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Section S1. X-ray Crystallography

(*a*) (*b*)

Figure S1. 1. Images of inverted reaction vessels with reaction mixtures [Mn(hfac)$_2$] + NN-Pz-CHF$_2$ (*a*) and [Mn(hfac)$_2$] + NN-Pz-CH$_2$CH$_2$F (*b*) after incubation at –15 °C for 24 h.

Fragments of crystal structures of complexes with shown cell axes

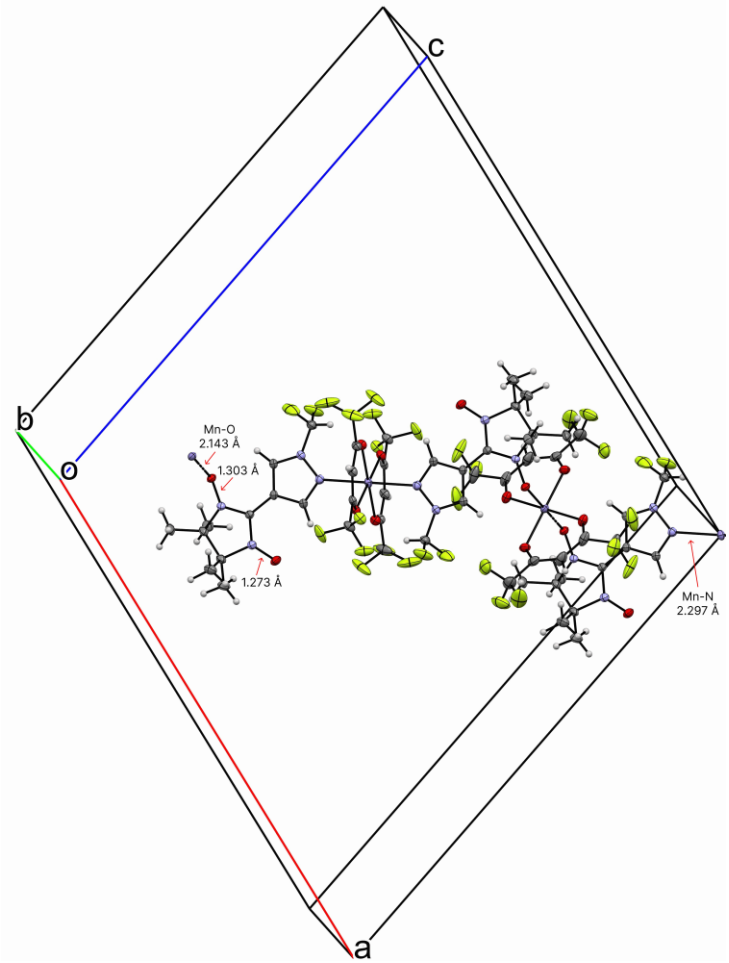

Figure S1.2. View of a fragment of the chain in 1. Hereinafter, thermal ellipsoids are drawn with 50% probability.

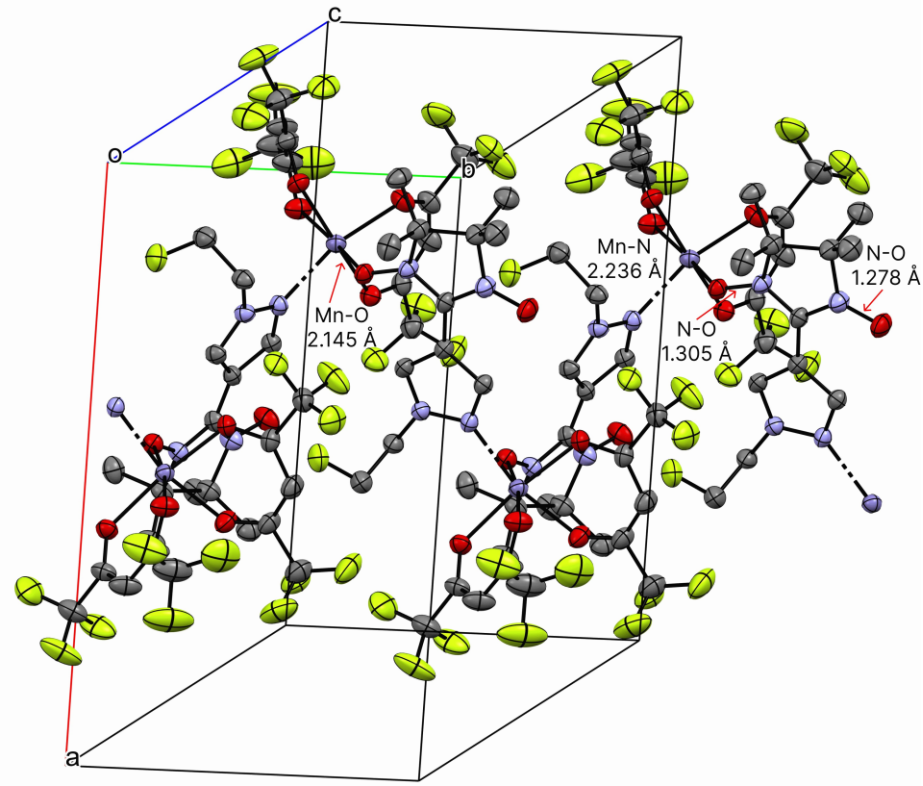

Figure S1.3. View of a fragment of the chain in 2.

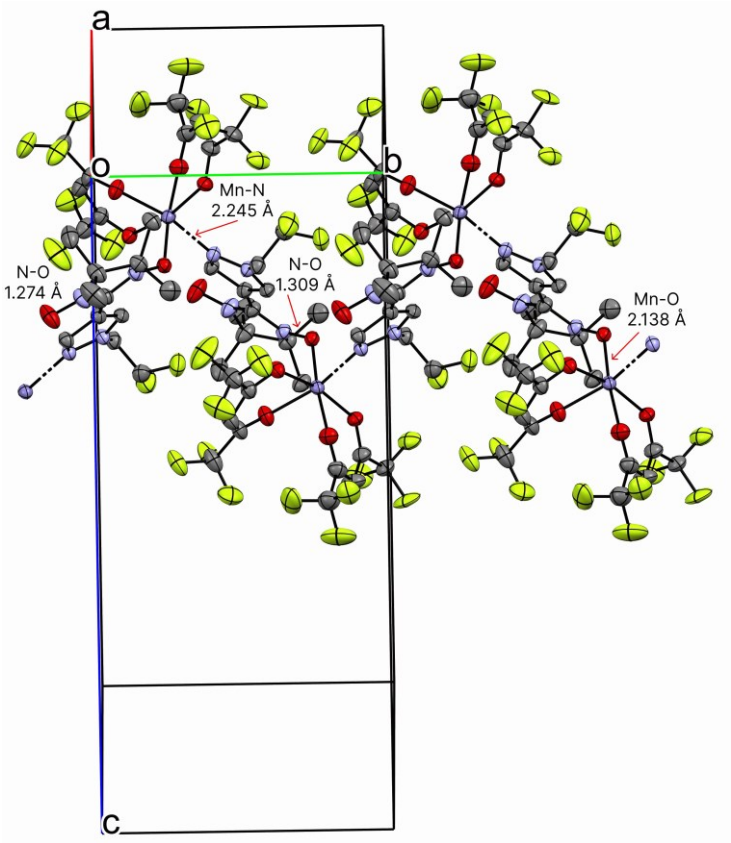

Figure S1.4. View of a fragment of the chain in 3·C_7H_8.

