SUPPORTING INFORMATION

Table A. Atomic Coordinates and Thermal Displacement Parameters $(Å)^2$ for α-FOX-7 at 200 K obtained from a Single Crystal Investigation.

atom	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
O11	0.0228	0.05808	0.75066	0.0213	0.0281	0.0131	0.0037	-0.0042	0.0031	0.0208
	(2)	(18)	(10)	(8)	(6)	(5)	(4)	(5)	(5)	(3)
O12	0.0811	0.2005	0.58111	0.0141	0.0421	0.0180	0.0071	0.0036	-0.0009	0.0247
	(2)	(2)	(11)	(8)	(7)	(6)	(5)	(5)	(5)	(3)
O21	-0.5194	0.05748	0.71268	0.0174	0.0318	0.0142	0.0013	0.0002	-0.0078	0.0211
	(2)	(18)	(9)	(7)	(6)	(5)	(4)	(5)	(5)	(3)
O22	-0.3037	0.16566	0.83645	0.0217	0.0396	0.0080	-0.0023	-0.0017	-0.0012	0.0231
	(2)	(19)	(11)	(8)	(6)	(5)	(4)	(5)	(5)	(3)
N11	-0.0358	0.14420	0.65806	0.0148	0.0193	0.0110	0.0002	-0.0004	0.0009	0.0150
	(2)	(18)	(12)	(8)	(6)	(6)	(4)	(5)	(5)	(3)
N12	-0.3570	0.12732	0.73397	0.0143	0.0184	0.0092	0.0015	0.0006	0.0009	0.0140
	(2)	(17)	(12)	(8)	(5)	(5)	(4)	(5)	(5)	(3)
C1	-0.2323	0.1685	0.63730	0.0134	0.0188	0.0083	0.0007	0.0007	-0.0010	0.0135
	(2)	(2)	(13)	(9)	(6)	(6)	(5)	(6)	(5)	(3)
C2	-0.3140	0.2406	0.52542	0.0183	0.0150	0.0081	-0.0006	-0.0008	0.0009	0.0138
	(3)	(2)	(12)	(9)	(5)	(6)	(4)	(6)	(5)	(3)
N21	-0.2015	0.3002	0.43882	0.0203	0.0322	0.0095	0.0054	0.0012	0.0024	0.0207
	(3)	(2)	(12)	(10)	(7)	(6)	(5)	(6)	(6)	(3)
H11	-0.254	0.344	0.367							0.036
	(5)	(3)	(3)							(7)
H12	-0.058	0.304	0.459							0.043
	(6)	(4)	(3)							(8)
N22	-0.5027	0.25428	0.51024	0.0172	0.0241	0.0121	0.0030	-0.0033	0.0007	0.0178
	(2)	(18)	(12)	(9)	(6)	(6)	(4)	(6)	(6)	(3)
H21	-0.550	0.297	0.442							0.031
	(5)	(4)	(3)							(7)
H22	-0.587	0.206	0.562							0.020
	(4)	(3)	(2)							(5)

Table B. Atomic Coordinates and Thermal Displacement Parameters (Å)^2 for α-FOX-7 at 298 K obtained from a Single Crystal Investigation.

