/3\sum_i\sum_j U_{ij}a_i^*a_j^*a_i\bullet a_j$$

	x	y	z	U(eq)
O(1)	1826(3)	7962(2)	7042(1)	66(1)
O(2)	3964(2)	6466(2)	6941(1)	56(1)
O(3)	2306(2)	4604(2)	4888(1)	51(1)
O(4)	5487(3)	1876(2)	4914(1)	77(1)
O(5)	2523(2)	1942(2)	4581(1)	62(1)
C(1)	2254(3)	4996(2)	6192(1)	39(1)
C(2)	4219(3)	5408(2)	6437(1)	46(1)
C(3)	5377(3)	4345(3)	6749(1)	55(1)
C(4)	5327(3)	3252(2)	6179(1)	50(1)
C(5)	3470(3)	2938(2)	5727(1)	41(1)
C(6)	2561(3)	4206(2)	5513(1)	38(1)
C(7)	2066(3)	2140(2)	6174(1)	47(1)
C(8)	1855(4)	2851(2)	6902(1)	56(1)
C(9)	1284(3)	4242(2)	6786(1)	52(1)
C(10)	1407(3)	6314(2)	6096(1)	48(1)
C(11)	2326(3)	7036(2)	6727(1)	51(1)
C(12)	3965(3)	2202(2)	5034(1)	48(1)
C(13)	2830(5)	1202(3)	3933(2)	75(1)
C(14)	169(3)	2034(3)	5770(2)	61(1)
C(15)	2793(4)	802(3)	6338(2)	65(1)

Table 3. Bond lengths [Å] and angles [°] for jeff.

O(1)-C(11)	1.196(3)	O(2)-C(11)	1.372(3)
O(2)-C(2)	1.456(3)	O(3)-C(6)	1.209(2)
O(4)-C(12)	1.199(3)	O(5)-C(12)	1.322(3)
O(5)-C(13)	1.437(3)	C(1)-C(6)	1.512(3)
C(1)-C(10)	1.521(3)	C(1)-C(2)	1.540(3)
C(1)-C(9)	1.545(3)	C(2)-C(3)	1.490(3)
C(3)-C(4)	1.541(3)	C(4)-C(5)	1.575(3)
C(5)-C(6)	1.526(3)	C(5)-C(12)	1.537(3)
C(5)-C(7)	1.588(3)	C(7)-C(15)	1.523(3)
C(7)-C(14)	1.530(4)	C(7)-C(8)	1.530(3)
C(8)-C(9)	1.528(4)	C(10)-C(11)	1.494(3)
C(11)-O(2)-C(2)	107.5(2)	C(12)-O(5)-C(13)	117.2(2)
C(6)-C(1)-C(10)	119.1(2)	C(6)-C(1)-C(2)	101.7(2)
C(10)-C(1)-C(2)	98.3(2)	C(6)-C(1)-C(9)	112.7(2)
C(10)-C(1)-C(9)	110.0(2)	C(2)-C(1)-C(9)	113.9(2)
O(2)-C(2)-C(3)	115.2(2)	O(2)-C(2)-C(1)	103.8(2)
C(3)-C(2)-C(1)	113.4(2)	C(2)-C(3)-C(4)	108.3(2)
C(3)-C(4)-C(5)	119.1(2)	C(6)-C(5)-C(12)	110.6(2)
C(6)-C(5)-C(4)	107.3(2)	C(12)-C(5)-C(4)	106.7(2)
C(6)-C(5)-C(7)	107.6(2)	C(12)-C(5)-C(7)	110.3(2)
C(4)-C(5)-C(7)	114.2(2)	O(3)-C(6)-C(1)	123.4(2)
O(3)-C(6)-C(5)	125.3(2)	C(1)-C(6)-C(5)	110.8(2)
C(15)-C(7)-C(14)	108.7(2)	C(15)-C(7)-C(8)	109.6(2)
C(14)-C(7)-C(8)	107.9(2)	C(15)-C(7)-C(5)	110.8(2)
C(14)-C(7)-C(5)	113.0(2)	C(8)-C(7)-C(5)	106.7(2)
C(9)-C(8)-C(7)	112.9(2)	C(8)-C(9)-C(1)	116.7(2)
C(11)-C(10)-C(1)	102.3(2)	O(1)-C(11)-O(2)	120.5(2)
O(1)-C(11)-C(10)	129.8(2)	O(2)-C(11)-C(10)	109.7(2)
O(4)-C(12)-O(5)	122.8(2)	O(4)-C(12)-C(5)	124.3(2)
O(5)-C(12)-C(5)	112.9(2)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for jeff. The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33} +2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23})$

	U11	U22	U33	U23	U13	U12
O(1)	73(1)	55(1)	69(1)	-19(1)	3(1)	0(1)
O(2)	52(1)	61(1)	53(1)	-13(1)	-9(1)	-2(1)
O(3)	64(1)	54(1)	33(1)	5(1)	-2(1)	2(1)
O(4)	55(1)	98(2)	80(1)	-30(1)	16(1)	10(1)
O(5)	62(1)	74(1)	50(1)	-19(1)	-2(1)	12(1)
C(1)	37(1)	45(1)	36(1)	1(1)	-1(1)	3(1)
C(2)	41(1)	55(1)	41(1)	-4(1)	-4(1)	-3(1)
C(3)	40(1)	73(2)	51(1)	-6(1)	-9(1)	5(1)
C(4)	38(1)	61(2)	49(1)	2(1)	-1(1)	9(1)
C(5)	39(1)	50(1)	34(1)	3(1)	2(1)	7(1)
C(6)	33(1)	48(1)	34(1)	1(1)	0(1)	-3(1)
C(7)	50(1)	46(1)	45(1)	7(1)	8(1)	4(1)
C(8)	67(2)	60(2)	42(1)	9(1)	15(1)	-1(1)
C(9)	54(1)	56(2)	47(1)	-1(1)	13(1)	1(1)
C(10)	51(1)	50(1)	44(1)	-3(1)	-2(1)	5(1)
C(11)	54(1)	48(1)	50(1)	-7(1)	3(1)	-5(1)
C(12)	51(1)	47(1)	46(1)	3(1)	3(1)	5(1)
C(13)	96(2)	74(2)	55(2)	-22(2)	8(2)	3(2)
C(14)	50(1)	61(2)	72(2)	0(1)	11(1)	-8(1)
C(15)	78(2)	52(2)	65(2)	13(1)	9(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for jeff.