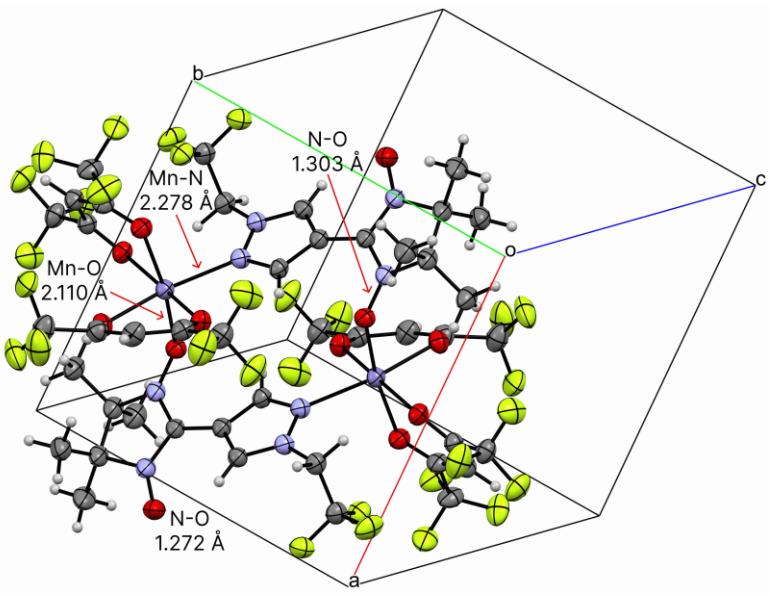

Figure S1.5. View of a fragment of the chain in 4·C_7H_8.

In one of the experiments, co–crystals of $[Mn(hfac)_2(NN–Pz–CH_2CHF_2)]_n$ with $[Mn(hfac)_2(NN–Pz–CH_2CHF_2)H_2O]$ were isolated and successfully characterised by the single–crystal X–ray analysis (Figure S1.6). The structure of the complex is formed by packing of chains with geometry similar to that in $[Mn(hfac)_2(NN–Pz–CH_2CHF_2)]_n$ and molecular complexes $[Mn(hfac)_2(NN–Pz–CH_2CHF_2)H_2O]$ containing a coordinated water molecule. It is noteworthy here that in $[Mn(hfac)_2(NN–Pz–CH_2CHF_2)H_2O]$, the paramagnetic ligand is coordinated by the oxygen atom of the nitroxide group, consistently with the oxophilic nature of the Mn ion.

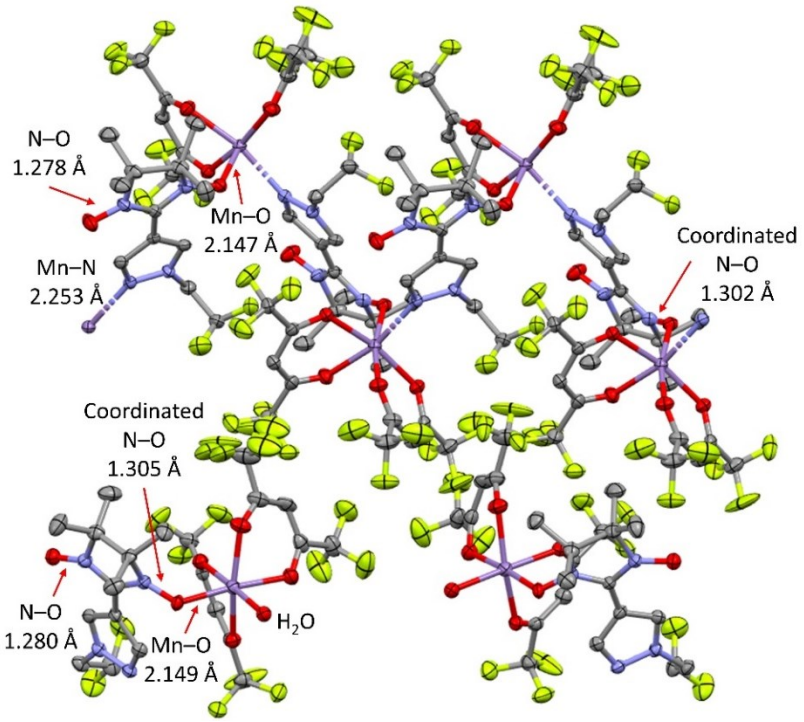

Figure S1.6. View of a fragment of the crystal structure of $[Mn(hfac)_2(NN–Pz–CH_2CHF_2)]_n \cdot n[Mn(hfac)_2(NN–Pz–CH_2CHF_2)H_2O]$.

Short inter-chain and inter-molecular contacts

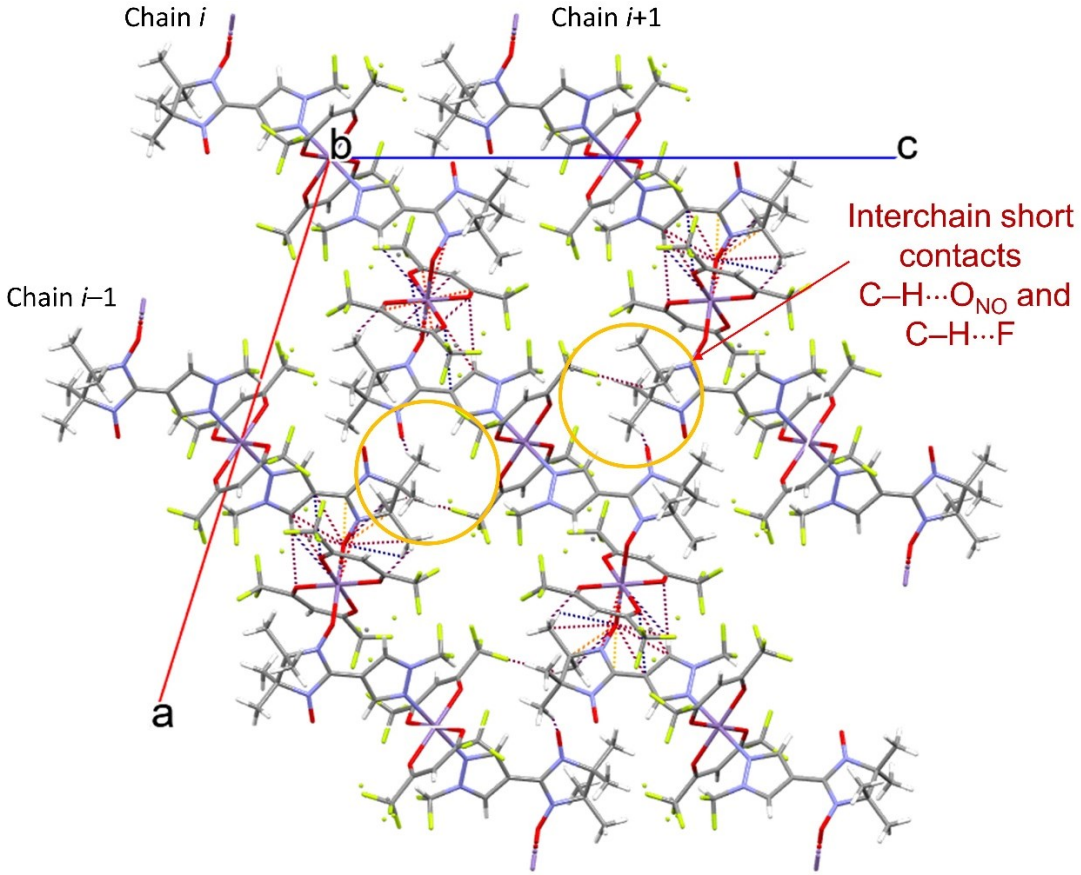

Figure S1.7. A fragment of crystal structure of 1 with short inter-chain contacts C–H···O$_{NO}$ (2.539 Å) and C–H···F (2.396 Å).

