Electronic Supplementary Information (ESI) for:

New π-Stacking Motifs for Molecular Semiconducting Materials: Bis(bis(8-quinolinyl)amide)metal(II) Complexes of Cr, Mn, Fe, and Zn

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Computational Results

Table S1 Cartesian coordinates in Å of optimized species:

$Zn(BQA)_2$ (PBEPBE/ Def2TZVP, multiplicity = 1):

a.n.	X	Y	Z
7	2.101049	-0.000064	-0.000211
6	2.705588	-1.039497	-0.645106
6	2.705890	1.039269	0.644558
6	4.045176	1.464745	0.552761
6	4.527845	2.570755	1.275867
6	3.721353	3.304709	2.125419
6	2.350091	2.96541	2.226889
6	1.833814	1.859486	1.475761
7	0.511110	1.550091	1.498774
6	-0.326269	2.249335	2.253754
6	0.098371	3.324532	3.058425
6	1.430749	3.681278	3.034047
6	1.833219	-1.859542	-1.476169
6	4.044811	-1.465216	-0.553539
6	4.527157	-2.571305	-1.276741
6	3.720386	-3.305100	-2.126165
6	2.349168	-2.965551	-2.227396
6	1.429559	-3.681243	-3.034406
1	4.727871	-0.955542	0.121695
1	5.577887	-2.847210	-1.160104
1	4.728030	0.954938	-0.122581
1	5.578605	2.846467	1.159047
1	4.114394	4.144713	2.700574
1	-0.624759	3.864366	3.670738
1	1.794883	4.523981	3.627118
1	-1.377911	1.952751	2.212673
1	4.113176	-4.145170	-2.701396
6	0.097242	-3.324255	-3.058551
7	0.510569	-1.549904	-1.498952
6	-0.327064	-2.248988	-2.253795
1	-1.378646	-1.952217	-2.212526
1	1.793439	-4.524007	-3.627549
1	-0.626092	-3.863951	-3.670745
30	0.000000	0.000139	0.000003
1	-1.793602	-4.523941	3.627555
1	0.625948	-3.863956	3.67077
6	-1.429692	-3.681189	3.034413
6	-0.097365	-3.32424	3.058569
1	-4.113320	-4.145039	2.701383
6	-3.720501	-3.304981	2.126153
6	-2.349274	-2.965472	2.227395
6	0.326979	-2.248987	2.253814
6	-4.527243	-2.571165	1.276721
1	1.378570	-1.952247	2.212552
6	-1.833287	-1.859480	1.476169
1	-5.57798	-2.847039	1.160076
7	-0.510628	-1.549880	1.498962
6	-4.044859	-1.465091	0.553521
6	-2.705625	-1.039410	0.645098
1	-4.728001	0.955093	0.122565
7	-2.101049	0.000004	0.000206
1	-4.727899	-0.955400	-0.121721
6	-4.045127	1.464877	-0.552774
6	-2.705854	1.039358	-0.644565
6	-4.527756	2.570904	-1.275881
1	-5.578508	2.846650	-1.159066
6	-1.833747	1.859549	-1.475761
7	-0.511053	1.550112	-1.498766
6	-3.721236	3.304833	-2.125429
6	-2.349984	2.965490	-2.22689
6	0.326353	2.249330	-2.253741
1	-4.114247	4.144850	-2.700584
6	-1.430615	3.681329	-3.034043
1	1.377986	1.952713	-2.212654
6	-0.098248	3.324541	-3.058413
1	-1.794719	4.524045	-3.627116
1	0.624903	3.864352	-3.670721

$Fe(BQA)_2$ (PBEPBE/ Def2TZVP, multiplicity = 1):

a.n.	X	Y	Z
7	-1.945946	-0.000217	0.000810
6	-2.534341	0.945365	-0.799694
6	-2.533304	-0.946121	0.801698
6	-3.885824	-1.305960	0.955721
6	-4.261811	-2.320030	1.854750
6	-3.340172	-3.006588	2.626705
6	-1.962048	-2.706881	2.493292
6	-1.569432	-1.691252	1.571482
7	-0.250504	-1.370669	1.361636
6	0.694268	-2.010967	2.061046
6	0.384723	-3.009631	3.000470
6	-0.931708	-3.362708	3.215948
6	-1.571345	1.690952	-1.570143
6	-3.887137	1.304558	-0.952812

6	-4.264186	2.318518	-1.851524
6	-3.343381	3.005614	-2.623997
6	-1.965023	2.706560	-2.491520
6	-0.935446	3.363061	-3.214648
1	-4.662520	0.830314	-0.360108
1	-5.325095	2.563942	-1.936927
1	-4.661815	-0.832098	0.363508
1	-5.322545	-2.565959	1.940859
1	-3.655293	-3.782049	3.326634
1	1.197287	-3.496131	3.541151
1	-1.195369	-4.143447	3.932560
1	1.724134	-1.719339	1.858080
1	-3.659337	3.781027	-3.323603
6	0.381298	3.010627	-3.000004
7	-0.252145	1.370886	-1.361262
6	0.691905	2.011864	-2.061040
1	1.722027	1.720616	-1.858816
1	-1.199923	4.143827	-3.930929
1	1.193293	3.497696	-3.541027
26	0.000001	0.000113	-0.000018
1	1.199286	4.143954	3.930977
1	-1.193833	3.497475	3.541063
6	0.934926	3.363151	3.214692
6	-0.381765	3.010526	3.000042
1	3.658747	3.781533	3.323650
6	3.342913	3.006076	2.624038
6	1.964603	2.706807	2.491562
6	-0.692221	2.011720	2.061073
6	4.263823	2.319136	1.851551
1	-1.722300	1.720321	1.858847
6	1.571076	1.691144	1.570180
1	5.324692	2.564732	1.936945
7	0.251924	1.370880	1.361301
6	3.886926	1.305127	0.952831
6	2.534187	0.945718	0.799720
1	4.661928	-0.831551	-0.363339
7	1.945946	0.000054	-0.000799
1	4.662374	0.831020	0.360103
6	3.886019	-1.305480	-0.955608
6	2.533454	-0.945775	-0.801665
6	4.262157	-2.319503	-1.854627
1	5.322920	-2.565331	-1.940675
6	1.569702	-1.691001	-1.571508
7	0.250732	-1.370554	-1.361724
6	3.340632	-3.006137	-2.626651
6	1.962470	-2.706571	-2.493318
6	-0.693939	-2.010916	-2.061215
1	3.655875	-3.781555	-3.326575
6	0.932235	-3.362475	-3.216054
1	-1.723844	-1.719392	-1.858298
6	-0.384241	-3.009521	-3.000651
1	1.196010	-4.143173	-3.932669
1	-1.196726	-3.496081	-3.541398

$Fe(BQA)_2$ (PBEPBE/ Def2TZVP, multiplicity = 3):

a.n.	X	Y	Z
7	-1.914733	0.000084	-0.000005
6	-2.507687	1.033923	-0.690253
6	-2.507785	-1.033700	0.690244
6	-3.854679	-1.446337	0.716532
6	-4.246369	-2.531891	1.516220
6	-3.343702	-3.237308	2.300351
6	-1.969818	-2.887539	2.279420
6	-1.563703	-1.795428	1.457326
7	-0.250586	-1.418648	1.344452
6	0.684920	-2.072802	2.051436
6	0.361781	-3.142679	2.896027
6	-0.956197	-3.557302	3.011855
6	-1.563535	1.795560	-1.457338
6	-3.854543	1.446685	-0.716541
6	-4.246136	2.532263	-1.516243
6	-3.343405	3.237588	-2.300383
6	-1.969552	2.887700	-2.279442
6	-0.955868	3.557373	-3.011874
1	-4.598020	0.956327	-0.093924
1	-5.297702	2.826773	-1.513666
1	-4.598115	-0.955900	0.093928
1	-5.297961	-2.826307	1.513638
1	-3.673095	-4.071404	2.922080
1	1.160490	-3.639656	3.447291
1	-1.225938	-4.396876	3.655561
1	1.712070	-1.731867	1.927555
1	-3.672723	4.071704	-2.922125
6	0.362074	3.142639	-2.896034
7	-0.250450	1.418669	-1.344452
6	0.685116	2.072740	-2.051434
1	1.712235	1.731714	-1.927546
1	-1.225533	4.396965	-3.655586
1	1.160829	3.639547	-3.447293
26	-0.000156	-0.000001	-0.000001
1	1.225838	4.396861	3.655501
1	-1.160640	3.639948	3.446701
6	0.956089	3.557395	3.011653
6	-0.361863	3.142963	2.895543

1	3.673055	4.071151	2.922622
6	3.343706	3.237178	2.300710
6	1.969795	2.887587	2.279351
6	-0.684971	2.073220	2.050685
6	4.246433	2.531622	1.516818
1	-1.712165	1.732551	1.926477
6	1.563734	1.795619	1.457061
1	5.298089	2.825817	1.514541
7	0.250568	1.419123	1.343791
6	3.854810	1.446107	0.717009
6	2.507883	1.033644	0.690232
1	4.598351	-0.955923	-0.094707
7	1.914921	-0.000082	0.000007
1	4.598437	0.955525	0.094752
6	3.854691	-1.446434	-0.716980
6	2.507798	-1.033859	-0.690212
6	4.246231	-2.531971	-1.516800
1	5.297864	-2.826251	-1.514521
6	1.563589	-1.795751	-1.457051
7	0.250452	-1.419152	-1.343782
6	3.343451	-3.237446	-2.300703
6	1.969567	-2.887748	-2.279343
6	-0.685136	-2.073177	-2.050676
1	3.672736	-4.071439	-2.922623
6	0.955809	-3.557478	-3.011645
1	-1.712303	-1.732424	-1.926469
6	-0.362111	-3.142945	-2.895533
1	1.225493	-4.396963	-3.655494
1	-1.160927	-3.639871	-3.446688

$Fe(BQA)_2$ (PBEPBE/ Def2TZVP, multiplicity = 5):

7	1.903933	0.000014	0.000070
6	2.504712	0.995653	0.745172
6	2.504797	-0.995595	-0.745006
6	3.861376	-1.403789	-0.764221
6	4.263037	-2.442308	-1.609119
6	3.362863	-3.108099	-2.439671
6	1.982238	-2.778329	-2.409015
6	1.567062	-1.732700	-1.532418
7	0.252556	-1.388035	-1.383943
6	-0.685985	-2.023715	-2.120428
6	-0.353672	-3.032375	-3.021581
6	0.977180	-3.423719	-3.170326
6	1.566900	1.732723	1.532528
6	3.861272	1.403904	0.764464
6	4.262842	2.442440	1.609386
6	3.362593	3.108190	2.439890
6	1.981985	2.778362	2.409155
6	0.976858	3.423703	3.170418
1	4.589126	0.950514	0.097788
1	5.312913	2.740957	1.609301
1	4.589173	-0.950369	-0.097503
1	5.313121	-2.740781	-1.608976
1	3.701922	-3.911135	-3.096396
1	-1.148300	-3.508985	-3.595953
1	1.253488	-4.223250	-3.859803
1	-1.717206	-1.708706	-1.968065
1	3.701583	3.911238	3.096637
6	-0.353968	3.032298	3.021602
7	0.252416	1.388006	1.383973
6	-0.686190	2.023635	2.120419
1	-1.717389	1.708584	1.968000
1	1.253095	4.223239	3.859917
1	-1.148648	3.508866	3.595939
26	0.000007	-0.000013	-0.000001
1	-1.253155	4.223297	-3.859830
1	1.148615	3.509031	-3.595795
6	-0.976903	3.423745	-3.170357
6	0.353937	3.032399	-3.021509
1	-3.701653	3.911148	-3.096651
6	-3.362649	3.108096	-2.439917
6	-1.982025	2.778326	-2.409155
6	0.686174	2.023691	-2.120380
6	-4.262895	2.442275	-1.609465
1	1.717379	1.708658	-1.967966
6	-1.566920	1.732674	-1.532554
1	-5.312984	2.740731	-1.609416
7	-0.252430	1.387969	-1.384011
6	-3.861300	1.403745	-0.764547
6	-2.504717	0.995581	-0.745209
1	-4.589178	-0.950252	0.097635
7	-1.903917	-0.000010	-0.000070
1	-4.589153	0.950290	-0.097909
6	-3.861369	-1.403720	0.764313
6	-2.504778	-0.995582	0.745046
6	-4.263029	-2.442243	1.609208
1	-5.313124	-2.740678	1.609104
6	-1.567037	-1.732690	1.532444
7	-0.252533	-1.388006	1.383978
6	-3.362838	-3.108085	2.439705
6	-1.982207	-2.778342	2.409016
6	0.686023	-2.023761	2.120379
1	-3.701893	-3.911134	3.096417
6	-0.977135	-3.423789	3.170260

1	1.717242	-1.708746	1.968019
6	0.353721	-3.032474	3.021478
1	-1.253439	-4.223343	3.859712
1	1.148361	-3.509133	3.595794

$Fe(BQA)_2$ (Blyp/def2tzvp, multiplicity = 1):

a.n.	X	Y	Z
7	1.976144	0.000238	0.001077
6	2.564582	-0.944778	-0.811054
6	2.563295	0.945608	0.813731
6	3.921299	1.298742	0.974215
6	4.307340	2.307858	1.880171
6	3.389076	2.999616	2.655392
6	2.004624	2.709782	2.520246
6	1.599686	1.697060	1.591150
7	0.269883	1.391777	1.386216
6	-0.666774	2.042677	2.093756
6	-0.343462	3.037267	3.038172
6	0.979966	3.374918	3.250362
6	1.602051	-1.696807	-1.589258
6	3.922920	-1.297146	-0.970410
6	4.310241	-2.306216	-1.875876
6	3.392989	-2.998706	-2.651642
6	2.008259	-2.709632	-2.517674
6	0.984529	-3.375698	-3.248243
1	4.694679	-0.820531	-0.380936
1	5.371151	-2.541107	-1.962469
1	4.693786	0.822641	0.385281
1	5.368045	2.543344	1.967642
1	3.709872	3.767781	3.357206
1	-1.146884	3.529828	3.582624
1	1.252873	4.148202	3.968012
1	-1.698575	1.765719	1.896743
1	3.714784	-3.766902	-3.352964
6	-0.339262	-3.038789	-3.037101
7	0.271929	-1.392067	-1.385570
6	-0.663850	-2.043919	-2.093427
1	-1.695947	-1.767358	-1.897389
1	1.258412	-4.149129	-3.965361
1	-1.141998	-3.532126	-3.581862
26	0.000039	-0.000157	-0.000014
1	-1.258258	-4.148670	3.965915
1	1.142142	-3.531625	3.582406
6	-0.984384	-3.375312	3.248714
6	0.339403	-3.038378	3.037569
1	-3.714634	-3.766603	3.353408
6	-3.392850	-2.998483	2.651999
6	-2.008123	-2.709371	2.518045
6	0.663980	-2.043596	2.093793
6	-4.310113	-2.306115	1.876125
1	1.696071	-1.767014	1.897756
6	-1.601917	-1.696643	1.589524
1	-5.371019	-2.541022	1.962722
7	-0.271805	-1.391856	1.385849
6	-3.922798	-1.297137	0.970554
6	-2.564468	-0.944774	0.811198
1	-4.693766	0.822226	-0.385210
7	-1.976089	0.000168	-0.001014
1	-4.694537	-0.820568	0.380996
6	-3.921352	1.298335	-0.974256
6	-2.563318	0.945337	-0.813798
6	-4.307497	2.307293	-1.880344
1	-5.368222	2.542694	-1.967806
6	-1.599785	1.696695	-1.591391
7	-0.269961	1.391467	-1.386494
6	-3.389306	2.998989	-2.655720
6	-2.004824	2.709246	-2.520622
6	0.666632	2.042272	-2.094211
1	-3.710184	3.767024	-3.357637
6	-0.980234	3.374295	-3.250911
1	1.698454	1.765371	-1.897233
6	0.343220	3.036703	-3.038763
1	-1.253212	4.147457	-3.968665
1	1.146590	3.529195	-3.583354