Atom	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
O11	0.0233	0.0619	0.74999	0.0305	0.0476	0.0219	0.0059	-0.0064	0.0044	0.0333
	(2)	(2)	(12)	(9)	(7)	(6)	(5)	(6)	(5)	(3)
O12	0.0813	0.2026	0.58134	0.0221	0.0690	0.0282	0.0120	0.0051	-0.0007	0.0398
	(3)	(3)	(13)	(9)	(9)	(7)	(6)	(6)	(6)	(4)
O21	-0.5174	0.0619	0.71255	0.0273	0.0528	0.0213	0.0019	0.0009	-0.0117	0.0338
	(2)	(2)	(10)	(8)	(8)	(6)	(5)	(5)	(6)	(4)
O 22	-0.3018	0.16770	0.83548	0.0320	0.0666	0.0126	-0.0031	-0.0019	-0.0034	0.0371
	(3)	(2)	(12)	(9)	(9)	(5)	(5)	(5)	(6)	(4)
N11	-0.0351	0.14690	0.65802	0.0221	0.00331	0.0174	0.0007	-0.0009	0.0013	0.0242
	(2)	(19)	(12)	(9)	(7)	(6)	(5)	(5)	(5)	(3)
N12	-0.3552	0.13025	0.73365	0.0245	0.0307	0.0137	0.0018	0.0003	0.0007	0.0230
	(2)	(19)	(12)	(9)	(6)	(5)	(4)	(5)	(5)	(3)
C1	-0.2311	0.1707	0.63705	0.0205	0.0308	0.0128	0.0013	0.0007	-0.0003	0.0214
	(3)	(2)	(14)	(10)	(7)	(7)	(5)	(6)	(6)	(4)
C2	-0.3131	0.2409	0.52561	0.0266	0.0255	0.0134	-0.0005	-0.0007	0.0019	0.0218
	(3)	(2)	(13)	(10)	(6)	(6)	(5)	(6)	(6)	(4)
N21	-0.2005	0.2991	0.43933	0.0317	0.0534	0.0153	0.0095	0.0025	0.0041	0.0335
	(3)	(3)	(13)	(12)	(8)	(6)	(6)	(6)	(7)	(4)
H11	-0.249	0.340	0.365							0.060
	(6)	(4)	(3)							(9)
H12	-0.067	0.304	0.455							0.039
	(6)	(4)	(3)							(7)
N22	-0.5008	0.2538	0.51035	0.0273	0.0400	0.0191	0.0043	-0.0044	0.0003	0 .0288
	(3)	(2)	(13)	(10)	(7)	(7)	(5)	(7)	(7)	(4)
H21	-0.546	0.298	0.440							0.063
	(7)	(5)	(4)							(9)
H22	-0.583	0.211	0.560							0.028
	(5)	(3)	(2)							(5)

Table C. Atomic Coordinates and Thermal Displacement Parameters (Å)^2 for α-FOX-7 at 333 K obtained from a Single Crystal Investigastion.

atom	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
O11	0.0238	0.0636	0.74970	0.0354	0.0539	0.0293	0.0065	-0.0078	0.0055	0.0395
	(2)	(2)	(12)	(10)	(7)	(6)	(5)	(6)	(6)	(4)
O12	0.0813	0.2035	0.58148	0.0254	0.0774	0.0372	0.0128	0.0062	-0.0015	0.0467
	(3)	(3)	(14)	(10)	(9)	(7)	(7)	(7)	(7)	(4)
O21	-0.5167	0.0637	0.71266	0.0314	0.0607	0.0283	0.0027	0.0011	-0.0129	0.0401
	(3)	(2)	(12)	(9)	(8)	(6)	(5)	(6)	(7)	(4)
O 22	-0.3011	0.1686	0.83497	0.0369	0.0769	0.0177	-0.0033	-0.0019	-0.0033	0.0438
	(3)	(2)	(12)	(10)	(10)	(6)	(6)	(6)	(7)	(4)
N11	-0.0349	0.1478	0.65792	0.0264	0.0379	0.0227	0.0006	-0.0012	0.0008	0.0290
	(3)	(2)	(12)	(9)	(7)	(7)	(5)	(5)	(5)	(4)
N12	-0.3543	0.13162	0.73335	0.0278	0.0351	0.0196	0.0016	-0.0001	0.0011	0.0275
	(3)	(19)	(12)	(10)	(6)	(6)	(5)	(6)	(5)	(3)
C1	-0.2313	0.1719	0.63709	0.0247	0.0350	0.0187	0.0009	0.0006	0.0003	0.0261
	(3)	(2)	(15)	(11)	(7)	(7)	(6)	(7)	(6)	(4)
C2	-0.3126	0.2411	0.52573	0.0312	0.0285	0.0190	-0.0012	-0.0013	0.0015	0.0262
	(3)	(2)	(13)	(11)	(6)	(6)	(5)	(7)	(6)	(4)
N21	-0.2005	0.2985	0.43950	0.0357	0.0609	0.0214	0.0107	0.0025	0.0043	0.0393
	(3)	(3)	(14)	(13)	(9)	(7)	(7)	(7)	(7)	(4)
H11	-0.247	0.343	0.370							0.057
	(5)	(4)	(3)							(9)
H12	-0.069	0.300	0.454							0.047
	(6)	(4)	(3)							(7)
N22	-0.5002	0.2540	0.51029	0.0318	0.0462	0.0246	0.0052	-0.0052	0.0007	0.0342
	(3)	(2)	(14)	(11)	(8)	(7)	(5)	(8)	(7)	(4)
H21	-0.539	0.298	0.446							0.053
	(6)	(4)	(3)							(8)
H22	-0.580	0.207	0.561							0.038
	(5)	(3)	(2)							(6)