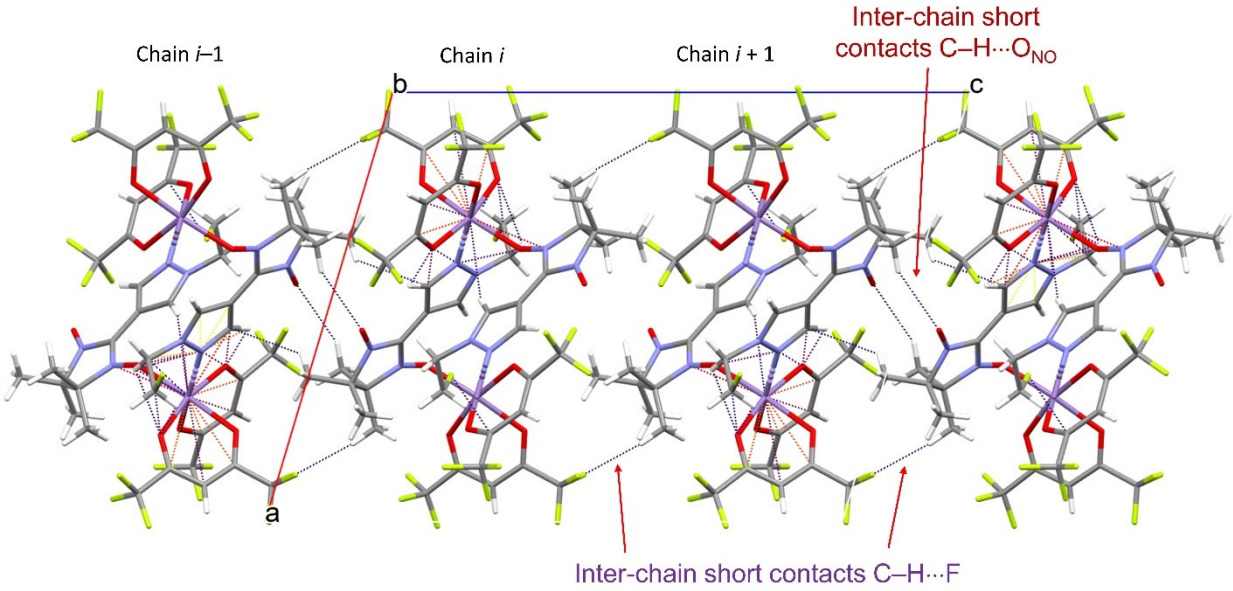

Figure S1.8. A fragment of crystal structure of 2 with short inter-chain contacts C–H···O$_{NO}$ (2.665 Å) and C–H···F (2.557 Å).

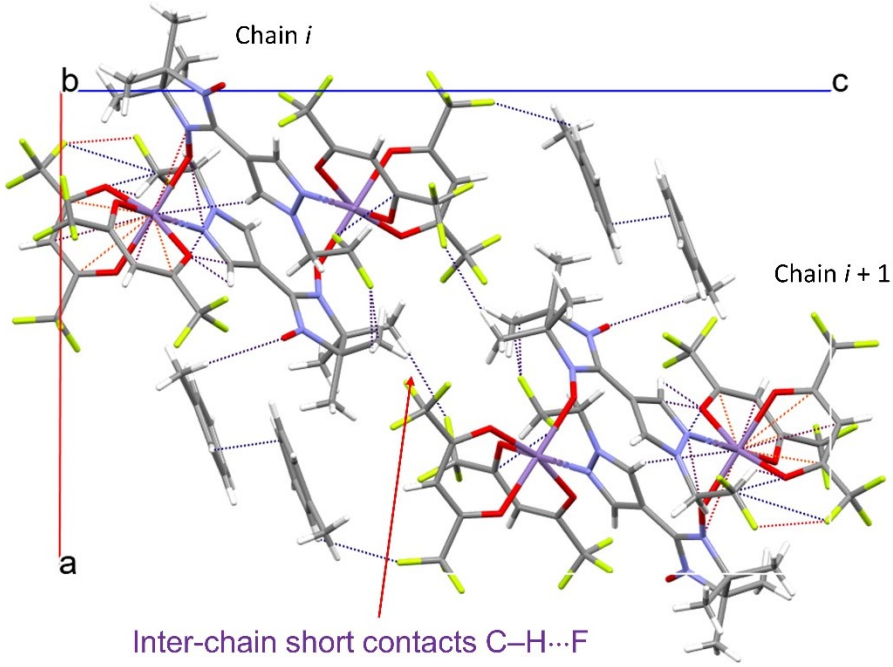

Figure S1.9. A fragment of crystal structure of 3·C_7H_8 with short inter-chain contacts C–H···F (2.576 Å).

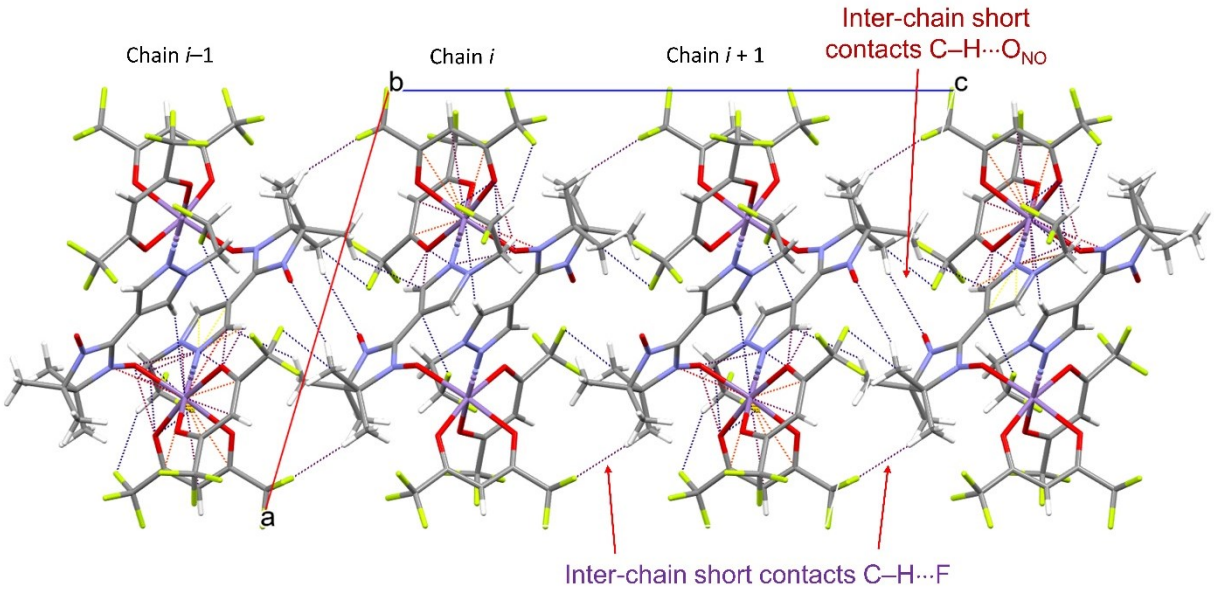

Figure S1.10. A fragment of crystal structure of 3 with short inter-chain contacts C–H···O_{NO} (2.640 Å) and C–H···F (2.490 Å).