$Fe(BQA)_2$ (Olyp/def2tzvp, multiplicity = 1):

a.n.	X	Y	Z
7	1.951745	0.000028	-0.000147
6	2.540282	0.968757	0.770265
6	2.540191	-0.968682	-0.770656
6	3.888551	-1.360233	-0.875443
6	4.276887	-2.389369	-1.749163
6	3.370883	-3.063969	-2.546749
6	1.994886	-2.741029	-2.457292
6	1.586787	-1.713281	-1.553764
7	0.267324	-1.382324	-1.376919
6	-0.658648	-2.015217	-2.104424
6	-0.336072	-3.017710	-3.033428
6	0.979894	-3.388263	-3.207520
6	1.586941	1.713400	1.553412
6	3.888654	1.360293	0.874952
6	4.277042	2.389512	1.748555
6	3.371088	3.064216	2.546108
6	1.995081	2.741281	2.456764
6	0.980124	3.388667	3.206908

1	4.650671	0.902757	0.261110
1	5.331893	2.655532	1.793528
1	4.650599	-0.902751	-0.261598
1	5.331733	-2.655401	-1.794214
1	3.695624	-3.846003	-3.228388
1	-1.136710	-3.493226	-3.594174
1	1.251827	-4.173724	-3.909663
1	-1.688238	-1.721541	-1.938836
1	3.695873	3.846340	3.227623
6	-0.335857	3.018121	3.032901
7	0.267471	1.382383	1.376710
6	-0.658476	2.015450	2.104107
1	-1.688071	1.721720	1.938644
1	1.252091	4.174246	3.908905
1	-1.136474	3.493768	3.593566
26	0.000002	0.000009	-0.000013
1	-1.252649	4.174174	-3.908845
1	1.136002	3.493971	-3.593569
6	-0.980576	3.388603	-3.206878
6	0.335452	3.018209	-3.032907
1	-3.696379	3.845957	-3.227539
6	-3.371491	3.063851	-2.546052
6	-1.995445	2.741075	-2.456738
6	0.658204	2.015545	-2.104150
6	-4.277353	2.389015	-1.748504
1	1.687835	1.721926	-1.938715
6	-1.587167	1.713216	-1.553422
1	-5.332238	2.654908	-1.793456
7	-0.267656	1.382347	-1.376762
6	-3.888829	1.359819	-0.874936
6	-2.540407	0.968445	-0.770273
1	-4.650489	-0.903323	0.261621
7	-1.951748	-0.000238	0.000101
1	-4.650783	0.902169	-0.261101
6	-3.888379	-1.360700	0.875465
6	-2.540066	-0.968992	0.770651
6	-4.276578	-2.389867	1.749211
1	-5.331391	-2.656023	1.794285
6	-1.586562	-1.713456	1.553763
7	-0.267142	-1.382334	1.376898
6	-3.370479	-3.064348	2.546790
6	-1.994522	-2.741246	2.457305
6	0.658919	-2.015120	2.104386
1	-3.695115	-3.846414	3.228443
6	-0.979440	-3.388357	3.207517
1	1.688470	-1.721318	1.938787
6	0.336479	-3.017651	3.033397
1	-1.251267	-4.173848	3.909668
1	1.137185	-3.493072	3.594126

$Cr(BQA)_2$ (PBEPBE/def2tzvp, multiplicity = 3):

a.n.	X	Y	Z
7	2.007345	-0.000013	-0.000073
6	2.603639	-0.990009	-0.752463
6	2.603734	0.989936	0.752302
6	3.952659	1.378790	0.814735
6	4.364727	2.425424	1.660985
6	3.476092	3.116859	2.463231
6	2.095786	2.797743	2.409501
6	1.667405	1.750422	1.540884
7	0.336047	1.424688	1.400084
6	-0.576460	2.089377	2.127534
6	-0.226313	3.111454	3.020761
6	1.100772	3.473347	3.162511
6	1.667223	-1.750467	-1.540970
6	3.952542	-1.378928	-0.814975
6	4.364505	-2.425600	-1.661229
6	3.475786	-3.117010	-2.463403
6	2.095499	-2.797826	-2.409592
6	1.100405	-3.473399	-3.162525
1	4.696941	-0.902782	-0.184289
1	5.423827	-2.691035	-1.678191
1	4.696994	0.902626	0.183987
1	5.424063	2.690809	1.677886
1	3.815065	3.916430	3.123945
1	-1.013088	3.612723	3.585471
1	1.396842	4.276384	3.840391
1	-1.615535	1.793833	1.979726
1	3.814679	-3.916612	-3.124121
6	-0.226653	-3.111439	-3.020699
7	0.335889	-1.424668	-1.400090
6	-0.576695	-2.089327	-2.127470
1	-1.615747	-1.793731	-1.979604
1	1.396394	-4.276464	-3.840407
1	-1.013488	-3.612681	-3.585349
24	0.000000	0.000023	0.000004
1	-1.396540	-4.276424	3.840405
1	1.013362	-3.612710	3.585363
6	-1.100525	-3.473366	3.162526
6	0.226545	-3.111445	3.020708
1	-3.814811	-3.916502	3.124105
6	-3.475891	-3.116909	2.463390
6	-2.095594	-2.797765	2.409587
6	0.576621	-2.089342	2.127482

6	-4.364586	-2.425471	1.661212
1	1.615683	-1.793776	1.979622
6	-1.667284	-1.750416	1.540969
1	-5.423915	-2.690877	1.678168
7	-0.335940	-1.424656	1.400098
6	-3.952587	-1.378810	0.814963
6	-2.603673	-0.989929	0.752459
1	-4.696967	0.902771	-0.184002
7	-2.007346	0.000052	0.000077
1	-4.696969	-0.902642	0.184274
6	-3.952615	1.378912	-0.814746
6	-2.603701	0.990017	-0.752305
6	-4.364646	2.425556	-1.661000
1	-5.423974	2.690973	-1.677907
6	-1.667345	1.750474	-1.540883
7	-0.335997	1.424701	-1.400075
6	-3.475986	3.116964	-2.463241
6	-2.095690	2.797807	-2.409503
6	0.576534	2.089364	-2.127519
1	-3.814932	3.916545	-3.123958
6	-1.100652	3.473383	-3.162507
1	1.615599	1.793790	-1.979705
6	0.226422	3.111452	-3.020748
1	-1.396694	4.276429	-3.840388
1	1.013215	3.612699	-3.585452

$Cr(BQA)_2$ (PBEPBE/def2tzvp, multiplicity = 5):

a.n.	X	Y	Z
7	-2.000587	0.000009	-0.000018
6	-2.599815	1.005852	-0.731708
6	-2.599843	-1.005818	0.731670
6	-3.950468	-1.407032	0.757718
6	-4.374017	-2.463284	1.580813
6	-3.498060	-3.159739	2.399437
6	-2.120216	-2.833259	2.378643
6	-1.677155	-1.772797	1.528572
7	-0.348480	-1.452205	1.423146
6	0.562474	-2.113409	2.155081
6	0.201872	-3.141184	3.032965
6	-1.132026	-3.50646	3.142250
6	-1.677102	1.772819	-1.528592
6	-3.950433	1.407090	-0.757773
6	-4.373951	2.463355	-1.580866
6	-3.497970	3.159800	-2.399473
6	-2.120132	2.833295	-2.378662
6	-1.131918	3.506483	-3.142250
1	-4.680702	0.928166	-0.112176
1	-5.431123	2.737278	-1.569230
1	-4.680719	-0.928101	0.112106
1	-5.431194	-2.737188	1.569163
1	-3.847920	-3.968325	3.043093
1	0.976606	-3.646587	3.609836
1	-1.436476	-4.316794	3.808050
1	1.601057	-1.80909	2.021297
1	-3.847806	3.968397	-3.043128
6	0.201971	3.141183	-3.032948
7	-0.348434	1.452203	-1.423149
6	0.562542	2.113395	-2.155067
1	1.601118	1.809056	-2.021270
1	-1.436345	4.316828	-3.808048
1	0.976722	3.646576	-3.609805
24	0.000000	-0.000004	0.000001
1	1.436412	4.316808	3.808046
1	-0.976665	3.646588	3.609810
6	1.131973	3.506467	3.142250
6	-0.201922	3.141184	3.032953
1	3.847866	3.968344	3.043122
6	3.498018	3.159751	2.399469
6	2.120175	2.833264	2.378661
6	-0.562508	2.113399	2.155074
6	4.373988	2.463293	1.58086
1	-1.601088	1.809072	2.021282
6	1.677130	1.772794	1.528593
1	5.431164	2.737202	1.569222
7	0.348457	1.452193	1.423155
6	3.950454	1.407034	0.757768
6	2.599831	1.005814	0.731706
1	4.680707	-0.928163	-0.112116
7	2.000587	-0.000020	0.000018
1	4.680716	0.928100	0.11217
6	3.950448	-1.407086	-0.757725
6	2.599828	-1.005854	-0.731673
6	4.373980	-2.463343	-1.580821
1	5.431154	-2.737261	-1.569175
6	1.677127	-1.772821	-1.528573
7	0.348457	-1.452210	-1.423144
6	3.498012	-3.159788	-2.399442
6	2.120172	-2.833289	-2.378644
6	-0.562508	-2.113404	-2.155076
1	3.847859	-3.968379	-3.043098
6	1.131970	-3.506478	-3.142247
1	-1.601087	-1.809070	-2.02129
6	-0.201922	-3.141185	-3.032958
1	1.436409	-4.316818	-3.808046

1	-0.976664	-3.646579	-3.609826

$[Cr(BQA)_2]^+$ (PBEPBE/def2tzvp, multiplicity = 2):

a.n.	X	Y	Z
7	1.955333	0.000189	-0.000001
6	2.574804	-1.072026	-0.626413
6	2.574595	1.072522	0.626416
6	3.903726	1.498883	0.547430
6	4.337503	2.616633	1.289912
6	3.478420	3.326541	2.107473
6	2.108757	2.961179	2.181029
6	1.666615	1.846627	1.417127
7	0.348839	1.453901	1.378307
6	-0.538439	2.127859	2.125382
6	-0.174902	3.222211	2.926533
6	1.139898	3.647669	2.955598
6	1.666975	-1.846308	-1.417125
6	3.904017	-1.498131	-0.547422
6	4.338011	-2.615799	-1.289901
6	3.479067	-3.325874	-2.107462
6	2.109334	-2.960776	-2.181024
6	1.140609	-3.647456	-2.955593
1	4.611115	-0.994915	0.108184
1	5.382685	-2.920593	-1.210935
1	4.610924	0.995805	-0.108176
1	5.382118	2.921629	1.210949
1	3.834283	4.181207	2.684644
1	-0.944622	3.726098	3.511077
1	1.441003	4.504547	3.560697
1	-1.572896	1.787159	2.074660
1	3.835096	-4.180474	-2.684631
6	-0.174272	-3.222251	-2.926533
7	0.349124	-1.453836	-1.378311
6	-0.538023	-2.127967	-2.125387
1	-1.572545	-1.787464	-2.074669
1	1.441882	-4.504277	-3.560689
1	-0.943893	-3.726287	-3.511078
24	-0.000001	0.000000	-0.000003
1	-1.441006	-4.504548	3.560694
1	0.944618	-3.726098	3.511075
6	-1.139901	-3.647670	2.955596
6	0.174898	-3.222212	2.926531
1	-3.834284	-4.181212	2.684637
6	-3.478421	-3.326544	2.107468
6	-2.108759	-2.961180	2.181026
6	0.538436	-2.127860	2.125381
6	-4.337504	-2.616638	1.289904
1	1.572893	-1.787159	2.074659
6	-1.666618	-1.846627	1.417125
1	-5.382118	-2.921638	1.210938
7	-0.348843	-1.453901	1.378306
6	-3.903728	-1.498888	0.547423
6	-2.574598	-1.072522	0.626413
1	-4.611114	0.994932	0.108190
7	-1.955336	-0.000188	-0.000002
1	-4.610924	-0.995815	-0.108187
6	-3.904015	1.498142	-0.547420
6	-2.574804	1.072029	-0.626414
6	-4.338006	2.615810	-1.289900
1	-5.382678	2.920610	-1.210931
6	-1.666974	1.846308	-1.417128
7	-0.349123	1.453834	-1.378313
6	-3.479061	3.325880	-2.107465
6	-2.109330	2.960777	-2.181027
6	0.538025	2.127962	-2.125390
1	-3.835088	4.180480	-2.684633
6	-1.140604	3.647453	-2.955599
1	1.572547	1.787457	-2.074672
6	0.174277	3.222245	-2.926539
1	-1.441874	4.504274	-3.560695
1	0.943899	3.726279	-3.511084

$[Cr(BQA)_2]^+$ (PBEPBE/def2tzvp, multiplicity = 4):

a.n.	X	Y	Z
7	1.997990	0.000016	0.000091
6	2.601156	-0.99610	-0.746049
6	2.601035	0.996178	0.746266
6	3.944828	1.390911	0.791463
6	4.369418	2.440558	1.632546
6	3.493912	3.130091	2.447346
6	2.11509	2.805798	2.408795
6	1.676718	1.757538	1.545085
7	0.346633	1.441925	1.426506
6	-0.559651	2.098200	2.154669
6	-0.202354	3.119498	3.050533
6	1.126484	3.475067	3.171188
6	1.676948	-1.757507	-1.54495
6	3.944975	-1.390753	-0.791143
6	4.369695	-2.440367	-1.632202
6	3.494293	-3.129947	-2.447076
6	2.115450	-2.805737	-2.40863
6	1.126941	-3.475064	-3.1711
1	4.685001	-0.91646	-0.15361
1	5.428448	-2.705121	-1.632471

1	4.684932	0.916654	0.153995
1	5.428155	2.705375	1.632896
1	3.840761	3.928734	3.10394
1	-0.979638	3.621002	3.626479
1	1.429739	4.276812	3.847808
1	-1.600316	1.803856	2.012931
1	3.841242	-3.928566	-3.103647
6	-0.201928	-3.119576	-3.050545
7	0.346835	-1.44197	-1.426476
6	-0.559355	-2.0983	-2.154709
1	-1.600047	-1.804016	-2.013052
1	1.430297	-4.276788	-3.847699
1	-0.979137	-3.621128	-3.62655
24	0.000001	-0.00003	-0.000007
1	-1.430187	-4.276802	3.847714
1	0.979231	-3.621085	3.626558
6	-1.126852	-3.475074	3.17111
6	0.202009	-3.119555	3.05055
1	-3.841142	-3.928641	3.103663
6	-3.494213	-3.130018	2.447086
6	-2.115377	-2.805776	2.408637
6	0.559410	-2.098276	2.154707
6	-4.369632	-2.440463	1.63221
1	1.600096	-1.803967	2.013047
6	-1.676901	-1.757541	1.54495
1	-5.428379	-2.705242	1.632483
7	-0.346796	-1.441972	1.426472
6	-3.944939	-1.390845	0.791144
6	-2.601129	-0.996161	0.746046
1	-4.684956	0.916529	-0.154003
7	-1.997988	-0.000036	-0.000102
1	-4.684976	-0.916572	0.153609
6	-3.944864	1.390811	-0.791466
6	-2.601061	0.996114	-0.746271
6	-4.369482	2.440450	-1.632544
1	-5.428226	2.705238	-1.632893
6	-1.676764	1.757502	-1.545088
7	-0.34667	1.441922	-1.426511
6	-3.493994	3.130012	-2.447341
6	-2.115164	2.805754	-2.408792
6	0.559597	2.098225	-2.154672
1	-3.840865	3.928649	-3.103930
6	-1.126575	3.475053	-3.171182
1	1.600269	1.803907	-2.012936
6	0.202272	3.119518	-3.050529
1	-1.429852	4.276794	-3.847797
1	0.979543	3.621046	-3.626474

$Mn(BQA)_2$ (PBEPBE/def2tzvp, multiplicity = 2):

a.n.	X	Y	Z
7	1.965265	0.000000	0.000040
6	2.562241	0.971981	0.772001
6	2.562286	-0.971964	-0.771908
6	3.91165	-1.356810	-0.861968
6	4.306195	-2.387369	-1.734984
6	3.404368	-3.056488	-2.544015
6	2.026785	-2.731609	-2.470051
6	1.615304	-1.714550	-1.559799
7	0.292449	-1.378850	-1.390152
6	-0.633414	-1.989889	-2.145445
6	-0.300435	-2.975631	-3.087624
6	1.017296	-3.359648	-3.245600
6	1.615217	1.714558	1.559850
6	3.911596	1.356850	0.862109
6	4.306090	2.387424	1.735129
6	3.404222	3.056536	2.544121
6	2.026646	2.731633	2.470109
6	1.017118	3.359662	3.245614
1	4.667912	0.889900	0.238903
1	5.364109	2.655620	1.773784
1	4.667935	-0.889855	-0.238728
1	5.364219	-2.655548	-1.773601
1	3.733885	-3.839191	-3.229216
1	-1.097393	-3.436046	-3.672611
1	1.295922	-4.139472	-3.957173
1	-1.666986	-1.688368	-1.977465
1	3.733700	3.839251	3.229327
6	-0.300601	2.975622	3.087594
7	0.292373	1.378835	1.390157
6	-0.633528	1.989864	2.145411
1	-1.667089	1.688324	1.977396
1	1.295705	4.139498	3.957191
1	-1.097588	3.436028	3.672547
25	-0.000001	-0.000012	-0.000002
1	-1.295740	4.139497	-3.957183
1	1.097558	3.436044	-3.672543
6	-1.017148	3.359661	-3.245608
6	0.300574	2.97563	-3.087591
1	-3.733731	3.839232	-3.229316
6	-3.404247	3.056517	-2.544113
6	-2.026670	2.731623	-2.470104
6	0.633509	1.989872	-2.145411
6	-4.306110	2.387397	-1.735123
1	1.667073	1.688339	-1.977399