	x	y	z	U(eq)
H(2A)	4793	5742	6003	80
H(3A)	4913	4048	7209	80
H(3B)	6627	4635	6852	80
H(4A)	5729	2482	6438	80
H(4B)	6228	3444	5825	80
H(8A)	944	2419	7176	80
H(8B)	3009	2822	7197	80
H(9A)	1494	4685	7254	80
H(9B)	-23	4263	6657	80
H(10A)	1672	6687	5625	80
H(10B)	91	6286	6132	80
H(13A)	1690	1078	3649	80
H(13B)	3336	388	4078	80
H(13C)	3670	1645	3638	80
H(14A)	-303	2873	5664	80
H(14B)	-641	1589	6077	80
H(14C)	263	1574	5316	80
H(15A)	3983	856	6593	80
H(15B)	2882	346	5882	80
H(15C)	1974	359	6642	80

Table 6. Selected Torsion angles [°] for jeff.

C(11)-O(2)-C(2)-C(3)	-153.1(2)	C(11)-O(2)-C(2)-C(1)	-28.5(2)
C(6)-C(1)-C(2)-O(2)	163.3(2)	C(10)-C(1)-C(2)-O(2)	41.1(2)
C(9)-C(1)-C(2)-O(2)	-75.2(2)	C(6)-C(1)-C(2)-C(3)	-71.0(2)
C(10)-C(1)-C(2)-C(3)	166.9(2)	C(9)-C(1)-C(2)-C(3)	50.6(3)
O(2)-C(2)-C(3)-C(4)	173.8(2)	C(1)-C(2)-C(3)-C(4)	54.3(3)
C(2)-C(3)-C(4)-C(5)	-39.2(3)	C(3)-C(4)-C(5)-C(6)	40.9(3)
C(3)-C(4)-C(5)-C(12)	159.5(2)	C(3)-C(4)-C(5)-C(7)	-78.3(3)
C(10)-C(1)-C(6)-O(3)	6.2(3)	C(2)-C(1)-C(6)-O(3)	-100.3(2)
C(9)-C(1)-C(6)-O(3)	137.4(2)	C(10)-C(1)-C(6)-C(5)	178.3(2)
C(2)-C(1)-C(6)-C(5)	71.9(2)	C(9)-C(1)-C(6)-C(5)	-50.5(2)
C(12)-C(5)-C(6)-O(3)	-2.0(3)	C(4)-C(5)-C(6)-O(3)	114.0(2)
C(7)-C(5)-C(6)-O(3)	-122.6(2)	C(12)-C(5)-C(6)-C(1)	-173.9(2)
C(4)-C(5)-C(6)-C(1)	-57.9(2)	C(7)-C(5)-C(6)-C(1)	65.5(2)
C(6)-C(5)-C(7)-C(15)	174.0(2)	C(12)-C(5)-C(7)-C(15)	53.2(3)
C(4)-C(5)-C(7)-C(15)	-67.0(3)	C(6)-C(5)-C(7)-C(14)	51.7(3)
C(12)-C(5)-C(7)-C(14)	-69.1(2)	C(4)-C(5)-C(7)-C(14)	170.7(2)
C(6)-C(5)-C(7)-C(8)	-66.8(2)	C(12)-C(5)-C(7)-C(8)	172.4(2)
C(4)-C(5)-C(7)-C(8)	52.2(2)	C(15)-C(7)-C(8)-C(9)	175.1(2)
C(14)-C(7)-C(8)-C(9)	-66.7(3)	C(5)-C(7)-C(8)-C(9)	55.1(3)
C(7)-C(8)-C(9)-C(1)	-42.9(3)	C(6)-C(1)-C(9)-C(8)	39.1(3)
C(10)-C(1)-C(9)-C(8)	174.7(2)	C(2)-C(1)-C(9)-C(8)	-76.2(3)
C(6)-C(1)-C(10)-C(11)	-146.6(2)	C(2)-C(1)-C(10)-C(11)	-38.2(2)
C(9)-C(1)-C(10)-C(11)	81.0(2)	C(2)-O(2)-C(11)-O(1)	-177.7(2)
C(2)-O(2)-C(11)-C(10)	3.1(3)	C(1)-C(10)-C(11)-O(1)	-155.4(3)
C(1)-C(10)-C(11)-O(2)	23.7(3)	C(13)-O(5)-C(12)-O(4)	2.0(4)
C(13)-O(5)-C(12)-C(5)	-177.1(2)	C(6)-C(5)-C(12)-O(4)	121.0(3)
C(4)-C(5)-C(12)-O(4)	4.6(3)	C(7)-C(5)-C(12)-O(4)	-120.0(3)
C(6)-C(5)-C(12)-O(5)	-59.9(3)	C(4)-C(5)-C(12)-O(5)	-176.3(2)
C(7)-C(5)-C(12)-O(5)	59.1(3)		