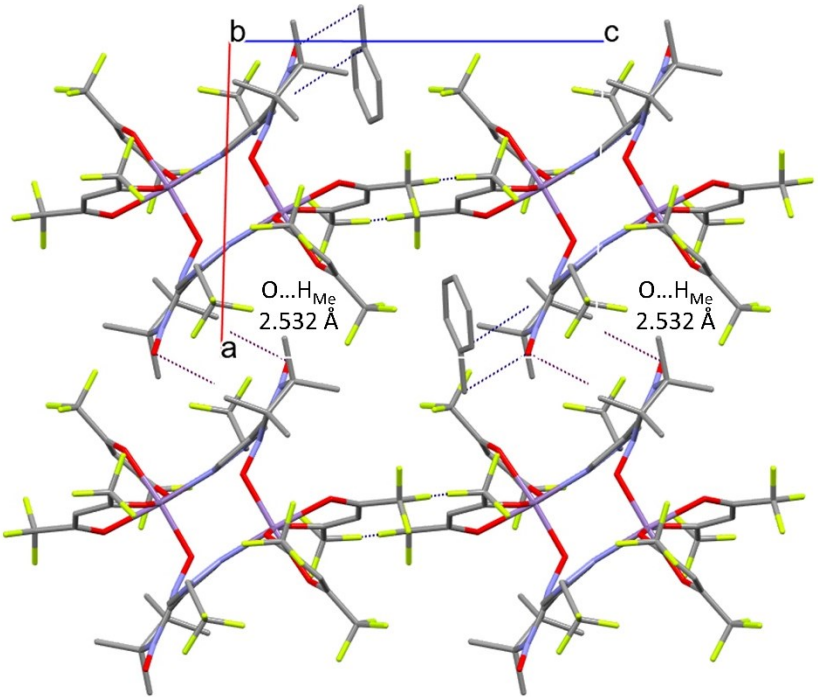

Figure S1.11. A fragment of crystal structure of 4·C_7H_8 (hydrogen atoms are not shown).

Table S1.1. Crystal data for complexes 1, 2, and 3.

Compound	**1**	**2**	**3**
Empirical formula	$C_{21}H_{17}F_{14}MnN_4O_6$	$C_{22}H_{20}F_{13}MnN_4O_6$	$C_{22}H_{19}F_{14}MnN_4O_6$
Formula weight	742.33	738.36	756.35
Temperature, K	100.0(1)	100.0(1)	100.0(1)
Wavelength, Å	1.54184	1.54184	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	I2/a	$P2_1/c$	$P2_1/c$
Unit cell dimensions			
a, Å	26.0180(2)	16.0023(4)	16.0909(8)
b, Å	9.42480(10)	9.7163(2)	9.9125(4)
c, Å	24.7301(2)	20.6248(5)	20.0481(9)
α, °	90	90	90
β, °	107.3830(10)	106.565(3)	106.374(3)
γ, °	90	90	90
Volume, Å^3	5787.22(9)	3073.72(13)	3068.0(2)
Z	8	4	4
Density (calcd.), g·cm^{-3}	1.704	1.596	1.637
Abs. coefficient, mm^{-1}	4.975	4.630	0.558
F(000)	2960	1480	1512
Crystal size, mm	0.70×0.11×0.07	0.05×0.03×0.02	0.23×0.31×0.39
Θ range, °	3.560 – 77.383	2.867 – 77.066	2.312 – 30.440
Index ranges	–32 ≤ h ≤ 31,	–20 ≤ h ≤19,	–17≤ h ≤ 21,
	–11 ≤ k ≤ 11,	–12 ≤ k ≤ 11,	–13 ≤ k ≤ 12,
	–30 ≤ l ≤ 31	–25 ≤ l ≤ 26	–26 ≤ l ≤ 22
Reflections			
collected	40209	40300	30917
independent [R_{int}]	6100 [0.0338]	6516 [0.0766]	7313 [0.0908]
observed with I > 2σ(I)	5800	5201	4577
Completeness to θ_{full} / θ_{max}	1.000 / 0.989	0.999 / 0.989	0.999 / 0.999
Data / restraints / parameters	6100 / 14 / 452	6516 / 0 / 420	7313/ 0 / 429
Goodness-of-fit on F^2	1.053	1.054	1.020
R1 / wR2 for $I > 2\sigma(I)$	0.0333 / 0.0827	0.0586 / 0.1601	0.0498 / 0.0975
R1 / wR2 (all data)	0.0352 / 0.0838	0.0714 / 0.1705	0.1009 / 0.1143
$\Delta\varrho_{max}$ / $\Delta\varrho_{min}$, e·Å^{-3}	0.491/ –0.526	0.626 / –0.588	0.474/ –0.520

Table S1.2. Crystal data for complexes 3·C_7H_8, 4·C_7H_8, and Mn(hfac)$_2$(NN–Pz–CH_2CHF_2)]$_n$·n[Mn(hfac)$_2$(NN–Pz–CH_2CHF_2)H_2O]).

Compound	**3·C_7H_8**	**4·C_7H_8**	**Mn(hfac)$_2$(NN–Pz–CH_2CHF_2)]$_n$· n[Mn(hfac)$_2$(NN–Pz–CH_2CHF_2)H_2O])**
Empirical formula	$C_{29}H_{27}F_{14}MnN_4O_6$	$C_{58}H_{52}F_{30}Mn_2N_8O_{12}$	$C_{22}H_{19}F_{14}MnN_4O_6$· $C_{22}H_{21}F_{14}MnN_4O_7$
Formula weight	848.48	1732.95	1530.72
Temperature, K	99.9(3)	99.9(3)	100
Wavelength, Å	1.54184	1.54184	0.71073, sealed tube
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	P $\bar{1}$	$P2_1/c$
Unit cell dimensions			
a, Å	14.9623(2)	11.01880(10)	30.298(3)
b, Å	9.98830(10)	12.9099(2)	9.7710(8)
c, Å	23.8702(4)	13.1514(2)	21.7394(18)
α, °	90	75.0990(10)	90
β, °	90.182(2)	88.1200(10)	110.106(3)
γ, °	90	76.9370(10)	90
Volume, Å^3	3567.33(8)	1760.47(4)	6043.5(9)
Z	4	1	4
Density (calcd.), g·cm^{-3}	1.580	1.635	1.682
Abs. coefficient, mm^{-1}	4.117	4.227	0.569
F(000)	1712	872	3064
Crystal size, mm	0.35×0.07×0.06	0.32×0.30×0.20	0.25×0.01×0.01
Θ range, °	3.436 – 77.000	3.465 – 76.624	1.874 – 26.085
Index ranges	–18 ≤ h ≤18, –10 ≤ k ≤ 12, –30 ≤ l ≤ 29	–13 ≤ h ≤13, –16 ≤ k ≤ 16, –16 ≤ l ≤ 16	–37 ≤ h ≤ 37, –12 ≤ k ≤ 12, –26 ≤ l ≤ 22
Reflections			
collected	25876	85727	38331
independent [R_{int}]	7243 [0.0507]	7377 [0.0968]	11939 [0.1009]
observed with I > 2σ(I)	6213	7099	6316
Completeness to θ_{full} / θ_{max}	0.977 / 0.951	0.999 / 0.987	0.999 / 0.996
Data / restraints / parameters	7243 / 298 / 602	7377 / 129 / 564	11939 / 48 / 875
Goodness-of-fit on F^2	1.076	1.077	1.018
R_1 / wR2 for $I > 2\sigma(I)$	0.0736 / 0.2032	0.0463 / 0.1268	0.0634 / 0.1400
R_1 / wR2 (all data)	0.0824 / 0.2096	0.0473 / 0.1275	0.1336 / 0.1786
ΔQ_{max} / ΔQ_{min}, e·Å^{-3}	1.049 / –0.559	0.643 / –0.650	1.032 / –0.578

Table S1.3. Selected bond distances in 1 (Å).