6	-1.615232	1.714549	-1.559849
1	-5.364130	2.655586	-1.773775
7	-0.292386	1.378834	-1.390158
6	-3.911607	1.356824	-0.862105
6	-2.562250	0.971963	-0.772001
1	-4.667928	-0.889898	0.238726
7	-1.965266	-0.000017	-0.000043
1	-4.667920	0.889868	-0.238900
6	-3.911639	-1.356845	0.861966
6	-2.562278	-0.971986	0.771906
6	-4.306174	-2.387407	1.734983
1	-5.364196	-2.655596	1.773600
6	-1.615289	-1.714564	1.559797
7	-0.292437	-1.378852	1.390149
6	-3.404341	-3.056518	2.544014
6	-2.026760	-2.731627	2.470050
6	0.633432	-1.989884	2.145441
1	-3.733850	-3.839224	3.229215
6	-1.017266	-3.359657	3.245597
1	1.667002	-1.688354	1.977460
6	0.300463	-2.97563	3.087621
1	-1.295884	-4.139484	3.957171
1	1.097425	-3.436038	3.672607

$Mn(BQA)_2$ (PBEPBE/def2tzvp, multiplicity = 4):

a.n.	X	Y	Z
7	1.943118	0.000018	0.000143
6	2.542736	0.995730	0.751596
6	2.542910	-0.995622	-0.751266
6	3.892277	-1.391086	-0.799903
6	4.297380	-2.435033	-1.649625
6	3.403843	-3.115923	-2.461625
6	2.024307	-2.790457	-2.413527
6	1.606669	-1.743804	-1.539576
7	0.284326	-1.409293	-1.389452
6	-0.645764	-2.054967	-2.114832
6	-0.308283	-3.071085	-3.015696
6	1.018165	-3.448396	-3.165931
6	1.606337	1.743855	1.539773
6	3.892065	1.391302	0.800393
6	4.296979	2.435300	1.650141
6	3.403288	3.116136	2.462017
6	2.023784	2.790556	2.413756
6	1.017499	3.448427	3.166029
1	4.633868	0.922315	0.160934
1	5.353462	2.711192	1.664753
1	4.633963	-0.922058	-0.160338
1	5.353886	-2.710841	-1.664112
1	3.741605	-3.914753	-3.123792
1	-1.102212	-3.560158	-3.580697
1	1.299837	-4.250358	-3.850953
1	-1.679765	-1.749611	-1.957328
1	3.740904	3.915005	3.124209
6	-0.308899	3.071002	3.015644
7	0.284038	1.409236	1.389493
6	-0.646190	2.054843	2.114754
1	-1.680148	1.749402	1.957132
1	1.299024	4.250424	3.851071
1	-1.102936	3.560017	3.580544
25	-0.000002	-0.000039	-0.000003
1	-1.299178	4.250401	-3.851048
1	1.102806	3.560074	-3.580528
6	-1.017625	3.448407	-3.166013
6	0.308786	3.071026	-3.015632
1	-3.741045	3.914895	-3.124188
6	-3.403402	3.116031	-2.462002
6	-2.023888	2.790496	-2.413746
6	0.646111	2.054869	-2.114753
6	-4.297069	2.435162	-1.650128
1	1.680079	1.749460	-1.957137
6	-1.606405	1.743802	-1.539771
1	-5.353561	2.711020	-1.664736
7	-0.284095	1.409224	-1.389498
6	-3.892119	1.391173	-0.800386
6	-2.542777	0.995643	-0.751593
1	-4.633936	-0.922226	0.160356
7	-1.943123	-0.000051	-0.000144
1	-4.633906	0.922163	-0.160927
6	-3.892229	-1.391226	0.799916
6	-2.542876	-0.995712	0.751270
6	-4.297289	-2.435189	1.649638
1	-5.353786	-2.711034	1.664131
6	-1.606605	-1.743863	1.539574
7	-0.284273	-1.409304	1.389445
6	-3.403724	-3.116050	2.461629
6	-2.024199	-2.790536	2.413521
6	0.645844	-2.054956	2.114808
1	-3.741452	-3.914896	3.123793
6	-1.018029	-3.448449	3.165911
1	1.679834	-1.749563	1.957300
6	0.308405	-3.071094	3.015665
1	-1.299670	-4.250426	3.850929
1	1.102356	-3.560148	3.580653

$Mn(BQA)_2$ (PBEPBE/def2tzvp, multiplicity = 6):

a.n.	X	Y	Z
7	2.175426	-0.001795	-0.001064
6	2.793718	-1.058798	-0.609796
6	2.796756	1.053837	0.606947
6	4.128767	1.485720	0.460135
6	4.625145	2.610935	1.142713
6	3.839572	3.356221	2.003085
6	2.475413	3.008117	2.157335
6	1.946486	1.882408	1.446119
7	0.624907	1.559733	1.512128
6	-0.192857	2.270626	2.281939
6	0.248002	3.363914	3.051705
6	1.575731	3.732269	2.979008
6	1.940635	-1.885535	-1.447922
6	4.124957	-1.493574	-0.464575
6	4.618078	-2.619859	-1.147755
6	3.829862	-3.363423	-2.007193
6	2.466271	-3.012370	-2.159788
6	1.564033	-3.734572	-2.980374
1	4.790277	-0.970889	0.219373
1	5.661633	-2.904078	-0.992836
1	4.792126	0.961588	-0.224607
1	5.669127	2.892892	0.986539
1	4.243734	4.211558	2.547072
1	-0.460969	3.909280	3.675644
1	1.949848	4.590011	3.543584
1	-1.243582	1.967571	2.280615
1	4.231516	-4.219623	-2.551680
6	0.237008	-3.363371	-3.051426
7	0.619673	-1.560032	-1.512291
6	-0.200563	-2.269162	-2.281092
1	-1.250640	-1.963885	-2.278415
1	1.935617	-4.593099	-3.545427
1	-0.473897	-3.907208	-3.674499
25	0.000002	0.000667	0.000203
1	-1.943709	-4.589821	3.545606
1	0.466683	-3.907246	3.675837
6	-1.570664	-3.731830	2.980700
6	-0.243163	-3.362458	3.052389
1	-4.238617	-4.213182	2.550758
6	-3.835511	-3.357569	2.006422
6	-2.471502	-3.008415	2.159645
6	0.196295	-2.268883	2.282226
6	-4.622286	-2.612937	1.146589
1	1.246793	-1.965049	2.280068
6	-1.943956	-1.882347	1.447977
1	-5.666168	-2.895698	0.991200
7	-0.622579	-1.558657	1.512987
6	-4.127267	-1.487379	0.463583
6	-2.795484	-1.054472	0.609393
1	-4.790866	0.968656	0.223273
7	-2.175421	0.001611	0.000862
1	-4.791534	-0.963788	-0.220695
6	-4.126456	1.491899	-0.461131
6	-2.794983	1.058159	-0.607354
6	-4.620943	2.617842	-1.143879
1	-5.664603	2.901247	-0.988176
6	-1.943162	1.885598	-1.446067
7	-0.621995	1.561113	-1.511441
6	-3.833932	3.362073	-2.003849
6	-2.470186	3.012079	-2.157473
6	0.197128	2.270920	-2.280811
1	-4.236645	4.217999	-2.547982
6	-1.569106	3.735029	-2.978674
1	1.247435	1.966423	-2.278974
6	-0.241850	3.364849	-3.050739
1	-1.941767	4.593311	-3.543390
1	0.468178	3.909272	-3.674300

Table S2 Absolute energies (a.u.) computed with method/Def2TZVP.

Molecule	Multiplicity	Method	Absolute energy
$Zn(BQA)_2$	1	PBEPBE	-3492.5578851
$Cr(BQA)_2$	1	PBEPBE	Did not converge
$Cr(BQA)_2$	3	PBEPBE	-2757.7576040
$Cr(BQA)_2$	5	PBEPBE	-2757.7346991
$[Cr(BQA)_2]^+$	2	PBEPBE	-2757.5661227
$[Cr(BQA)_2]^+$	4	PBEPBE	-2757.5883125
$Mn(BQA)_2$	2	PBEPBE	-2864.2641805
$Mn(BQA)_2$	4	PBEPBE	-2864.2397968
$Mn(BQA)_2$	6	PBEPBE	-2864.2369049
$Fe(BQA)_2$	1	PBEPBE	-2976.9923581
$Fe(BQA)_2$	3	PBEPBE	-2976.9532000
$Fe(BQA)_2$	5	PBEPBE	-2976.9038425
$Fe(BQA)_2$	1	BLYP	-2978.7464030
$Fe(BQA)_2$	1	OLYP	-2978.9492766

Table S3 Average metal to nitrogen bond length in the complexes as determined by XRD and computed at PBEPBE/Def2TZVP.

	Av. Len. M – N_{amide} / Å		Av. Len. M - $N_{quinolinyl}$ / Å	
Molecule	XRD	Calc.	XRD	Calc.
$Zn(BQA)_2$	2.07	2.10	2.18	2.22
$Cr(BQA)_2$[a]	1.98	2.01	2.04	2.03
$Mn(BQA)_2$[b]	2.17	2.18	2.24	2.26
$Fe(BQA)_2$	1.93	1.95	1.94	1.95

[a] Multiplicity for the calculation was set to 3

[b] Multiplicity for the calculation was set to 6

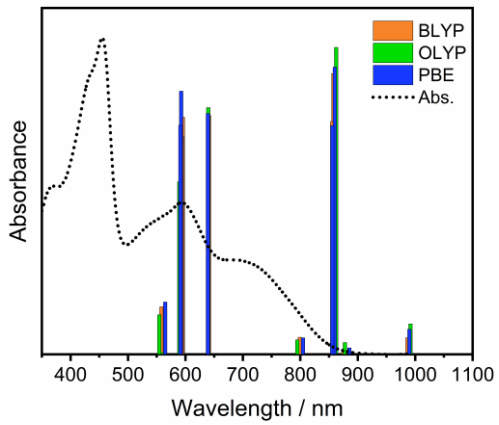

Fig. S1 Calculated absorbance for $Fe(BQA)_2$ in vacuo by different functionals and a Def2TZVP basis set compared to the experimental spectrum in solution.

Supplementary Measurement Data

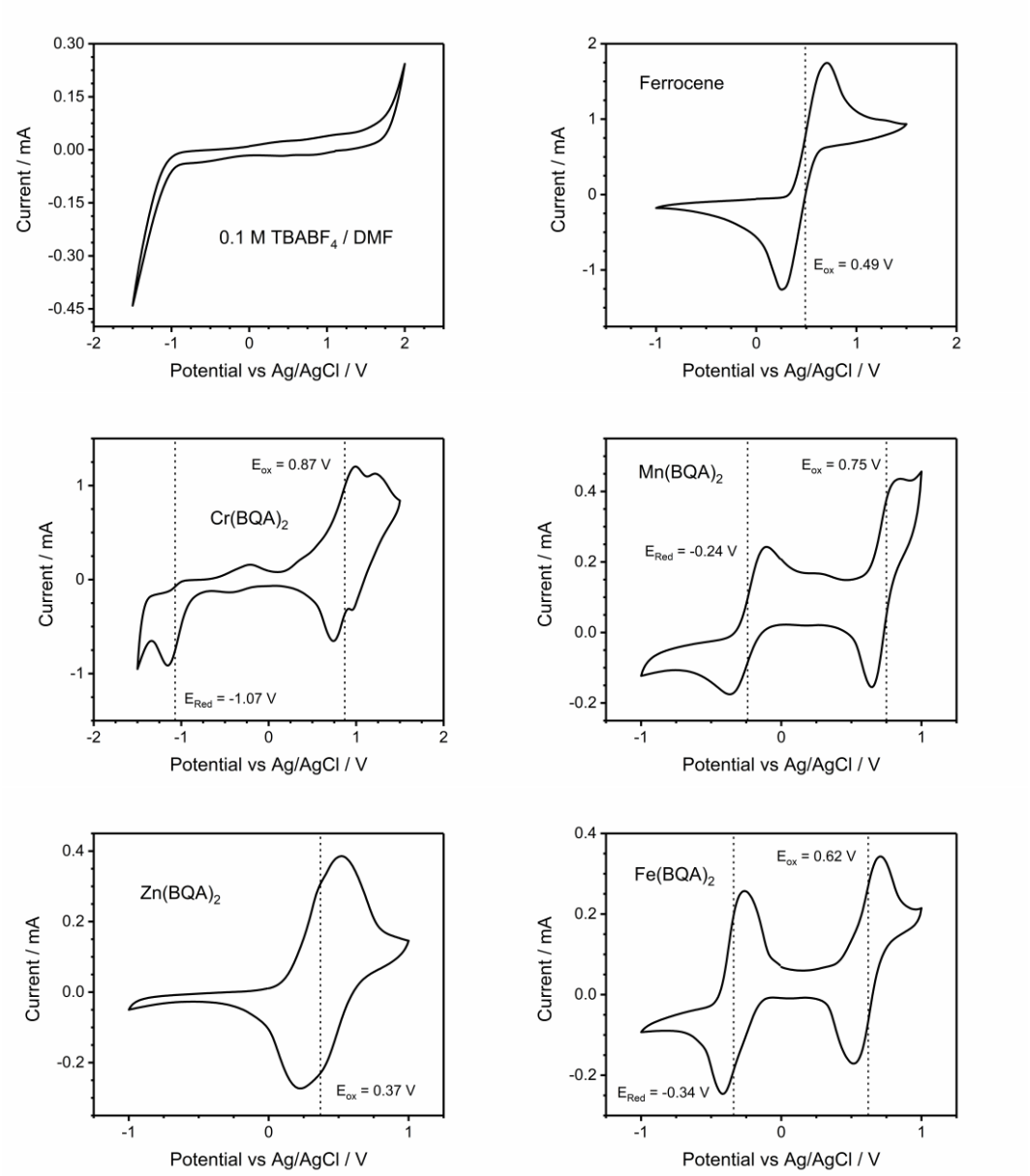

Fig. S2 Cyclic voltammograms of all complexes in this study, the DMF/$TBABF_4$ electrolyte background and the external ferrocene reference.

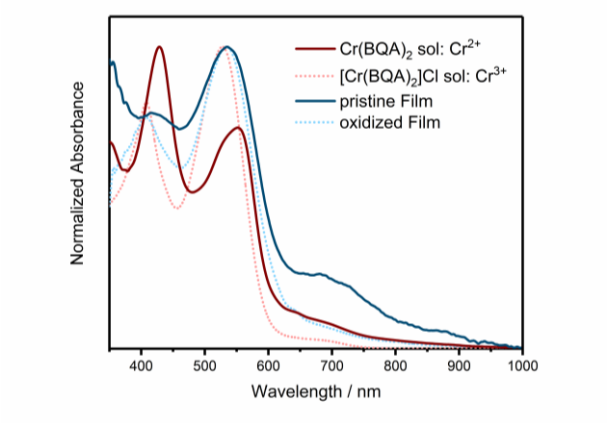

Fig. S3 Investigation on the oxidation state of the $Cr(BQA)_2$ powder. $[Cr(BQA)_2]Cl$ was explicitly synthesized to compare to $Cr(BQA)_2$. The absorbance of a 20 nm thick film of $Cr(BQA)_2$ is also given. The film was then left at air for a week, leading to (partial) oxidation seen in a significant decrease of the absorbance above 600 nm.