Table D. Donor (D)-Acceptor (A) Geometry (Å, ^{o}) for Hydrogen Bonds in α-FOX-7 at 200 K Obtained from a Single Crystal Investigation. Intramolecular Bonds are marked *.

D – H ··· A	D-H (Å)	H···A (Å)	D···A (Å)	D – H···A (^{o})
N21-H11··· O11	0.94	2.12	2.999	156
N21-H11··· O21	0.94	2.46	2.994	116
N21-H12···O12*	1.02	1.81	2.611	133
N21-H12···O22	1.02	2.25	2.995	129
N22-H21···O22	0.89	2.13	2.906	147
N22-H21···O11	0.89	2.41	3.179	146
N22-H22···O21*	0.89	2.02	2.624	125
N22-H22···O12	0.89	2.31	3.011	137
averaged	0.93	2.19	3.01	136

D – H: ± 0.04 Å, H···A: ± 0.04 Å, D···A: ± 0.004 Å, ∠ D - H···A: ± 2 ^{o}

Table E. Donor (D)-Acceptor (A) Geometry (Å, ^{o}) for Hydrogen Bonds in α-FOX-7 at 298 K Obtained from a Single Crystal Investigation. Intramolecular Bonds are marked *.

D – H ··· A	D-H (Å)	H···A (Å)	D···A (Å)	D – H···A (^{o})
N21-H11··· O11	0.95	2.15	3.015	152
N21-H11··· O21	0.95	2.44	3.008	118
N21-H12···O12*	0.94	1.88	2.608	132
N21-H12···O22	0.94	2.30	3.013	133
N22-H21···O22	0.93	2.12	2.921	143
N22-H21···O11	0.93	2.36	3.193	148
N22-H22···O21*	0.85	2.04	2.619	125
N22-H22···O12	0.85	2.34	3.027	138
averaged	0.92	2.20	3.03	136

D – H: ± 0.04 Å, H···A: ± 0.04 Å, D···A: ± 0.004 Å, ∠ D - H···A: ± 2 ^{o}

Table F. Donor (D)-Acceptor (A) Geometry (Å, ^{o}) for Hydrogen Bonds in α-FOX-7 at 333 K obtained from a Single Crystal Investigation. Intramolecular Bonds are marked *.

D – H ··· A	D-H (Å)	H···A (Å)	D···A (Å)	D – H···A (^{o})
N21-H11··· O11	0.90	2.18	3.020	154
N21-H11··· O21	0.90	2.48	3.014	119
N21-H12···O12*	0.93	1.89	2.608	132
N21-H12···O22	0.93	2.30	3.024	134
N22-H21···O22	0.83	2.22	2.926	143
N22-H21···O11	0.83	2.45	3.197	150
N22-H22···O21*	0.86	2.02	2.622	127
N22-H22···O12	0.86	2.36	3.034	136
averaged	0.92	2.24	3.04	137

D – H: ± 0.04 Å, H···A: ± 0.04 Å, D···A: ± 0.004 Å, ∠ D - H···A: ± 2 ^{o}