Bond	Distance	Bond	Distance	Bond	Distance
Mn(1)–O(2)#1	2.1428(11)	F(1)–C(4)	1.332(2)	F(8)–C(16)	1.326(3)
Mn(1)–O(2)	2.1427(11)	F(2)–C(4)	1.324(2)	C(17A)–F(9A)	1.318(4)
Mn(1)–O(3)#1	2.1420(12)	C(12A)–F(3A)	1.348(4)	C(17A)–F(10A)	1.322(4)
Mn(1)–O(3)	2.1420(12)	C(12A)–F(4A)	1.313(4)	C(17A)–F(11A)	1.333(4)
Mn(1)–O(4)	2.1363(12)	C(12A)–F(5A)	1.330(3)	C(17A)–C(18)	1.535(4)
Mn(1)–O(4)#1	2.1362(12)	C(12A)–C(13)	1.548(3)	C(17B)–F(9B)	1.319(2)
Mn(2)–O(5)#2	2.1321(11)	C(12B)–F(3B)	1.348(4)	C(17B)–F(10B)	1.323(3)
Mn(2)–O(5)	2.1322(11)	C(12B)–F(4B)	1.313(4)	C(17B)–F(11B)	1.334(3)
Mn(2)–O(6)	2.1378(11)	C(12B)–F(5B)	1.330(3)	C(17B)–C(18)	1.536(2)
Mn(2)–O(6)#2	2.1378(11)	C(12B)–C(13)	1.547(3)	F(12)–C(21)	1.336(2)
Mn(2)–N(2)	2.2966(13)	F(6)–C(16)	1.335(3)	F(13)–C(21)	1.334(2)
Mn(2)–N(2)#2	2.2966(13)	F(7)–C(16)	1.332(2)	F(14)–C(21)	1.326(2)
O(1)–N(3)	1.2730(18)	N(1)–C(3)	1.345(2)	C(1)–C(2)	1.418(2)
O(2)–N(4)	1.3027(17)	N(1)–C(4)	1.439(2)	C(2)–C(3)	1.380(2)
O(3)–C(13)	1.247(2)	N(2)–C(1)	1.325(2)	C(2)–C(5)	1.439(2)
O(4)–C(15)	1.255(2)	N(3)–C(5)	1.356(2)	C(6)–C(7)	1.519(2)
O(5)–C(18)	1.259(2)	N(3)–C(6)	1.504(2)	C(6)–C(8)	1.530(2)
O(6)–C(20)	1.250(2)	N(4)–C(5)	1.336(2)	C(6)–C(9)	1.554(2)
N(1)–N(2)	1.3694(18)	N(4)–C(9)	1.5027(19)	C(9)–C(10)	1.532(2)
C(9)–C(11)	1.522(2)	C(14)–C(15)	1.387(3)	C(18)–C(19)	1.388(2)
C(13)–C(14)	1.397(3)	C(15)–C(16)	1.537(3)	C(19)–C(20)	1.397(2)
C(20)–C(21)	1.539(2)				

Table S1.4. Selected bond distances in 2 (Å).

Bond	Distance	Bond	Distance	Bond	Distance
Mn(1)–O(1)	2.145(2)	O(6)–C(21)	1.254(4)	C(20)–C(21)	1.386(5)
Mn(1)–O(3)	2.130(2)	N(1)–C(1)	1.324(4)	C(21)–C(22)	1.524(5)
Mn(1)–O(4)	2.176(2)	N(1)–C(2)	1.501(3)	C(4)–C(6)	1.408(4)
Mn(1)–O(5)	2.144(2)	N(2)–C(1)	1.354(4)	C(11)–C(12)	1.498(5)
Mn(1)–O(6)	2.173(2)	N(2)–C(3)	1.506(4)	C(13)–C(14)	1.532(5)
Mn(1)–N(3)#1	2.236(2)	N(3)–N(4)	1.365(3)	C(14)–C(15)	1.390(5)
F(1)–C(12)	1.400(4)	N(3)–C(6)	1.331(4)	C(15)–C(16)	1.384(5)
F(2)–C(13)	1.335(5)	N(4)–C(5)	1.345(4)	C(16)–C(17)	1.539(4)
F(3)–C(13)	1.327(5)	N(4)–C(11)	1.457(4)	C(18)–C(19)	1.530(4)
F(4)–C(13)	1.327(4)	C(1)–C(4)	1.439(4)	C(19)–C(20)	1.380(5)
F(5)–C(17)	1.333(4)	C(2)–C(3)	1.558(4)	F(11)–C(22)	1.327(5)
F(6)–C(17)	1.327(4)	C(2)–C(7)	1.515(4)	F(12)–C(22)	1.355(6)
F(7)–C(17)	1.313(4)	C(2)–C(8)	1.535(5)	F(13)–C(22)	1.339(6)
F(8)–C(18)	1.320(4)	C(3)–C(9)	1.524(5)	O(1)–N(1)	1.305(3)
F(9)–C(18)	1.333(5)	C(3)–C(10)	1.522(4)	O(2)–N(2)	1.278(3)
F(10)–C(18)	1.316(5)	C(4)–C(5)	1.391(4)	O(3)–C(14)	1.256(4)
O(4)–C(16)	1.256(3)	O(5)–C(19)	1.259(3)		

Table S1.5. Selected bond distances in 3·C_7H_8 (Å).