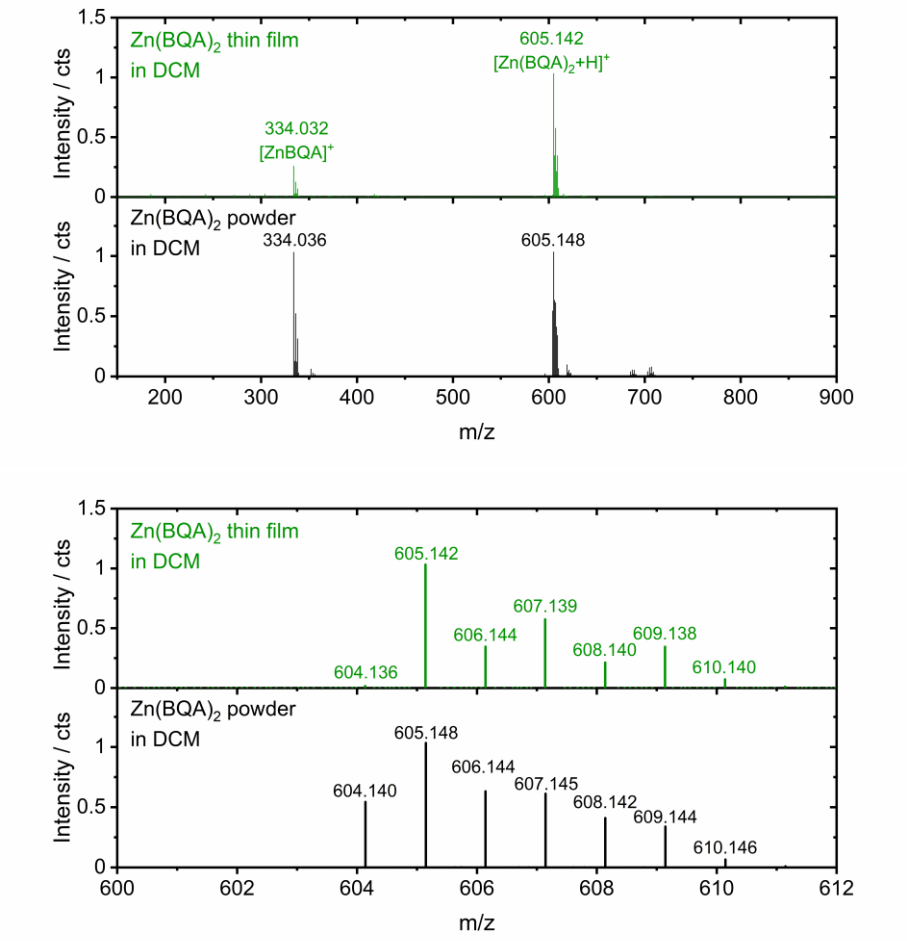

Fig. S4 Electrospray ionization mass spectra following dissolution of a vapour-deposited $Zn(BQA)_2$ thin film in DCM and the respective source material as powder. The bottom graph shows a limited m/z range. The evaporation source was filled at air.

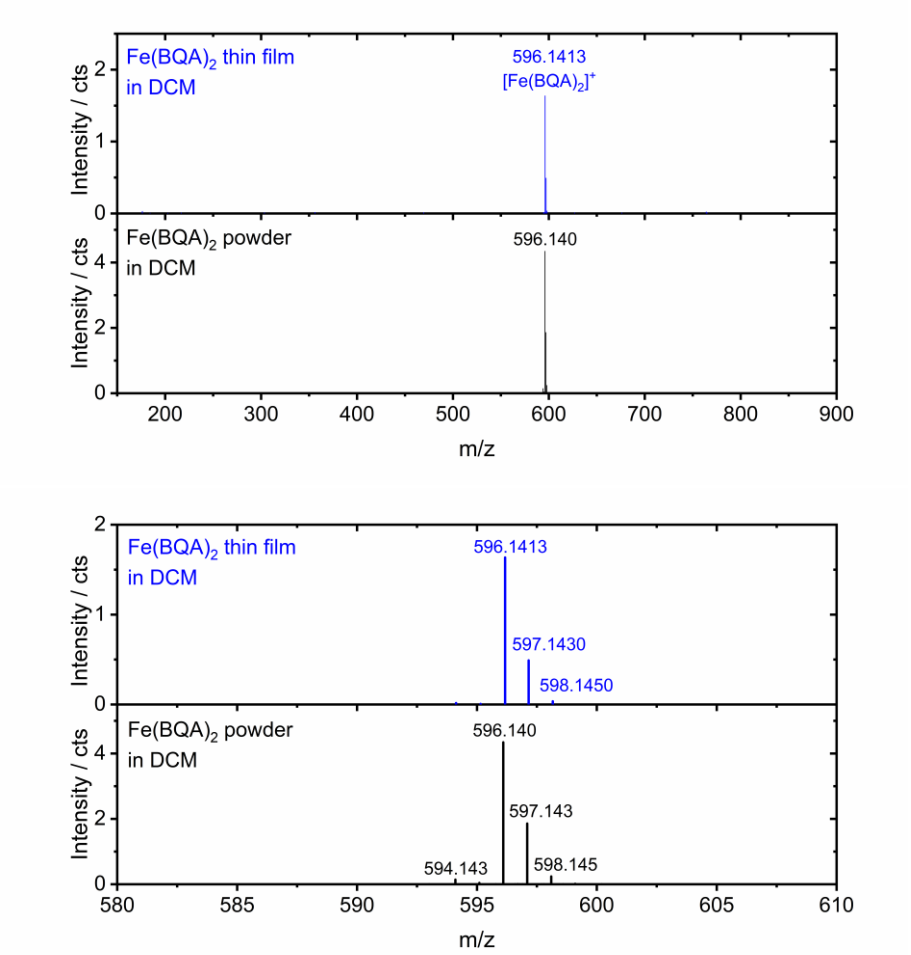

Fig. S5 Electrospray ionization mass spectra from solutions in DCM of a vapour-deposited $Fe(BQA)_2$ thin film and the respective source material as powder. The bottom graph shows a limited m/z range. The evaporation source was filled at air.

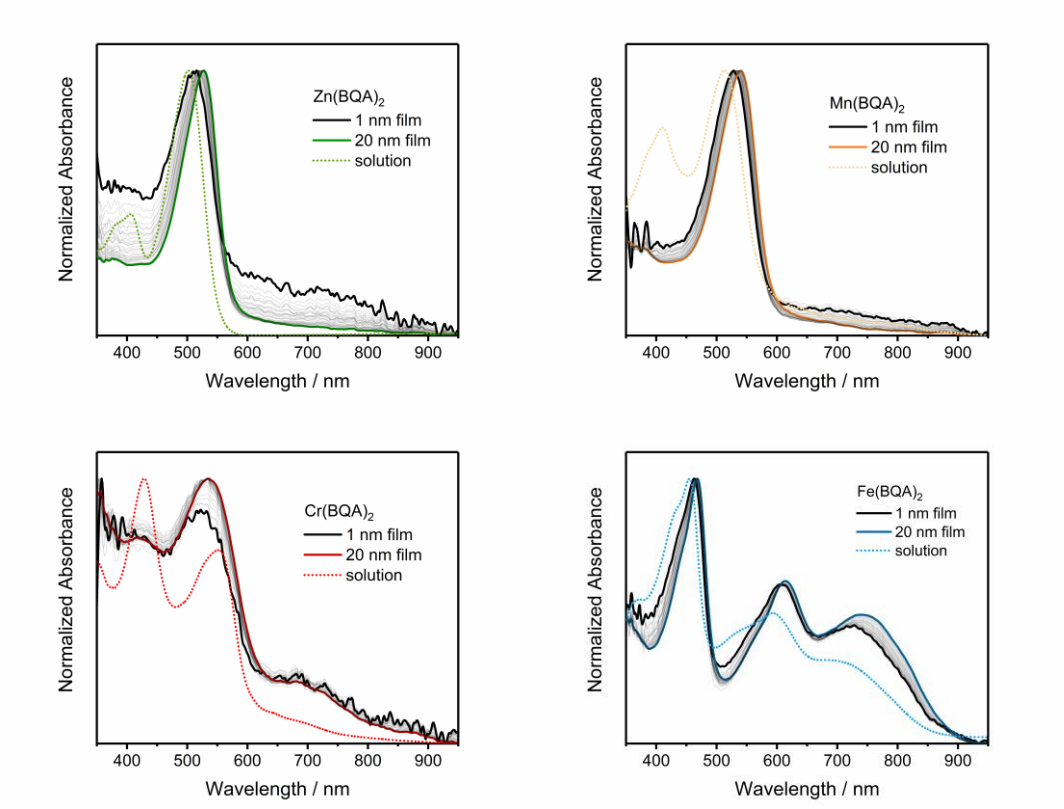

Fig. S6 Optical absorbance of thin films dependent on film thickness. The absorbance of the source material in DMF solution is also shown.

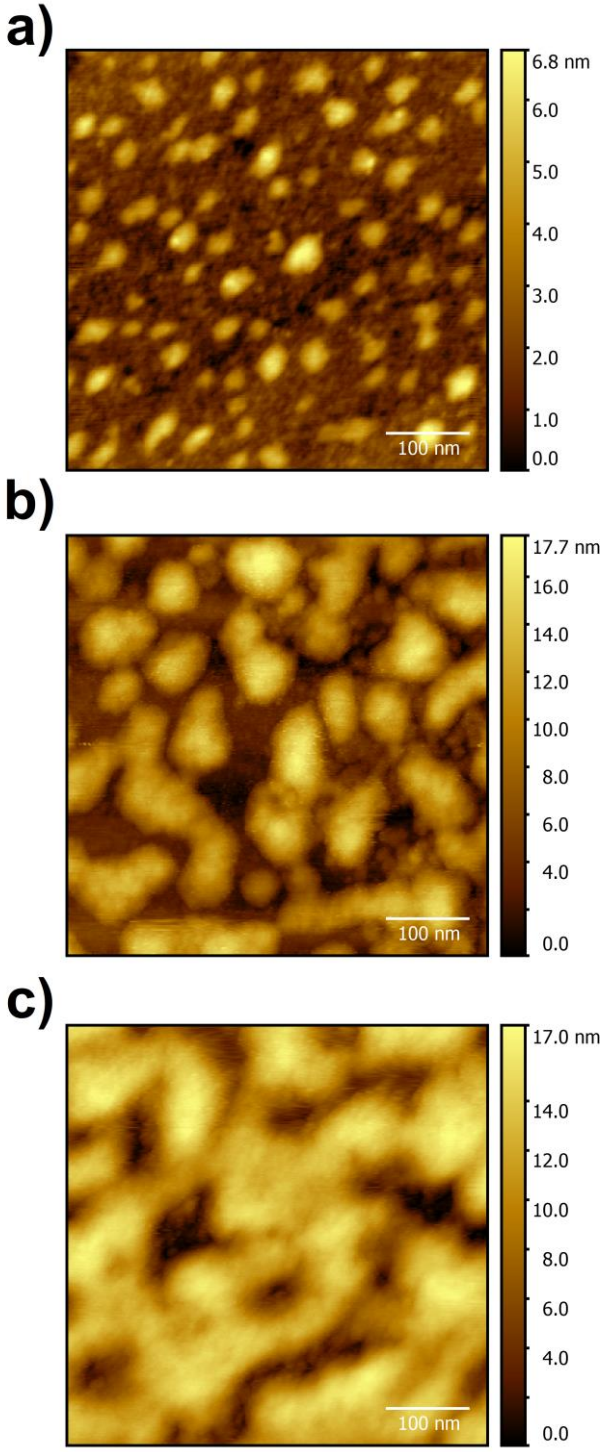

Fig. S7 AFM images of a) 1 nm b) 5 nm and c) 12 nm $Fe(BQA)_2$ vapor-deposited on quartz glass.

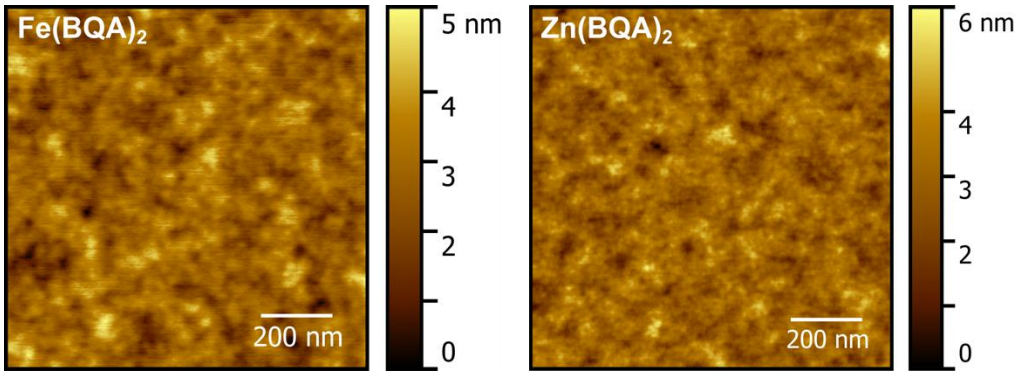

Fig. S8 AFM images of $Fe(BQA)_2$ and $Zn(BQA)_2$ deposited on SiO_2 coated silicon wafers. The film thickness of $Zn(BQA)_2$ was 72 nm and its evaporation source was filled at air.

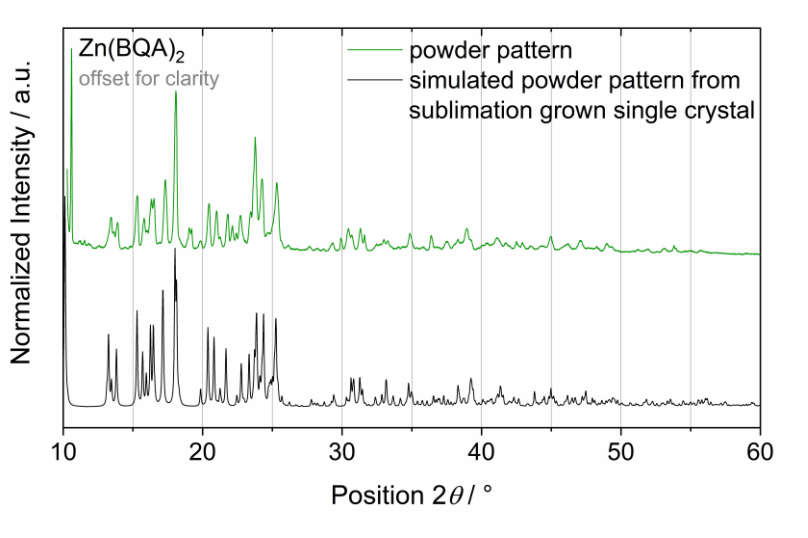

Fig. S9 Powder XRD pattern of $Zn(BQA)_2$ source material. A reference pattern simulated from the single crystal XRD data is shown to prove the identity of the solid state structures.

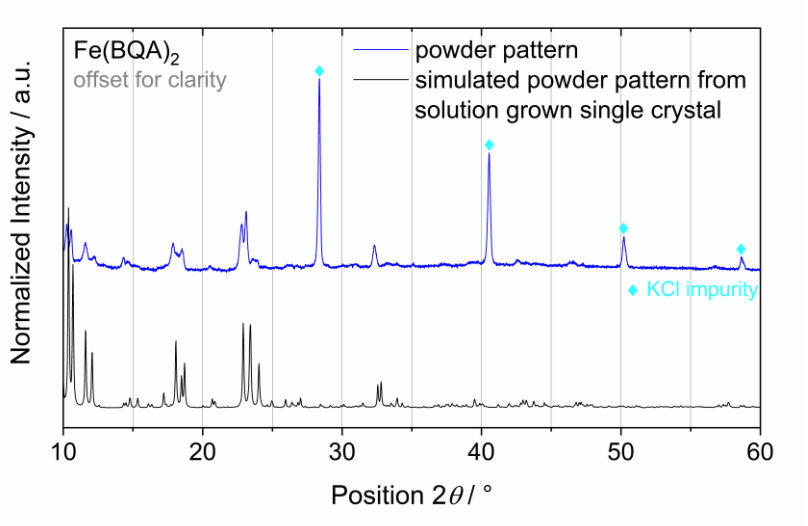

Fig. S10 Powder XRD pattern of $Fe(BQA)_2$ source material. A reference pattern simulated from single crystal XRD data is shown to prove the identity of the solid state structures.