Bond	Distance	Bond	Distance	Bond	Distance
Mn(1)–O(1)	2.138(3)	C(24)–F(12A)	1.326(3)	C(11B)–C(12B)	1.503(8)
Mn(1)–O(3)	2.138(3)	C(24)–F(13A)	1.325(3)	F(1B)–C(12B)	1.382(8)
Mn(1)–O(4)	2.169(2)	C(24)–F(11B)	1.326(4)	C(12B)–F(14B)	1.281(9)
Mn(1)–O(5)	2.126(2)	C(24)–F(12B)	1.326(4)	C(16)–C(17)	1.380(5)
Mn(1)–O(6)	2.157(3)	C(24)–F(13B)	1.326(4)	C(17)–C(18)	1.391(5)
Mn(1)–N(4)#1	2.244(3)	C(24)–F(11C)	1.326(4)	C(21)–C(22)	1.392(6)
F(2A)–C(15A)	1.337(3)	C(24)–F(12C)	1.326(4)	C(22)–C(23)	1.390(6)
F(3A)–C(15A)	1.337(3)	C(24)–F(13C)	1.326(4)	C(25A)–C(26A)	1.378(3)
F(4A)–C(15A)	1.337(3)	C(24)–C(23)	1.539(7)	C(25A)–C(30A)	1.377(3)
C(15A)–C(16)	1.544(12)	O(1)–N(1)	1.309(4)	C(25A)–C(31A)	1.483(10)
F(2B)–C(15B)	1.337(4)	O(2)–N(2)	1.274(4)	C(26A)–C(27A)	1.379(3)
F(3B)–C(15B)	1.337(4)	O(3)–C(16)	1.260(5)	C(27A)–C(28A)	1.377(3)
F(4B)–C(15B)	1.337(4)	O(4)–C(18)	1.252(5)	C(28A)–C(29A)	1.377(3)
C(15B)–C(16)	1.55(2)	O(5)–C(21)	1.248(5)	C(29A)–C(30A)	1.378(3)
F(5A)–C(19A)	1.313(3)	O(6)–C(23)	1.242(5)	C(25B)–C(26B)	1.378(4)
F(6A)–C(19A)	1.314(3)	N(1)–C(1)	1.331(4)	C(25B)–C(30B)	1.379(4)
F(7A)–C(19A)	1.318(3)	N(1)–C(2)	1.493(4)	C(25B)–C(31B)	1.484(10)
C(19A)–C(18)	1.538(5)	N(2)–C(1)	1.355(5)	C(26B)–C(27B)	1.378(4)
F(5B)–C(19B)	1.314(4)	N(2)–C(3)	1.497(5)	C(27B)–C(28B)	1.378(4)
F(6B)–C(19B)	1.315(4)	N(3)–N(4)	1.366(4)	C(28B)–C(29B)	1.378(4)
F(7B)–C(19B)	1.315(4)	N(3)–C(10)	1.341(4)	C(29B)–C(30B)	1.378(4)
C(19B)–C(18)	1.538(6)	N(3)–C(11A)	1.455(5)		
C(20A)–F(8A)	1.343(3)	N(3)–C(11B)	1.455(5)		
C(20A)–F(9A)	1.343(3)	N(4)–C(9)	1.325(4)		
C(20A)–F(10A)	1.343(3)	C(1)–C(8)	1.431(5)		
C(20A)–C(21)	1.529(6)	C(2)–C(3)	1.552(6)		
C(20B)–F(8B)	1.340(4)	C(2)–C(4)	1.521(5)		
C(20B)–F(9B)	1.340(4)	C(2)–C(5)	1.522(6)		
C(20B)–F(10B)	1.340(4)	C(3)–C(6)	1.531(7)		
C(20B)–C(21)	1.526(6)	C(3)–C(7)	1.516(7)		
C(20C)–F(8C)	1.343(4)	C(8)–C(9)	1.414(5)		
C(20C)–F(9C)	1.343(4)	C(8)–C(10)	1.394(5)		
C(20C)–F(10C)	1.343(4)	C(11A)–C(12A)	1.503(8)		
C(20C)–C(21)	1.529(6)	F(1A)–C(12A)	1.382(8)		
C(24)–F(11A)	1.326(3)	C(12A)–F(14A)	1.283(8)		

Table S1.6. Selected bond distances in 3 (Å).

Bond	Distance	Bond	Distance	Bond	Distance
Mn(1)—O(1)	2.1467 (18)	O(1)—N(1)	1.310 (3)	C(2)—C(3)	1.551 (4)
Mn(1)—O(3)	2.1606 (19)	O(2)—N(2)	1.277 (3)	C(2)—C(7)	1.532 (4)
Mn(1)—O(4)	2.1392 (19)	O(3)—C(13)	1.249 (3)	C(2)—C(8)	1.513 (4)
Mn(1)—O(5)	2.126 (2)	O(4)—C(15)	1.262 (3)	C(3)—C(9)	1.521 (4)
Mn(1)—O(6)	2.1780 (19)	O(5)—C(20)	1.251 (3)	C(3)—C(10)	1.528 (4)
Mn(1)—N(4)^{i}	2.248 (2)	O(6)—C(18)	1.258 (3)	C(4)—C(5)	1.388 (4)
F(1)—C(12)	1.363 (3)	N(1)—C(1)	1.329 (3)	C(4)—C(6)	1.396 (4)
F(2)—C(12)	1.370 (3)	N(1)—C(2)	1.495 (3)	C(11)—C(12)	1.499 (4)
F(3)—C(16)	1.328 (4)	N(2)—C(1)	1.355 (3)	C(13)—C(14)	1.398 (4)
F(4)—C(16)	1.348 (4)	N(2)—C(3)	1.509 (4)	C(13)—C(16)	1.538 (4)
F(5)—C(16)	1.327 (3)	N(3)—N(4)	1.359 (3)	C(14)—C(15)	1.378 (4)
F(6)—C(17)	1.310 (3)	N(3)—C(5)	1.334 (3)	C(15)—C(17)	1.528 (4)
F(7)—C(17)	1.335 (4)	N(3)—C(11)	1.459 (3)	C(18)—C(19)	1.381 (4)
F(8)—C(17)	1.328 (4)	N(4)—Mn(1)^{ii}	2.248 (2)	C(18)—C(22)	1.531 (4)
F(9)—C(21)	1.328 (4)	N(4)—C(6)	1.326 (3)	C(19)—C(20)	1.394 (4)
F(10)—C(21)	1.334 (4)	C(1)—C(4)	1.438 (4)	C(20)—C(21)	1.534 (4)
F(11)—C(21)	1.313 (4)				
F(12)—C(22)	1.332 (3)				
F(13)—C(22)	1.336 (3)				
F(14)—C(22)	1.327 (3)				

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+3/2.

Table S1.7. Selected bond distances in 4·C_7H_8 (Å).

Bond	Distance	Bond	Distance	Bond	Distance
Mn(1)–O(2)	2.1101(14)	O(5)–C(19)	1.248(3)	C(4)–C(3)	1.4328(16)
Mn(1)–O(3)	2.1534(14)	O(6)–C(21)	1.260(3)	C(24)–C(23)	1.4331(16)
Mn(1)–O(4)	2.1776(15)	N(1)–C(1)	1.345(3)	C(1)–C(5)	1.4866(16)
Mn(1)–O(5)	2.1769(15)	N(1)–C(2)	1.507(3)	C(2)–C(3)	1.3707(17)
Mn(1)–O(6)	2.1327(14)	N(2)–C(1)	1.336(3)	C(3)–C(12)	1.5150(15)
Mn(1)–N(4)#1	2.2779(18)	N(2)–C(3)	1.502(2)	C(23)–C(32)	1.5108(15)
F(1)–C(12)	1.336(3)	N(3)–N(4)	1.372(2)	C(21)–C(25)	1.4861(15)
F(2)–C(12)	1.337(2)	N(3)–C(9)	1.343(3)	C(15)–C(14)	1.5147(16)
F(3)–C(12)	1.332(3)	N(3)–C(11)	1.451(2)	C(15)–C(16)	1.3892(18)
F(4)–C(13)	1.319(3)	N(4)–C(10)	1.331(3)	C(15)–C(20)	1.3918(17)
F(5)–C(13)	1.328(3)	C(1)–C(8)	1.443(3)	C(32)–C(33)	1.4957(16)
F(6)–C(13)	1.328(3)	C(2)–C(3)	1.563(3)	C(5)–C(10)	1.3924(18)
F(7A)–C(17A)	1.334(5)	C(2)–C(4)	1.522(3)	C(23B)–C(29B)	1.507(7)
F(8A)–C(17A)	1.311(5)	C(2)–C(5)	1.522(4)	C(24B)–C(25B)	1.384(3)
F(9A)–C(17A)	1.332(5)	C(3)–C(6)	1.532(3)	C(25B)–C(26B)	1.385(3)
C(17A)–C(16)	1.541(4)	C(3)–C(7)	1.519(3)	C(26B)–C(27B)	1.386(3)
F(7B)–C(17B)	1.341(6)	C(8)–C(9)	1.390(3)	C(27B)–C(28B)	1.386(3)
F(8B)–C(17B)	1.319(6)	C(8)–C(10)	1.399(3)	C(25A)–C(26A)	1.383(3)
F(9B)–C(17B)	1.339(5)	C(11)–C(12)	1.510(3)	C(26A)–C(27A)	1.383(3)
C(17B)–C(16)	1.549(4)	C(13)–C(14)	1.537(3)	C(27A)–C(28A)	1.384(3)
F(7C)–C(17C)	1.334(6)	C(14)–C(15)	1.388(3)	C(23B)–C(24B)	1.384(3)
F(8C)–C(17C)	1.312(6)	C(15)–C(16)	1.399(3)	C(23B)–C(28B)	1.386(3)
F(9C)–C(17C)	1.332(5)	C(19)–C(20)	1.401(3)	F(13)–C(22)	1.333(3)
C(17C)–C(16)	1.542(4)	C(20)–C(21)	1.388(3)	F(14)–C(22)	1.328(3)
F(10A)–C(18A)	1.324(4)	C(21)–C(22)	1.537(3)	F(15)–C(22)	1.326(3)
F(11A)–C(18A)	1.336(4)	C(23A)–C(24A)	1.388(3)	O(1)–N(1)	1.272(3)
F(12A)–C(18A)	1.335(4)	C(23A)–C(28A)	1.385(3)	O(2)–N(2)	1.304(2)
C(18A)–C(19)	1.543(3)	C(23A)–C(29A)	1.510(6)	O(3)–C(14)	1.247(3)
F(10B)–C(18B)	1.330(5)	C(24A)–C(25A)	1.384(3)	O(4)–C(16)	1.245(3)
F(11B)–C(18B)	1.340(5)	F(12B)–C(18B)	1.339(4)	C(18B)–C(19)	1.550(4)

Section S2. Powder X-ray Diffraction Data

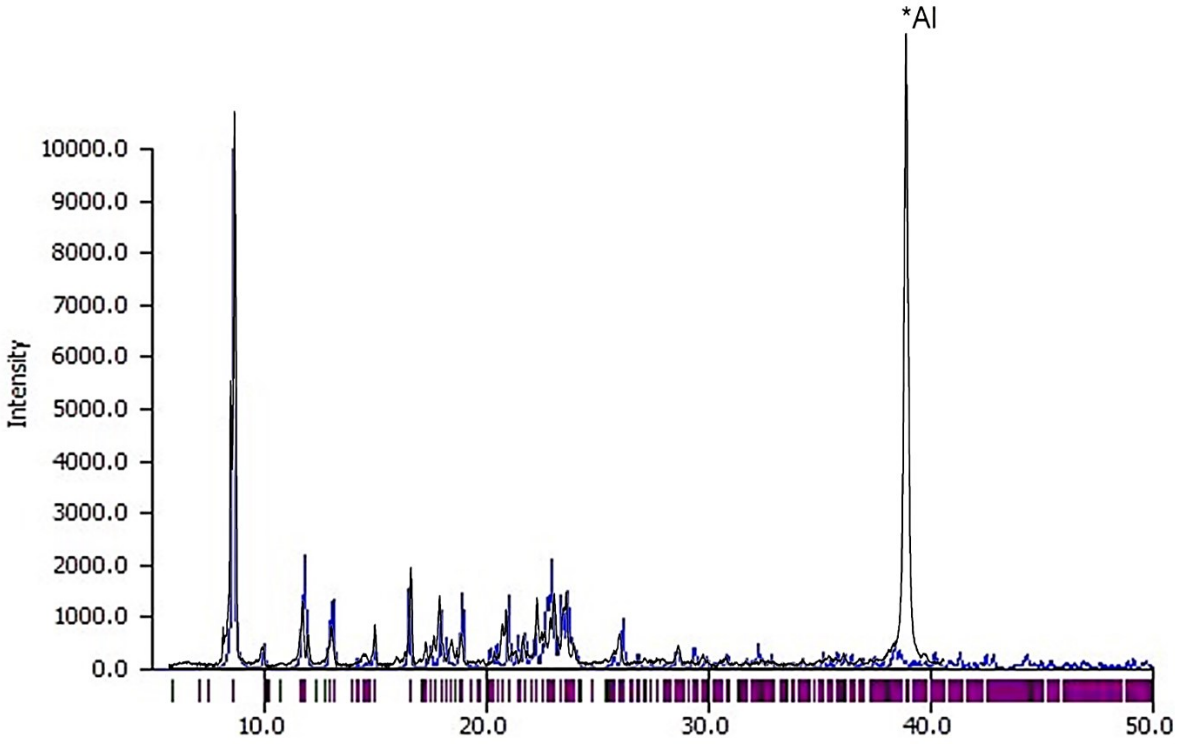

Figure S2.1. Experimental (black) and calculated (blue) powder X-ray diffraction pattern of 1.

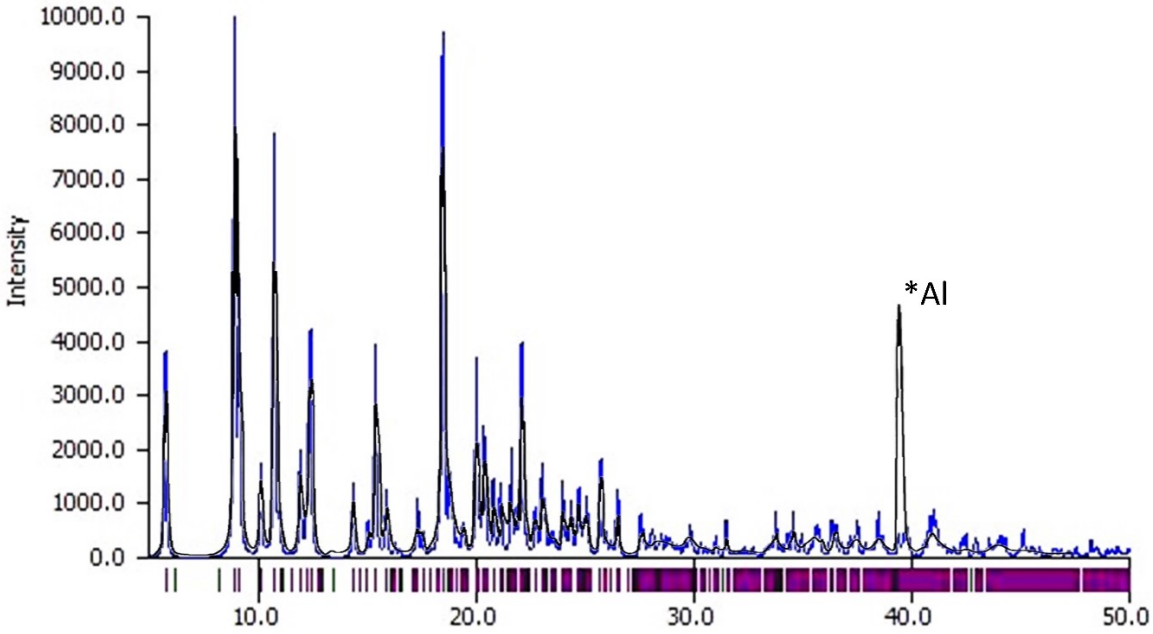

Figure S2.2. Experimental (black) and calculated (blue) powder X-ray diffraction pattern of 2.