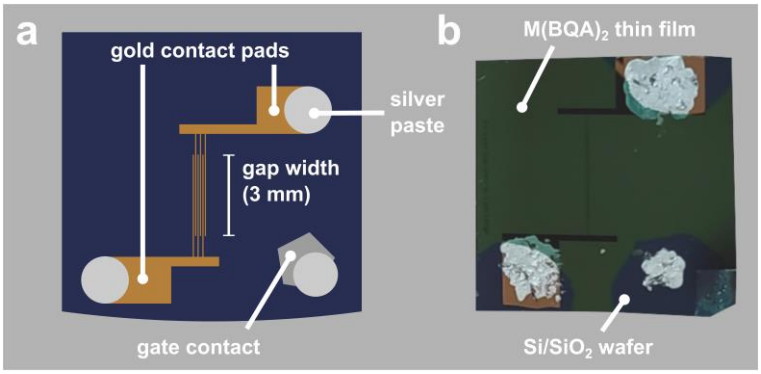

Fig. S11 Sample structure for electrical characterisation in bottom-gate bottom-contact field-effect transistor geometry. (a) Scheme and (b) Photography.

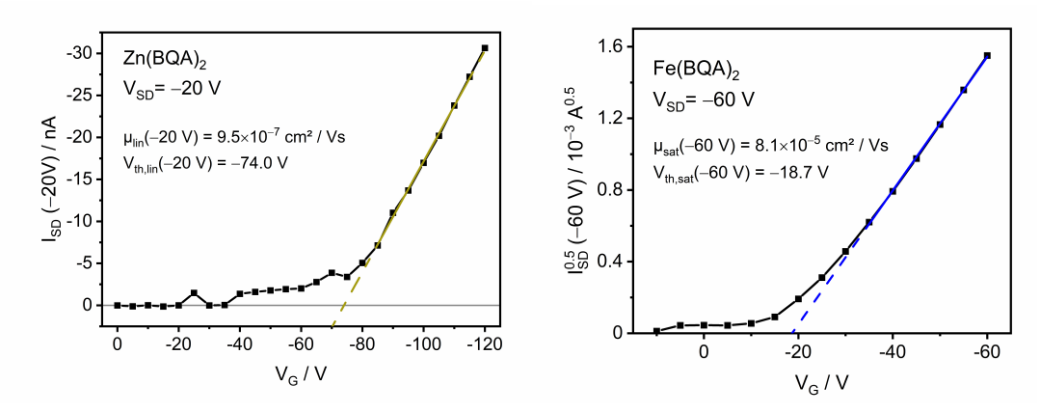

Fig. S12 Transfer curves of thin films of $Zn(BQA)_2$ (d=88 nm) and $Fe(BQA)_2$.

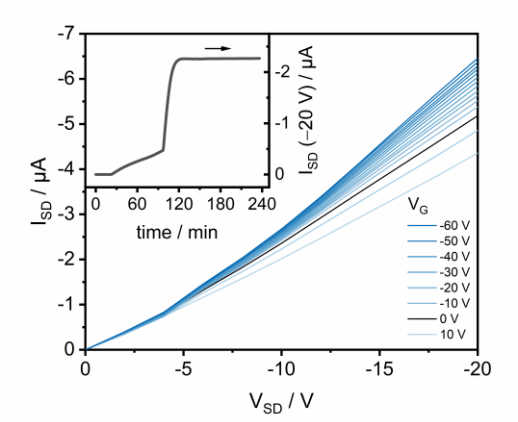

Fig. S13 Output characteristics of a $Fe(BQA)_2$ thin film at air after several hours. Inset: Current evolution during venting.

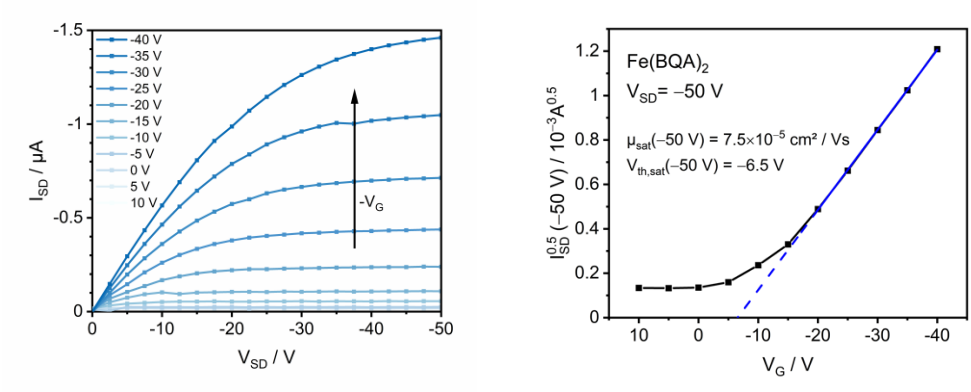

Fig. S14 Output and transfer characteristics of an $Fe(BQA)_2$ thin film (10 µm channel length and 30 mm channel width). The evaporation source was filled at air.

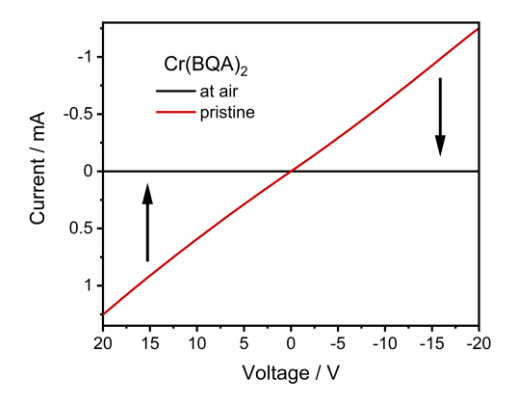

Fig. S15 Current supported by a $Cr(BQA)_2$ thin film in between interdigitated electrodes. Film thickness was 69 nm. After venting the preparation chamber, the current falls below the detection limit, as indicated by the arrows.