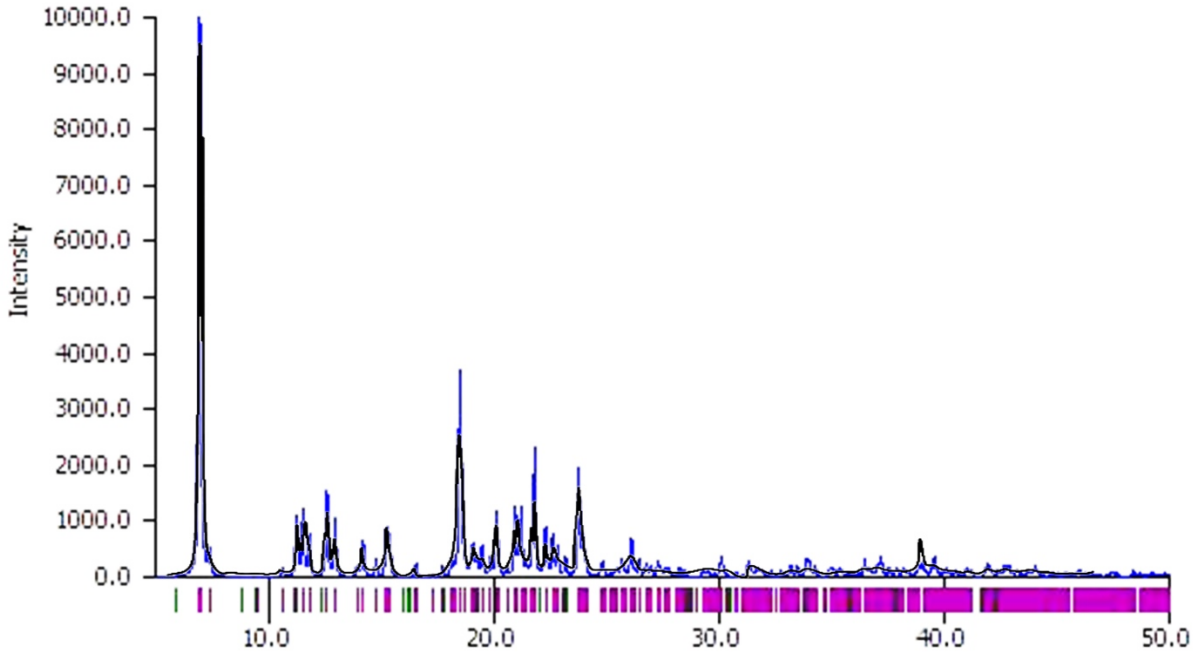

Figure S2.3. Experimental (black) and calculated (blue) powder X-ray diffraction pattern of 3·C_7H_8.

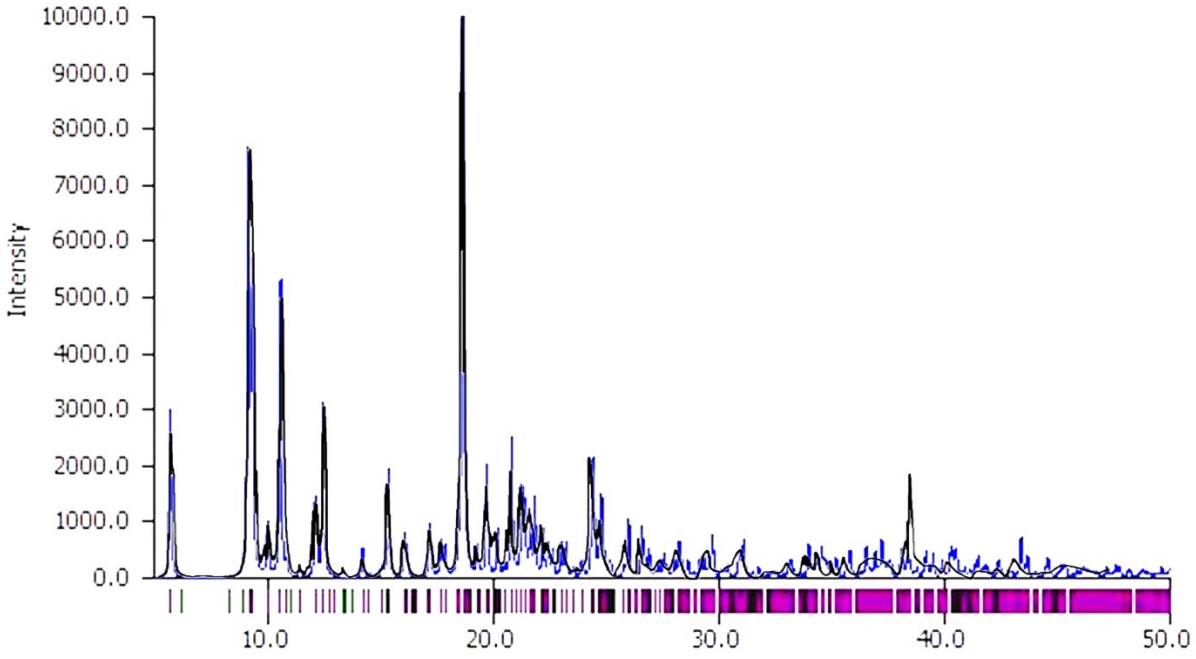

Figure S2.4. Experimental (black) and calculated (blue) powder X-ray diffraction pattern of 3.

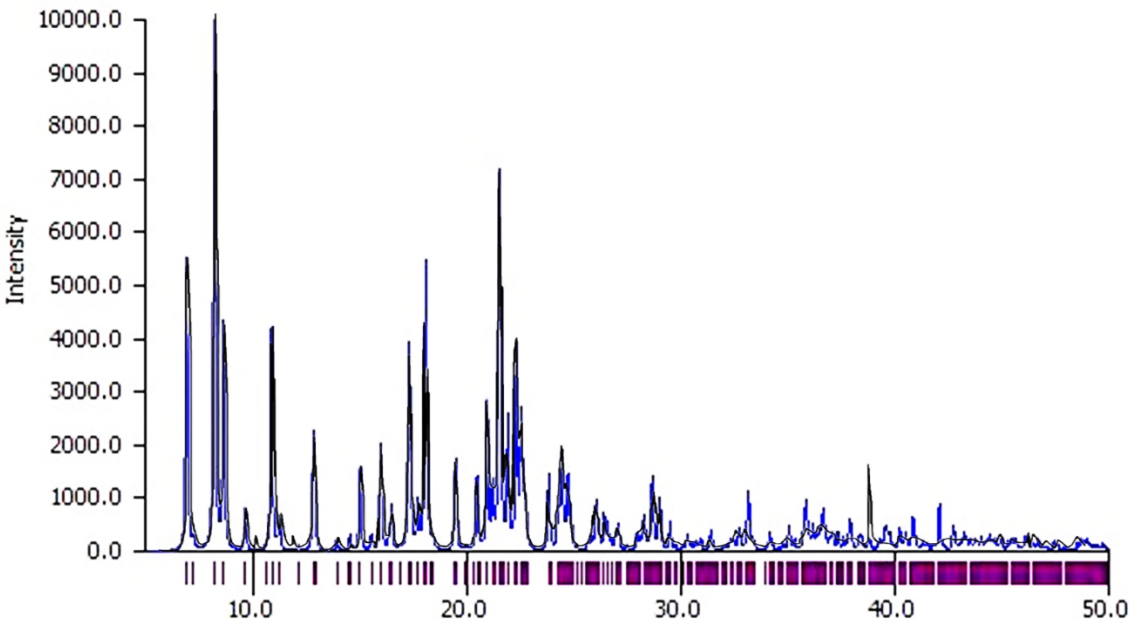

Figure S2.5. Experimental (black) and calculated (blue) powder X-ray diffraction pattern of 4·C_7H_8.