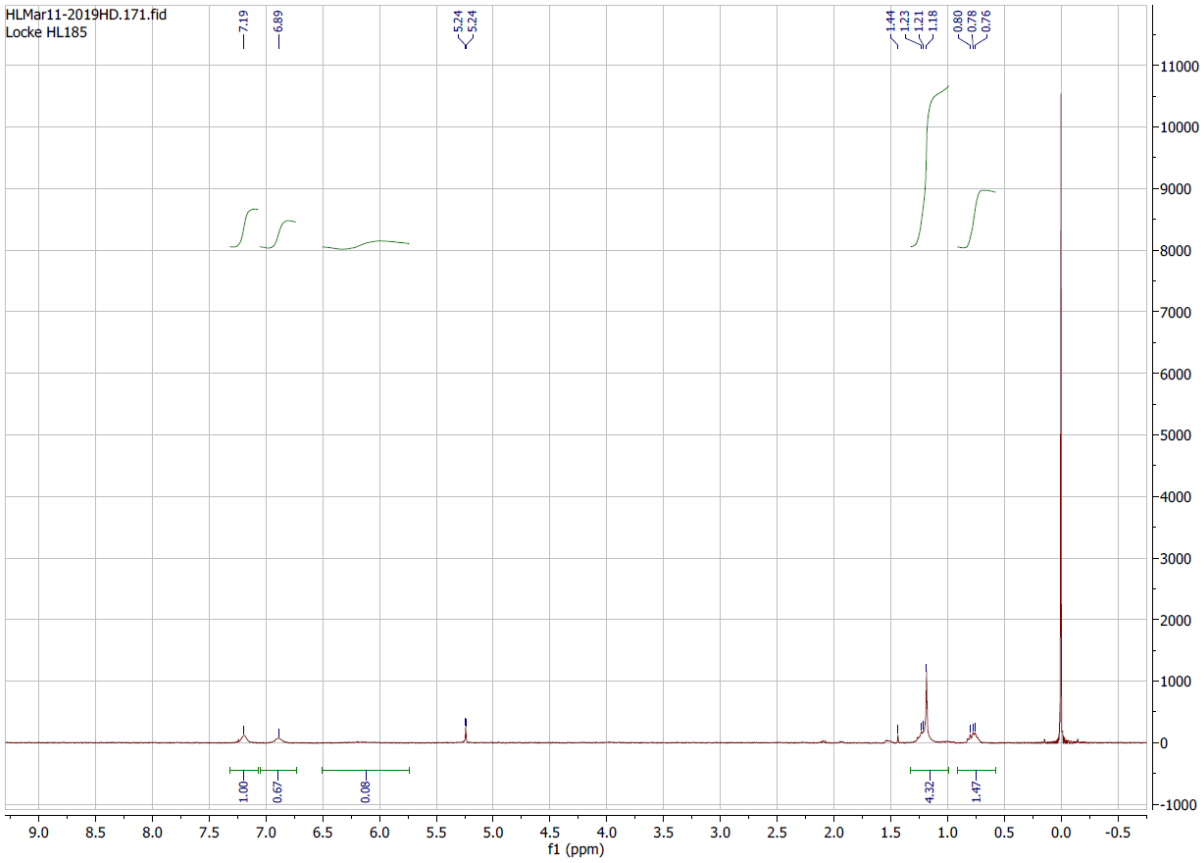

Fig. S16 ^{1}H-NMR (CD_2Cl_2) spectrum of $Fe(BQA)_2$

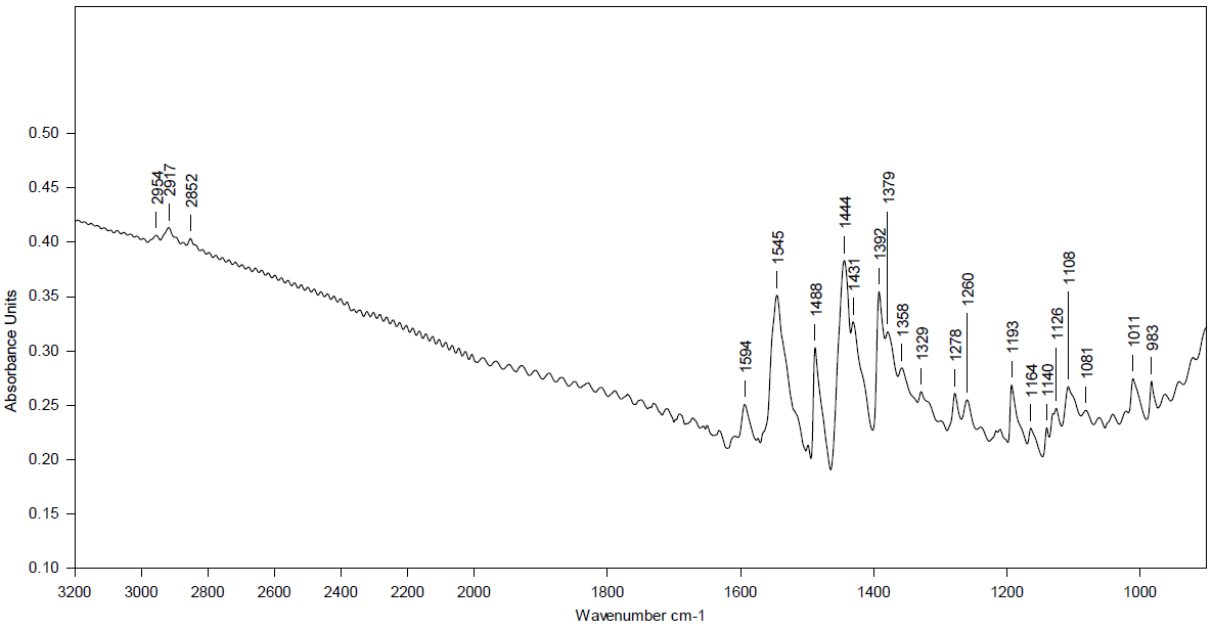

Fig. S17 IR spectrum of $Fe(BQA)_2$

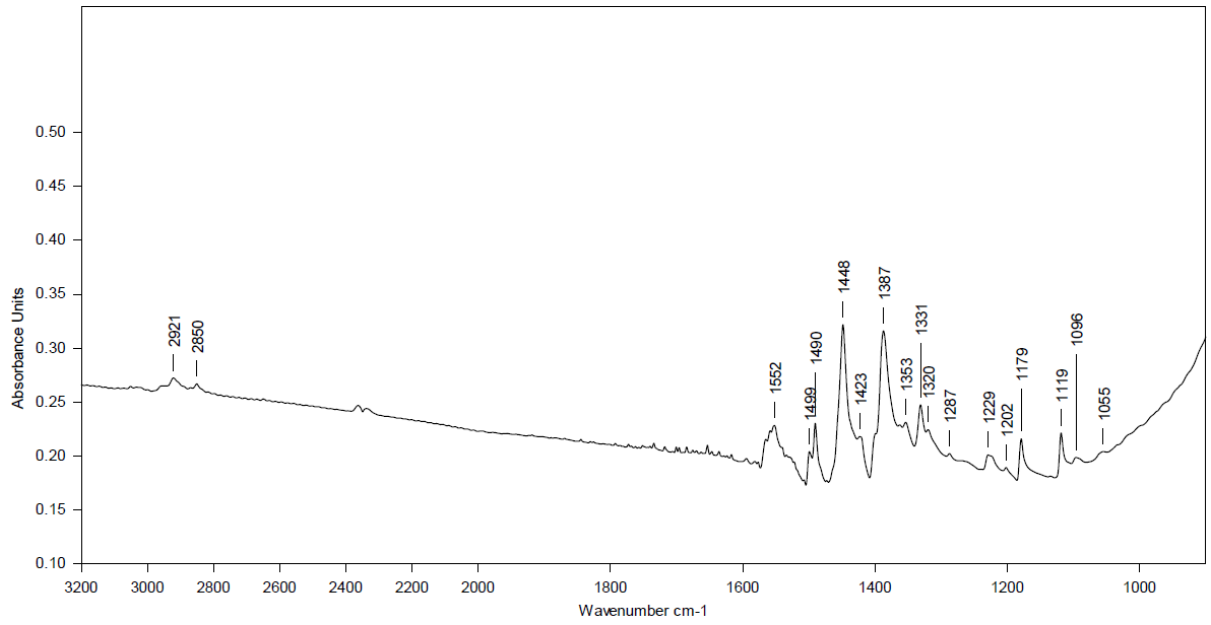

Fig. S18 IR spectrum of $Mn(BQA)_2$

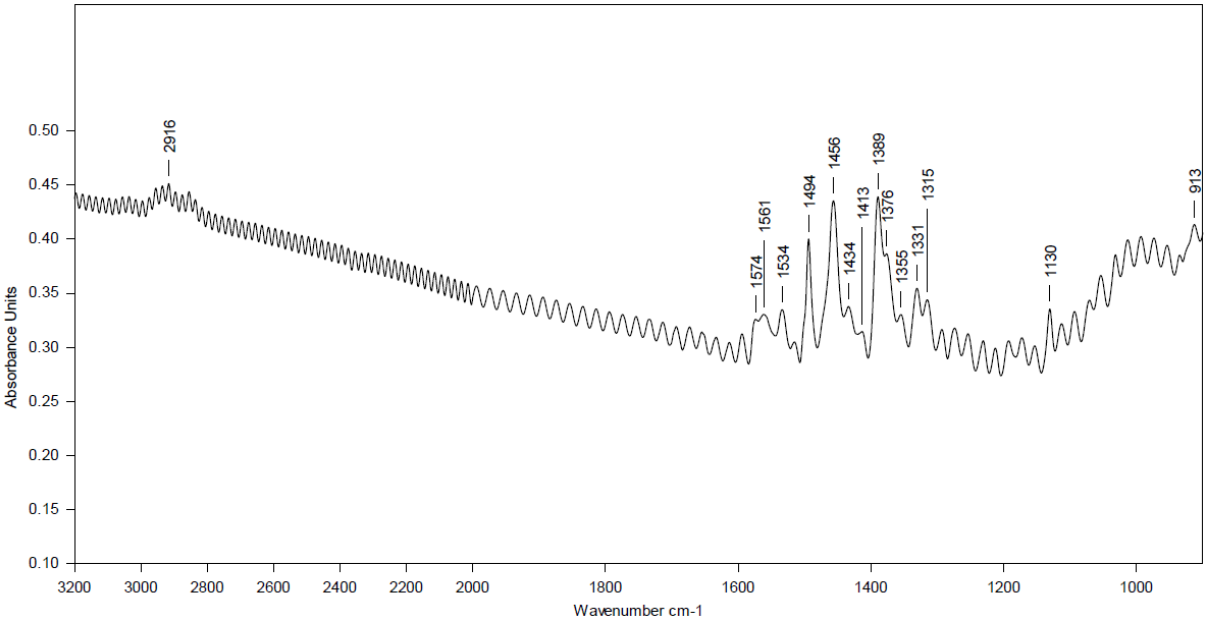

Fig. S19 IR spectrum of $Cr(BQA)_2$

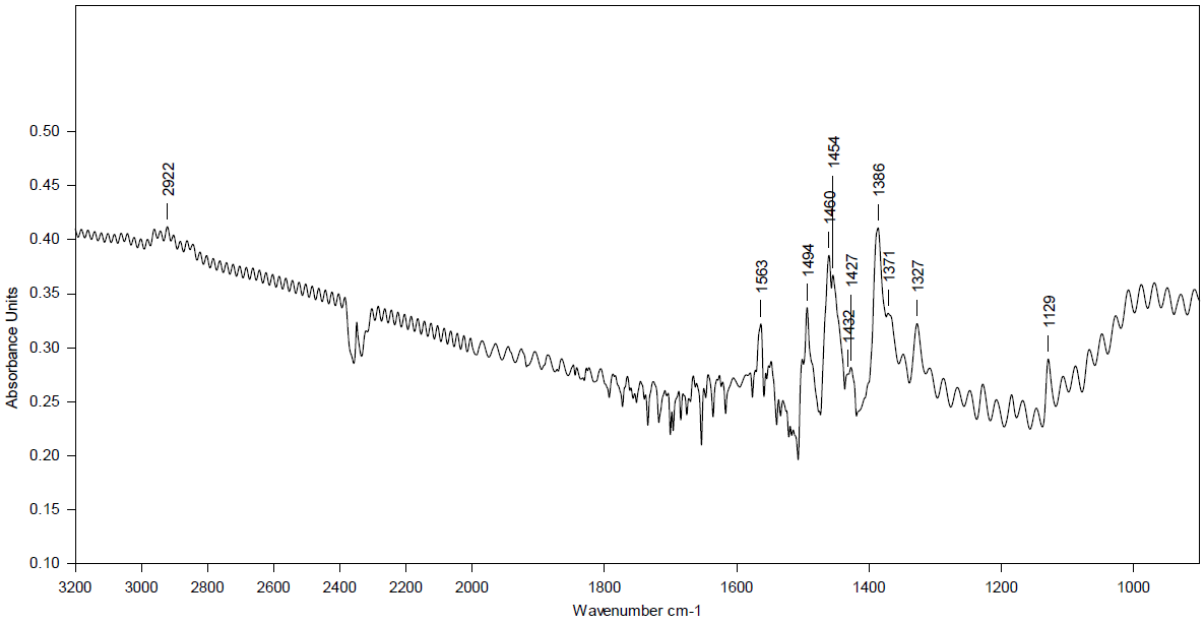

Fig. S20 IR spectrum of $[Cr(BQA)_2]Cl$

Crystallography

Crystallographic data were collected at low temperatures (100 K) using φ- and ω-scans on a BRUKER D8 Venture system equipped with dual IμS microfocus sources, a PHOTON100 detector and an OXFORD CRYOSYSTEMS 700 low temperature system. Mo-K_α radiation with wavelength 0.71073 Å or Cu-K_α radiation with wavelength 1.54178 Å and a collimating Quazar multilayer mirror were used. Semi-empirical absorption corrections from equivalents were applied using SADABS-2016/2 [1] the space groups were determined by systematic absences using XPREP and the structures were solved by direct methods using SHELXT. [2]

Refinement for all structures was performed against F^2 on all data by full-matrix least squares using SHELXL. [3] All non-hydrogen atoms were refined anisotropically and C-H hydrogen atoms were positioned at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2x or 1.5x (CH_3 hydrogens) the U_{eq} value of the atoms they are linked to.

The crystallographic data were deposited at the Cambridge Crystallographic Data Centre as CCDC 1897889-1897893 and 2057276 and can be obtained free of charge. [4]

[Zn(BQA)$_2$]

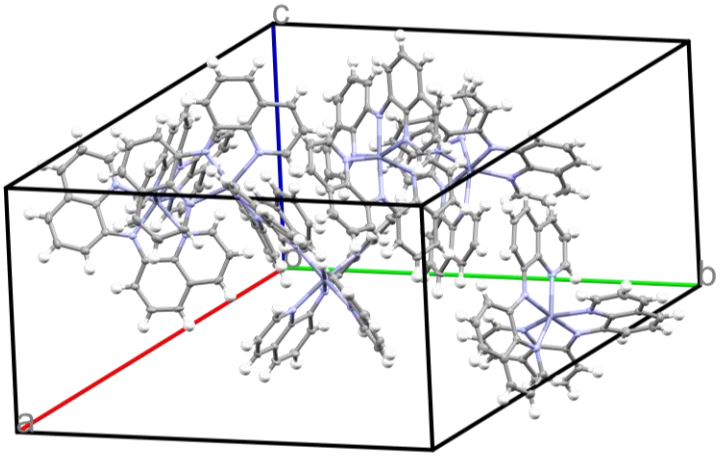

Fig. S21 Unit cell with complete molecules of $Zn(BQA)_2$ crystallized from THF

The unit cell of [$Zn(BQA)_2$] was determined using 9567 reflections and the structure was solved in the hexagonal space group $P6_1$. Partial racemic twinning was found and the twin ratio was refined and converged to 0.035(9). The asymmetric unit contains one molecule of [$Zn(BQA)_2$] as well as heavily disordered solvent molecules. The SQUEEZE [5] method as implemented in Platon[6] was used to include a model for the disordered solvent molecules. The obtained model was added as .fab-file to the refinement using SHELXL. SQUEEZE found one independent void with disordered solvent, located at 0.0 0.0 0.0, with a volume of 1179 Å^3. The equivalent of 279 electrons were identified in the void. This number of electrons corresponds to approximately 7 molecules of THF in the unit cell; however, there could also be hexane from the vapor diffusion in the crystal lattice which would change the amount of solvent molecules slightly.

Table S4. Crystal data and structure refinement for $[Zn(BQA)_2]$.

CCDC No.	1897889	
Empirical formula	$C_{36}\ H_{24}\ N_6\ Zn$	
Formula weight	605.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	$P6_1$	
Unit cell dimensions	a = 20.6945(4) Å	α= 90°.
	b = 20.6945(4) Å	β= 90°.
	c = 13.5955(3) Å	γ = 120°.
Volume	5042.4(2) $Å^3$	
Z	6	
Density (calculated)	1.197 Mg/m^3	
Absorption coefficient	0.762 mm^{-1}	
F(000)	1872	
Crystal size	0.980 x 0.163 x 0.137 mm^3	
Theta range for data collection	2.273 to 29.129°.	
Index ranges	$-28 \le h \le 28$, $-28 \le k \le 28$, $-18 \le l \le 18$	
Reflections collected	149185	
Independent reflections	9051 [R(int) = 0.1439]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9051 / 1 / 389	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2σ(I)]	R1 = 0.0296, wR2 = 0.0645	
R indices (all data)	R1 = 0.0377, wR2 = 0.0664	
Absolute structure parameter	0.035(9)	
Largest diff. peak and hole	0.342 and -0.302 $e.Å^{-3}$	

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [$Zn(BQA)_2$]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	755(1)	5084(1)	4934(1)	16(1)
N(1)	412(1)	5842(1)	4385(1)	19(1)
N(2)	1058(1)	5853(1)	6072(1)	17(1)
N(3)	1287(1)	4700(1)	5987(1)	17(1)
N(11)	1738(1)	5591(1)	3970(1)	17(1)
N(12)	500(1)	4282(1)	3863(1)	18(1)
N(13)	-345(1)	4188(1)	5380(1)	18(1)
C(1)	104(1)	5818(2)	3522(2)	24(1)
C(2)	-39(2)	6378(2)	3199(2)	30(1)
C(3)	128(2)	6963(2)	3802(2)	29(1)
C(4)	459(2)	7020(2)	4726(2)	24(1)
C(5)	607(1)	6442(1)	4996(2)	18(1)
C(6)	977(1)	6462(1)	5906(2)	18(1)
C(7)	1233(2)	7111(2)	6468(2)	25(1)
C(8)	1079(2)	7680(2)	6200(2)	28(1)
C(9)	694(2)	7641(2)	5364(2)	31(1)
C(10)	1306(1)	5697(1)	6920(2)	16(1)
C(11)	1387(1)	6008(1)	7863(2)	19(1)
C(12)	1659(2)	5780(2)	8659(2)	25(1)
C(13)	1864(1)	5253(2)	8571(2)	22(1)
C(14)	1762(1)	4889(2)	7653(2)	20(1)
C(15)	1462(1)	5090(1)	6854(2)	17(1)
C(16)	1923(2)	4306(2)	7501(2)	25(1)
C(17)	1758(2)	3937(2)	6625(2)	27(1)
C(18)	1416(1)	4145(2)	5887(2)	22(1)
C(21)	2351(1)	6243(1)	4076(2)	20(1)
C(22)	2922(1)	6546(2)	3367(2)	21(1)
C(23)	2824(1)	6156(2)	2513(2)	21(1)
C(24)	2167(1)	5462(1)	2359(2)	18(1)
C(25)	1634(1)	5189(1)	3128(2)	16(1)
C(26)	944(1)	4479(1)	3045(2)	16(1)
C(27)	809(2)	4127(2)	2130(2)	21(1)
C(28)	1337(2)	4417(2)	1367(2)	24(1)

C(29)	2010(2)	5060(2)	1467(2)	23(1)
C(30)	-90(1)	3587(1)	4042(2)	18(1)
C(31)	-281(2)	2912(2)	3594(2)	27(1)
C(32)	-929(2)	2241(2)	3855(2)	31(1)
C(33)	-1400(2)	2214(2)	4570(2)	32(1)
C(34)	-1220(2)	2873(2)	5105(2)	23(1)
C(35)	-558(1)	3548(1)	4860(2)	18(1)
C(36)	-1647(2)	2898(2)	5894(2)	29(1)
C(37)	-1419(2)	3538(2)	6412(2)	29(1)
C(38)	-759(2)	4179(2)	6131(2)	24(1)

Table S6. Bond lengths [Å] and angles [°] for $[Zn(BQA)_2]$.

Zn(1)-N(12)	2.067(2)	C(3)-C(4)	1.407(4)
Zn(1)-N(2)	2.080(2)	C(3)-H(3)	0.9500
Zn(1)-N(1)	2.154(2)	C(4)-C(9)	1.420(4)
Zn(1)-N(3)	2.183(2)	C(4)-C(5)	1.423(4)
Zn(1)-N(13)	2.183(2)	C(5)-C(6)	1.445(3)
Zn(1)-N(11)	2.195(2)	C(6)-C(7)	1.399(3)
N(1)-C(1)	1.325(3)	C(7)-C(8)	1.412(4)
N(1)-C(5)	1.374(3)	C(7)-H(7)	0.9500
N(2)-C(10)	1.364(3)	C(8)-C(9)	1.367(4)
N(2)-C(6)	1.371(3)	C(8)-H(8)	0.9500
N(3)-C(18)	1.311(3)	C(9)-H(9)	0.9500
N(3)-C(15)	1.371(3)	C(10)-C(11)	1.407(3)
N(11)-C(21)	1.320(3)	C(10)-C(15)	1.447(3)
N(11)-C(25)	1.367(3)	C(11)-C(12)	1.406(3)
N(12)-C(30)	1.366(3)	C(11)-H(11)	0.9500
N(12)-C(26)	1.368(3)	C(12)-C(13)	1.359(4)
N(13)-C(38)	1.326(3)	C(12)-H(12)	0.9500
N(13)-C(35)	1.366(3)	C(13)-C(14)	1.418(3)
C(1)-C(2)	1.402(4)	C(13)-H(13)	0.9500
C(1)-H(1)	0.9500	C(14)-C(15)	1.413(3)
C(2)-C(3)	1.356(4)	C(14)-C(16)	1.419(4)
C(2)-H(2)	0.9500	C(16)-C(17)	1.362(4)

C(16)-H(16)	0.9500	N(2)-Zn(1)-N(3)	77.08(8)
C(17)-C(18)	1.413(4)	N(1)-Zn(1)-N(3)	154.40(8)
C(17)-H(17)	0.9500	N(12)-Zn(1)-N(13)	77.02(8)
C(18)-H(18)	0.9500	N(2)-Zn(1)-N(13)	103.31(8)
C(21)-C(22)	1.406(3)	N(1)-Zn(1)-N(13)	97.50(8)
C(21)-H(21)	0.9500	N(3)-Zn(1)-N(13)	90.64(8)
C(22)-C(23)	1.369(4)	N(12)-Zn(1)-N(11)	76.50(8)
C(22)-H(22)	0.9500	N(2)-Zn(1)-N(11)	103.05(8)
C(23)-C(24)	1.414(4)	N(1)-Zn(1)-N(11)	90.53(8)
C(23)-H(23)	0.9500	N(3)-Zn(1)-N(11)	92.88(7)
C(24)-C(29)	1.413(3)	N(13)-Zn(1)-N(11)	153.53(8)
C(24)-C(25)	1.417(3)	C(1)-N(1)-C(5)	119.2(2)
C(25)-C(26)	1.452(3)	C(1)-N(1)-Zn(1)	127.36(19)
C(26)-C(27)	1.399(3)	C(5)-N(1)-Zn(1)	113.18(16)
C(27)-C(28)	1.405(3)	C(10)-N(2)-C(6)	126.3(2)
C(27)-H(27)	0.9500	C(10)-N(2)-Zn(1)	116.85(16)
C(28)-C(29)	1.369(4)	C(6)-N(2)-Zn(1)	116.88(15)
C(28)-H(28)	0.9500	C(18)-N(3)-C(15)	119.7(2)
C(29)-H(29)	0.9500	C(18)-N(3)-Zn(1)	127.71(17)
C(30)-C(31)	1.388(4)	C(15)-N(3)-Zn(1)	112.54(16)
C(30)-C(35)	1.450(3)	C(21)-N(11)-C(25)	119.5(2)
C(31)-C(32)	1.410(4)	C(21)-N(11)-Zn(1)	127.70(17)
C(31)-H(31)	0.9500	C(25)-N(11)-Zn(1)	112.50(16)
C(32)-C(33)	1.358(4)	C(30)-N(12)-C(26)	124.9(2)
C(32)-H(32)	0.9500	C(30)-N(12)-Zn(1)	117.04(15)
C(33)-C(34)	1.422(4)	C(26)-N(12)-Zn(1)	117.98(17)
C(33)-H(33)	0.9500	C(38)-N(13)-C(35)	119.4(2)
C(34)-C(36)	1.407(4)	C(38)-N(13)-Zn(1)	128.17(18)
C(34)-C(35)	1.424(3)	C(35)-N(13)-Zn(1)	111.89(15)
C(36)-C(37)	1.360(4)	N(1)-C(1)-C(2)	122.8(3)
C(36)-H(36)	0.9500	N(1)-C(1)-H(1)	118.6
C(37)-C(38)	1.401(4)	C(2)-C(1)-H(1)	118.6
C(37)-H(37)	0.9500	C(3)-C(2)-C(1)	118.9(3)
C(38)-H(38)	0.9500	C(3)-C(2)-H(2)	120.6
		C(1)-C(2)-H(2)	120.6
N(12)-Zn(1)-N(2)	175.29(8)	C(2)-C(3)-C(4)	120.8(3)
N(12)-Zn(1)-N(1)	107.22(8)	C(2)-C(3)-H(3)	119.6
N(2)-Zn(1)-N(1)	77.44(8)	C(4)-C(3)-H(3)	119.6
N(12)-Zn(1)-N(3)	98.24(8)	C(3)-C(4)-C(9)	123.6(3)

C(3)-C(4)-C(5)	117.4(3)	C(16)-C(17)-H(17)	120.8
C(9)-C(4)-C(5)	118.9(2)	C(18)-C(17)-H(17)	120.8
N(1)-C(5)-C(4)	120.9(2)	N(3)-C(18)-C(17)	123.1(2)
N(1)-C(5)-C(6)	117.1(2)	N(3)-C(18)-H(18)	118.5
C(4)-C(5)-C(6)	122.0(2)	C(17)-C(18)-H(18)	118.5
N(2)-C(6)-C(7)	129.1(2)	N(11)-C(21)-C(22)	123.1(2)
N(2)-C(6)-C(5)	114.9(2)	N(11)-C(21)-H(21)	118.5
C(7)-C(6)-C(5)	115.9(2)	C(22)-C(21)-H(21)	118.5
C(6)-C(7)-C(8)	121.7(3)	C(23)-C(22)-C(21)	118.3(2)
C(6)-C(7)-H(7)	119.2	C(23)-C(22)-H(22)	120.8
C(8)-C(7)-H(7)	119.2	C(21)-C(22)-H(22)	120.8
C(9)-C(8)-C(7)	122.2(3)	C(22)-C(23)-C(24)	120.5(2)
C(9)-C(8)-H(8)	118.9	C(22)-C(23)-H(23)	119.8
C(7)-C(8)-H(8)	118.9	C(24)-C(23)-H(23)	119.8
C(8)-C(9)-C(4)	119.2(3)	C(29)-C(24)-C(23)	123.1(2)
C(8)-C(9)-H(9)	120.4	C(29)-C(24)-C(25)	119.6(2)
C(4)-C(9)-H(9)	120.4	C(23)-C(24)-C(25)	117.2(2)
N(2)-C(10)-C(11)	129.3(2)	N(11)-C(25)-C(24)	121.4(2)
N(2)-C(10)-C(15)	115.3(2)	N(11)-C(25)-C(26)	117.2(2)
C(11)-C(10)-C(15)	115.2(2)	C(24)-C(25)-C(26)	121.4(2)
C(12)-C(11)-C(10)	121.6(2)	N(12)-C(26)-C(27)	129.7(2)
C(12)-C(11)-H(11)	119.2	N(12)-C(26)-C(25)	114.3(2)
C(10)-C(11)-H(11)	119.2	C(27)-C(26)-C(25)	115.8(2)
C(13)-C(12)-C(11)	122.7(2)	C(26)-C(27)-C(28)	121.6(2)
C(13)-C(12)-H(12)	118.7	C(26)-C(27)-H(27)	119.2
C(11)-C(12)-H(12)	118.7	C(28)-C(27)-H(27)	119.2
C(12)-C(13)-C(14)	118.7(2)	C(29)-C(28)-C(27)	122.5(2)
C(12)-C(13)-H(13)	120.6	C(29)-C(28)-H(28)	118.7
C(14)-C(13)-H(13)	120.6	C(27)-C(28)-H(28)	118.7
C(15)-C(14)-C(13)	119.4(2)	C(28)-C(29)-C(24)	118.7(2)
C(15)-C(14)-C(16)	117.6(2)	C(28)-C(29)-H(29)	120.6
C(13)-C(14)-C(16)	122.9(2)	C(24)-C(29)-H(29)	120.6
N(3)-C(15)-C(14)	120.9(2)	N(12)-C(30)-C(31)	129.5(2)
N(3)-C(15)-C(10)	117.1(2)	N(12)-C(30)-C(35)	114.6(2)
C(14)-C(15)-C(10)	122.0(2)	C(31)-C(30)-C(35)	115.8(2)
C(17)-C(16)-C(14)	120.2(2)	C(30)-C(31)-C(32)	122.1(3)
C(17)-C(16)-H(16)	119.9	C(30)-C(31)-H(31)	119.0
C(14)-C(16)-H(16)	119.9	C(32)-C(31)-H(31)	119.0
C(16)-C(17)-C(18)	118.3(2)	C(33)-C(32)-C(31)	122.1(3)

C(33)-C(32)-H(32)	118.9	C(34)-C(35)-C(30)	121.5(2)
C(31)-C(32)-H(32)	118.9	C(37)-C(36)-C(34)	120.8(3)
C(32)-C(33)-C(34)	119.2(3)	C(37)-C(36)-H(36)	119.6
C(32)-C(33)-H(33)	120.4	C(34)-C(36)-H(36)	119.6
C(34)-C(33)-H(33)	120.4	C(36)-C(37)-C(38)	118.7(3)
C(36)-C(34)-C(33)	123.8(3)	C(36)-C(37)-H(37)	120.7
C(36)-C(34)-C(35)	117.2(3)	C(38)-C(37)-H(37)	120.7
C(33)-C(34)-C(35)	118.9(2)	N(13)-C(38)-C(37)	122.8(3)
N(13)-C(35)-C(34)	121.0(2)	N(13)-C(38)-H(38)	118.6
N(13)-C(35)-C(30)	117.5(2)	C(37)-C(38)-H(38)	118.6

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Zn(BQA)_2]$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	15(1)	20(1)	11(1)	-1(1)	0(1)	7(1)
N(1)	14(1)	23(1)	16(1)	0(1)	0(1)	7(1)
N(2)	16(1)	21(1)	12(1)	-1(1)	-1(1)	8(1)
N(3)	17(1)	24(1)	12(1)	2(1)	4(1)	11(1)
N(11)	17(1)	19(1)	12(1)	0(1)	-2(1)	8(1)
N(12)	15(1)	22(1)	13(1)	-1(1)	0(1)	7(1)
N(13)	17(1)	22(1)	15(1)	2(1)	0(1)	11(1)
C(1)	20(1)	26(1)	22(1)	-1(1)	-6(1)	7(1)
C(2)	24(1)	30(2)	29(1)	3(1)	-8(1)	9(1)
C(3)	23(2)	30(2)	38(2)	6(1)	-3(1)	16(1)
C(4)	19(1)	26(1)	29(1)	3(1)	4(1)	12(1)
C(5)	11(1)	20(1)	20(1)	1(1)	3(1)	5(1)
C(6)	14(1)	21(1)	16(1)	1(1)	4(1)	7(1)
C(7)	26(1)	25(1)	20(1)	-2(1)	3(1)	11(1)
C(8)	35(2)	21(1)	26(1)	-2(1)	6(1)	12(1)
C(9)	37(2)	29(2)	34(2)	4(1)	6(1)	23(1)
C(10)	11(1)	20(1)	14(1)	0(1)	3(1)	4(1)
C(11)	17(1)	23(1)	16(1)	-3(1)	2(1)	9(1)
C(12)	21(1)	31(2)	13(1)	-3(1)	-1(1)	6(1)

C(13)	16(1)	31(2)	14(1)	1(1)	-2(1)	8(1)
C(14)	15(1)	28(1)	16(1)	4(1)	3(1)	9(1)
C(15)	10(1)	23(1)	14(1)	1(1)	2(1)	6(1)
C(16)	23(1)	35(2)	20(1)	5(1)	0(1)	17(1)
C(17)	31(2)	36(2)	25(1)	1(1)	2(1)	24(1)
C(18)	23(1)	30(2)	17(1)	-1(1)	2(1)	15(1)
C(21)	19(1)	23(1)	17(1)	0(1)	-1(1)	10(1)
C(22)	15(1)	21(1)	24(1)	2(1)	0(1)	7(1)
C(23)	16(1)	27(1)	19(1)	9(1)	6(1)	12(1)
C(24)	18(1)	23(1)	16(1)	3(1)	3(1)	12(1)
C(25)	15(1)	21(1)	12(1)	1(1)	-1(1)	10(1)
C(26)	15(1)	21(1)	14(1)	0(1)	0(1)	10(1)
C(27)	20(1)	24(1)	15(1)	-3(1)	-2(1)	9(1)
C(28)	30(2)	33(2)	12(1)	-4(1)	0(1)	18(1)
C(29)	25(1)	34(2)	13(1)	1(1)	7(1)	16(1)
C(30)	18(1)	22(1)	13(1)	2(1)	-2(1)	9(1)
C(31)	31(2)	26(2)	21(1)	-3(1)	0(1)	13(1)
C(32)	37(2)	19(1)	27(1)	-3(1)	-4(1)	6(1)
C(33)	28(2)	23(2)	30(1)	4(1)	-3(1)	1(1)
C(34)	19(1)	26(1)	20(1)	6(1)	-2(1)	8(1)
C(35)	14(1)	22(1)	16(1)	4(1)	-1(1)	8(1)
C(36)	21(1)	31(2)	31(2)	14(1)	8(1)	10(1)
C(37)	27(2)	34(2)	29(2)	10(1)	12(1)	17(1)
C(38)	24(1)	27(2)	22(1)	5(1)	5(1)	15(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Zn(BQA)_2]$.

	x	y	z	U(eq)
H(1)	-26	5403	3103	29
H(2)	-249	6349	2568	36
H(3)	21	7338	3599	35
H(7)	1517	7171	7044	30
H(8)	1248	8104	6614	34
H(9)	585	8024	5212	37
H(11)	1255	6382	7965	23
H(12)	1701	6003	9284	30
H(13)	2072	5131	9114	26
H(16)	2147	4172	8012	30
H(17)	1870	3551	6514	33
H(18)	1273	3868	5291	27
H(21)	2410	6521	4658	24
H(22)	3364	7009	3477	25
H(23)	3200	6353	2020	25
H(27)	349	3680	2021	25
H(28)	1223	4157	758	29
H(29)	2364	5233	948	28
H(31)	35	2901	3095	32
H(32)	-1039	1795	3521	38
H(33)	-1845	1759	4711	39
H(36)	-2101	2462	6067	35
H(37)	-1702	3550	6955	35
H(38)	-600	4625	6494	28

Vacuum-grown [Zn(BQA)$_2$]

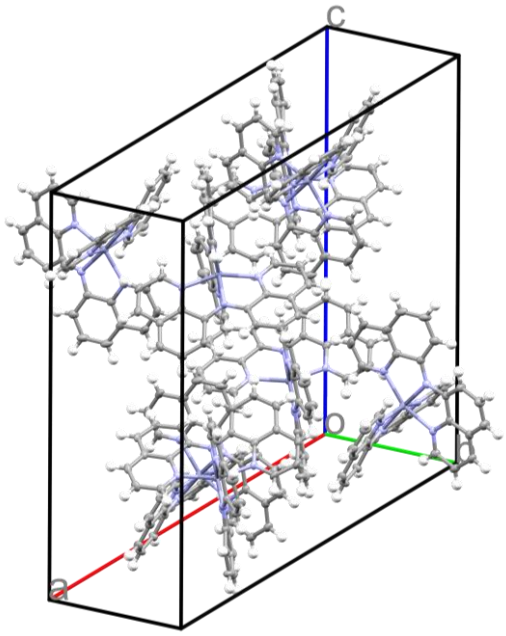

Fig. S22 Unit cell with complete molecules of vapor-grown Zn(BQA)$_2$

The unit cell of [Zn(BQA)$_2$] obtained from sublimation was determined using 9782 reflections and the structure was solved in the monoclinic space group *C*2/*c*. The structure was refined as a pseudo merohedral twin. The twin ratio was refined and converged to 0.035(9). The asymmetric unit contains one molecule of [Zn(BQA)$_2$].

Table S9. Crystal data and structure refinement for vacuum grown [Zn(BQA)$_2$].

CCDC No.	1897892	
Empirical formula	C_{36} H_{24} N_6 Zn	
Formula weight	605.98	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 19.5616(9) Å	α= 90°.
	b = 13.4711(6) Å	β= 113.988(3)°.
	c = 22.5945(14) Å	γ = 90°.
Volume	5439.8(5) Å^3	
Z	8	
Density (calculated)	1.480 Mg/m^3	
Absorption coefficient	1.556 mm^{-1}	
F(000)	2496	

Crystal size	0.058 x 0.057 x 0.036 mm^3
Theta range for data collection	2.140 to 72.109°.
Index ranges	$-24 \leq h \leq 24$, $-16 \leq k \leq 15$, $-27 \leq l \leq 27$
Reflections collected	95886
Independent reflections	5366 [R(int) = 0.1319]
Completeness to theta = 67.679°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5366 / 0 / 389
Goodness-of-fit on F^2	1.908
Final R indices [I>2σ(I)]	R1 = 0.1157, wR2 = 0.3658
R indices (all data)	R1 = 0.1249, wR2 = 0.3765
Largest diff. peak and hole	1.425 and -1.875 e.$Å^{-3}$

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for vacuum grown [$Zn(BQA)_2$]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	6618(1)	5680(1)	7012(1)	20(1)
N(1)	5642(3)	6657(4)	6626(3)	20(1)
N(2)	6909(3)	6715(4)	6465(3)	22(1)
N(3)	7705(3)	5175(4)	7101(3)	22(1)
N(21)	7092(3)	6199(4)	8012(3)	23(1)
N(22)	6308(3)	4575(4)	7496(3)	22(1)
N(23)	6053(3)	4608(4)	6241(3)	20(1)
C(1)	5003(4)	6554(5)	6686(4)	26(1)
C(2)	4407(4)	7241(6)	6418(4)	30(2)
C(3)	4499(4)	8047(6)	6085(4)	27(2)
C(4)	5173(4)	8198(5)	6025(3)	23(1)
C(5)	5334(4)	9043(5)	5728(3)	26(1)
C(6)	6016(5)	9131(5)	5716(4)	26(1)
C(7)	6576(4)	8390(5)	5953(3)	21(1)
C(8)	6446(4)	7514(5)	6227(3)	20(1)
C(9)	5742(4)	7453(5)	6294(3)	20(1)

C(11)	8096(5)	4427(5)	7456(4)	29(2)
C(12)	8758(5)	4088(6)	7422(4)	35(2)
C(13)	9006(4)	4542(6)	7000(4)	31(2)
C(14)	8593(4)	5330(5)	6603(3)	25(1)
C(15)	8792(4)	5786(6)	6140(4)	29(2)
C(16)	8353(5)	6540(6)	5769(4)	29(2)
C(17)	7718(4)	6885(5)	5852(3)	24(1)
C(18)	7501(4)	6474(5)	6323(3)	21(1)
C(19)	7944(4)	5642(5)	6683(3)	22(1)
C(21)	7504(5)	6991(6)	8248(4)	31(2)
C(22)	7782(5)	7256(7)	8907(5)	37(2)
C(23)	7626(4)	6655(7)	9327(4)	33(2)
C(24)	7183(4)	5786(6)	9095(4)	27(2)
C(25)	6960(5)	5170(6)	9493(4)	34(2)
C(26)	6464(6)	4411(6)	9207(4)	36(2)
C(27)	6211(5)	4201(5)	8540(4)	28(2)
C(28)	6463(4)	4723(5)	8133(3)	22(1)
C(29)	6924(4)	5584(5)	8421(3)	23(1)
C(31)	5923(4)	4694(5)	5624(4)	26(1)
C(32)	5565(5)	3943(6)	5168(4)	28(2)
C(33)	5369(5)	3092(5)	5387(4)	29(2)
C(34)	5529(4)	2954(6)	6048(4)	27(1)
C(35)	5416(5)	2041(6)	6307(4)	38(2)
C(36)	5636(6)	1968(6)	6969(4)	38(2)
C(37)	5925(5)	2782(5)	7383(4)	29(2)
C(38)	6027(4)	3715(5)	7154(3)	21(1)
C(39)	5864(4)	3764(5)	6470(3)	22(1)

Table S11. Bond lengths [Å] and angles [°] for vacuum grown [Zn(BQA)$_2$].

Zn(1)-N(22)	2.078(6)	Zn(1)-N(1)	2.187(6)
Zn(1)-N(2)	2.090(6)	N(1)-C(1)	1.319(10)
Zn(1)-N(3)	2.164(6)	N(1)-C(9)	1.368(9)
Zn(1)-N(21)	2.180(6)	N(2)-C(18)	1.361(9)
Zn(1)-N(23)	2.184(6)	N(2)-C(8)	1.369(9)

N(3)-C(11)	1.321(9)	C(21)-H(21)	0.9500
N(3)-C(19)	1.365(10)	C(22)-C(23)	1.372(14)
N(21)-C(21)	1.312(10)	C(22)-H(22)	0.9500
N(21)-C(29)	1.377(10)	C(23)-C(24)	1.424(12)
N(22)-C(28)	1.361(10)	C(23)-H(23)	0.9500
N(22)-C(38)	1.377(9)	C(24)-C(25)	1.415(12)
N(23)-C(31)	1.317(10)	C(24)-C(29)	1.423(10)
N(23)-C(39)	1.361(9)	C(25)-C(26)	1.377(14)
C(1)-C(2)	1.417(11)	C(25)-H(25)	0.9500
C(1)-H(1)	0.9500	C(26)-C(27)	1.409(12)
C(2)-C(3)	1.375(12)	C(26)-H(26)	0.9500
C(2)-H(2)	0.9500	C(27)-C(28)	1.396(10)
C(3)-C(4)	1.394(11)	C(27)-H(27)	0.9500
C(3)-H(3)	0.9500	C(28)-C(29)	1.452(10)
C(4)-C(5)	1.421(11)	C(31)-C(32)	1.410(10)
C(4)-C(9)	1.436(9)	C(31)-H(31)	0.9500
C(5)-C(6)	1.350(12)	C(32)-C(33)	1.365(11)
C(5)-H(5)	0.9500	C(32)-H(32)	0.9500
C(6)-C(7)	1.416(10)	C(33)-C(34)	1.408(11)
C(6)-H(6)	0.9500	C(33)-H(33)	0.9500
C(7)-C(8)	1.403(9)	C(34)-C(35)	1.418(12)
C(7)-H(7)	0.9500	C(34)-C(39)	1.422(10)
C(8)-C(9)	1.448(10)	C(35)-C(36)	1.381(13)
C(11)-C(12)	1.403(13)	C(35)-H(35)	0.9500
C(11)-H(11)	0.9500	C(36)-C(37)	1.402(11)
C(12)-C(13)	1.376(13)	C(36)-H(36)	0.9500
C(12)-H(12)	0.9500	C(37)-C(38)	1.404(10)
C(13)-C(14)	1.413(11)	C(37)-H(37)	0.9500
C(13)-H(13)	0.9500	C(38)-C(39)	1.446(10)
C(14)-C(15)	1.397(12)		
C(14)-C(19)	1.418(10)	N(22)-Zn(1)-N(2)	175.6(2)
C(15)-C(16)	1.373(11)	N(22)-Zn(1)-N(3)	102.2(2)
C(15)-H(15)	0.9500	N(2)-Zn(1)-N(3)	76.7(2)
C(16)-C(17)	1.409(11)	N(22)-Zn(1)-N(21)	77.1(2)
C(16)-H(16)	0.9500	N(2)-Zn(1)-N(21)	107.1(2)
C(17)-C(18)	1.409(10)	N(3)-Zn(1)-N(21)	90.9(2)
C(17)-H(17)	0.9500	N(22)-Zn(1)-N(23)	77.6(2)
C(18)-C(19)	1.447(9)	N(2)-Zn(1)-N(23)	98.1(2)
C(21)-C(22)	1.409(12)	N(3)-Zn(1)-N(23)	91.5(2)

N(21)-Zn(1)-N(23)	154.5(2)	C(5)-C(6)-C(7)	123.3(7)
N(22)-Zn(1)-N(1)	104.3(2)	C(5)-C(6)-H(6)	118.3
N(2)-Zn(1)-N(1)	76.5(2)	C(7)-C(6)-H(6)	118.3
N(3)-Zn(1)-N(1)	153.1(2)	C(8)-C(7)-C(6)	120.6(6)
N(21)-Zn(1)-N(1)	98.9(2)	C(8)-C(7)-H(7)	119.7
N(23)-Zn(1)-N(1)	90.2(2)	C(6)-C(7)-H(7)	119.7
C(1)-N(1)-C(9)	119.4(6)	N(2)-C(8)-C(7)	128.7(6)
C(1)-N(1)-Zn(1)	127.3(5)	N(2)-C(8)-C(9)	114.9(6)
C(9)-N(1)-Zn(1)	113.3(4)	C(7)-C(8)-C(9)	116.4(6)
C(18)-N(2)-C(8)	125.9(6)	N(1)-C(9)-C(4)	121.4(6)
C(18)-N(2)-Zn(1)	116.3(4)	N(1)-C(9)-C(8)	117.1(6)
C(8)-N(2)-Zn(1)	117.5(5)	C(4)-C(9)-C(8)	121.5(6)
C(11)-N(3)-C(19)	119.7(7)	N(3)-C(11)-C(12)	122.3(7)
C(11)-N(3)-Zn(1)	127.0(5)	N(3)-C(11)-H(11)	118.9
C(19)-N(3)-Zn(1)	113.0(4)	C(12)-C(11)-H(11)	118.9
C(21)-N(21)-C(29)	119.4(7)	C(13)-C(12)-C(11)	119.1(7)
C(21)-N(21)-Zn(1)	127.9(5)	C(13)-C(12)-H(12)	120.4
C(29)-N(21)-Zn(1)	112.7(5)	C(11)-C(12)-H(12)	120.4
C(28)-N(22)-C(38)	125.7(6)	C(12)-C(13)-C(14)	120.1(7)
C(28)-N(22)-Zn(1)	117.7(5)	C(12)-C(13)-H(13)	119.9
C(38)-N(22)-Zn(1)	116.3(5)	C(14)-C(13)-H(13)	119.9
C(31)-N(23)-C(39)	120.7(6)	C(15)-C(14)-C(13)	123.0(7)
C(31)-N(23)-Zn(1)	127.1(5)	C(15)-C(14)-C(19)	120.1(7)
C(39)-N(23)-Zn(1)	112.1(4)	C(13)-C(14)-C(19)	116.9(7)
N(1)-C(1)-C(2)	122.5(7)	C(16)-C(15)-C(14)	119.2(7)
N(1)-C(1)-H(1)	118.8	C(16)-C(15)-H(15)	120.4
C(2)-C(1)-H(1)	118.8	C(14)-C(15)-H(15)	120.4
C(3)-C(2)-C(1)	118.8(7)	C(15)-C(16)-C(17)	121.9(7)
C(3)-C(2)-H(2)	120.6	C(15)-C(16)-H(16)	119.1
C(1)-C(2)-H(2)	120.6	C(17)-C(16)-H(16)	119.1
C(2)-C(3)-C(4)	120.5(7)	C(18)-C(17)-C(16)	121.6(6)
C(2)-C(3)-H(3)	119.7	C(18)-C(17)-H(17)	119.2
C(4)-C(3)-H(3)	119.7	C(16)-C(17)-H(17)	119.2
C(3)-C(4)-C(5)	124.2(6)	N(2)-C(18)-C(17)	129.1(6)
C(3)-C(4)-C(9)	117.2(7)	N(2)-C(18)-C(19)	115.1(6)
C(5)-C(4)-C(9)	118.5(7)	C(17)-C(18)-C(19)	115.7(6)
C(6)-C(5)-C(4)	119.3(6)	N(3)-C(19)-C(14)	121.9(6)
C(6)-C(5)-H(5)	120.3	N(3)-C(19)-C(18)	116.8(6)
C(4)-C(5)-H(5)	120.3	C(14)-C(19)-C(18)	121.3(7)

N(21)-C(21)-C(22)	123.0(8)	N(23)-C(31)-C(32)	122.4(7)
N(21)-C(21)-H(21)	118.5	N(23)-C(31)-H(31)	118.8
C(22)-C(21)-H(21)	118.5	C(32)-C(31)-H(31)	118.8
C(23)-C(22)-C(21)	118.9(8)	C(33)-C(32)-C(31)	117.9(7)
C(23)-C(22)-H(22)	120.6	C(33)-C(32)-H(32)	121.1
C(21)-C(22)-H(22)	120.6	C(31)-C(32)-H(32)	121.1
C(22)-C(23)-C(24)	120.3(7)	C(32)-C(33)-C(34)	121.4(7)
C(22)-C(23)-H(23)	119.9	C(32)-C(33)-H(33)	119.3
C(24)-C(23)-H(23)	119.9	C(34)-C(33)-H(33)	119.3
C(25)-C(24)-C(29)	120.1(7)	C(33)-C(34)-C(35)	123.2(7)
C(25)-C(24)-C(23)	123.1(7)	C(33)-C(34)-C(39)	117.0(7)
C(29)-C(24)-C(23)	116.7(7)	C(35)-C(34)-C(39)	119.7(7)
C(26)-C(25)-C(24)	118.5(7)	C(36)-C(35)-C(34)	118.4(7)
C(26)-C(25)-H(25)	120.7	C(36)-C(35)-H(35)	120.8
C(24)-C(25)-H(25)	120.7	C(34)-C(35)-H(35)	120.8
C(25)-C(26)-C(27)	121.7(8)	C(35)-C(36)-C(37)	122.1(7)
C(25)-C(26)-H(26)	119.2	C(35)-C(36)-H(36)	118.9
C(27)-C(26)-H(26)	119.2	C(37)-C(36)-H(36)	118.9
C(28)-C(27)-C(26)	122.6(8)	C(36)-C(37)-C(38)	122.1(7)
C(28)-C(27)-H(27)	118.7	C(36)-C(37)-H(37)	118.9
C(26)-C(27)-H(27)	118.7	C(38)-C(37)-H(37)	118.9
N(22)-C(28)-C(27)	129.6(7)	N(22)-C(38)-C(37)	129.1(6)
N(22)-C(28)-C(29)	114.9(6)	N(22)-C(38)-C(39)	115.1(6)
C(27)-C(28)-C(29)	115.4(7)	C(37)-C(38)-C(39)	115.6(6)
N(21)-C(29)-C(24)	121.8(7)	N(23)-C(39)-C(34)	120.5(7)
N(21)-C(29)-C(28)	117.1(6)	N(23)-C(39)-C(38)	117.9(6)
C(24)-C(29)-C(28)	121.2(7)	C(34)-C(39)-C(38)	121.5(6)

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for vacuum grown $[Zn(BQA)_2]$. The anisotropic displacement factor exponent takes the form:
$-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	27(1)	13(1)	21(1)	1(1)	11(1)	0(1)

N(1)	24(3)	18(3)	20(3)	-4(2)	9(2)	-1(2)
N(2)	26(3)	16(3)	23(3)	4(2)	11(2)	1(2)
N(3)	27(3)	14(3)	23(3)	1(2)	9(2)	5(2)
N(21)	27(3)	17(3)	26(3)	-3(2)	12(2)	0(2)
N(22)	28(3)	15(2)	24(3)	3(2)	11(2)	0(2)
N(23)	24(3)	12(2)	23(3)	1(2)	8(2)	0(2)
C(1)	30(4)	21(3)	29(3)	-5(3)	13(3)	-3(3)
C(2)	25(3)	25(4)	42(4)	-8(3)	16(3)	-4(3)
C(3)	25(3)	25(3)	28(3)	-9(3)	7(3)	4(3)
C(4)	28(3)	16(3)	22(3)	-6(2)	7(3)	3(2)
C(5)	36(4)	16(3)	23(3)	-2(2)	9(3)	10(3)
C(6)	39(4)	8(3)	30(4)	2(2)	13(3)	2(3)
C(7)	22(3)	15(3)	28(3)	3(2)	11(3)	5(2)
C(8)	24(3)	14(3)	21(3)	-1(2)	8(2)	0(2)
C(9)	27(3)	11(3)	18(3)	-2(2)	6(2)	-1(2)
C(11)	40(4)	20(3)	21(3)	7(3)	8(3)	6(3)
C(12)	43(5)	28(4)	26(4)	7(3)	6(3)	14(3)
C(13)	30(4)	30(4)	26(4)	-1(3)	6(3)	9(3)
C(14)	27(3)	24(3)	24(3)	-3(3)	9(3)	5(3)
C(15)	24(3)	29(4)	34(4)	-4(3)	13(3)	3(3)
C(16)	37(4)	27(4)	30(4)	5(3)	22(3)	3(3)
C(17)	26(3)	22(3)	26(3)	6(2)	13(3)	3(3)
C(18)	23(3)	13(3)	24(3)	0(2)	9(3)	-2(2)
C(19)	25(3)	18(3)	20(3)	-1(2)	4(3)	0(2)
C(21)	31(4)	26(4)	40(4)	-5(3)	19(3)	-3(3)
C(22)	27(4)	40(4)	43(5)	-18(4)	14(3)	-10(3)
C(23)	28(4)	41(4)	28(4)	-16(3)	8(3)	-2(3)
C(24)	28(3)	26(4)	25(4)	-5(3)	7(3)	10(3)
C(25)	47(5)	32(4)	20(3)	2(3)	12(3)	11(3)
C(26)	64(6)	24(4)	28(4)	2(3)	27(4)	4(3)
C(27)	41(4)	21(3)	29(4)	1(3)	19(3)	2(3)
C(28)	26(3)	16(3)	22(3)	0(2)	9(3)	3(2)
C(29)	27(3)	19(3)	21(3)	1(2)	7(3)	5(3)
C(31)	32(4)	18(3)	26(3)	2(3)	11(3)	4(3)
C(32)	38(4)	23(3)	22(3)	-3(3)	9(3)	5(3)
C(33)	34(4)	23(3)	28(4)	-8(3)	10(3)	-2(3)
C(34)	28(3)	22(3)	31(4)	-4(3)	13(3)	-2(3)
C(35)	53(5)	27(4)	33(4)	-8(3)	17(4)	-10(4)
C(36)	58(5)	22(4)	37(4)	1(3)	23(4)	-11(3)

C(37)	44(4)	16(3)	27(3)	0(3)	15(3)	-5(3)
C(38)	23(3)	15(3)	25(3)	0(2)	10(3)	0(2)
C(39)	21(3)	16(3)	29(3)	0(2)	10(3)	1(2)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for vacuum grown [$Zn(BQA)_2$].

	x	y	z	U(eq)
H(1)	4940	5999	6919	31
H(2)	3952	7145	6468	36
H(3)	4100	8505	5894	33
H(5)	4965	9541	5539	31
H(6)	6125	9720	5540	31
H(7)	7043	8487	5926	26
H(11)	7924	4108	7744	35
H(12)	9030	3553	7686	42
H(13)	9456	4325	6976	37
H(15)	9224	5576	6082	34
H(16)	8482	6838	5447	35
H(17)	7429	7406	5584	29
H(21)	7621	7404	7961	37
H(22)	8071	7842	9059	44
H(23)	7814	6819	9774	40
H(25)	7148	5279	9947	40
H(26)	6287	4019	9465	43
H(27)	5856	3684	8361	34
H(31)	6075	5283	5481	31
H(32)	5464	4028	4723	34
H(33)	5119	2581	5087	35
H(35)	5193	1492	6032	45
H(36)	5590	1348	7149	45
H(37)	6056	2699	7834	34

[Mn(BQA)$_2$]

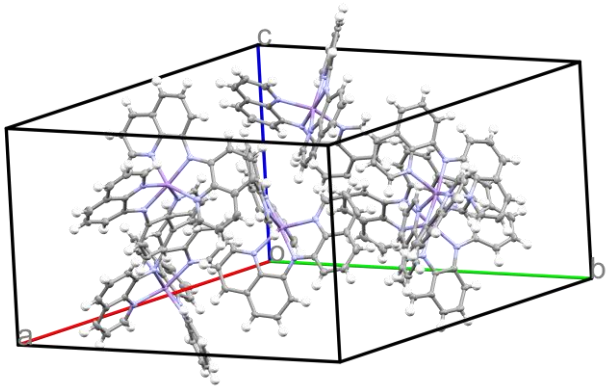

Fig. S23 Unit cell with complete molecules of Mn(BQA)$_2$

The unit cell of [Mn(BQA)$_2$] was determined using 9975 reflections and the structure was solved in the hexagonal space group *P*6$_5$. The asymmetric unit contains one molecule of [Mn(BQA)$_2$] as well as heavily disordered solvent molecules. SQUEEZE as implemented in Platon was used to include a model for the disordered solvent in the refinement. One independent void at 0.0 0.0 0.0 with a volume of 1156 Å^3 was found in the unit cell. The equivalent of 278 electrons were found in the void which corresponds to 6 to 7 molecules of the used solvents (thf and hexane). The obtained model was added as .fab-file to the refinement using SHELXL.

Table S14. Crystal data and structure refinement for [Mn(BQA)$_2$].

CCDC No.	1897890	
Empirical formula	C_{36} H_{24} Mn N_6	
Formula weight	595.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	*P*6$_5$	
Unit cell dimensions	a = 20.5446(5) Å	α= 90°.
	b = 20.5446(5) Å	β= 90°.
	c = 13.8346(4) Å	γ = 120°.
Volume	5057.0(3) Å^3	
Z	6	
Density (calculated)	1.173 Mg/m^3	
Absorption coefficient	0.423 mm^{-1}	
F(000)	1842	
Crystal size	0.420 x 0.038 x 0.034 mm^3	
Theta range for data collection	2.289 to 29.127°.	
Index ranges	-28 ≤ h ≤ 28, -28 ≤ k ≤ 28, -18 ≤ l ≤ 18	

Reflections collected	396141
Independent reflections	9056 [R(int) = 0.1489]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9056 / 1 / 388
Goodness-of-fit on F^2	1.029
Final R indices [I>2σ(I)]	R1 = 0.0330, wR2 = 0.0638
R indices (all data)	R1 = 0.0414, wR2 = 0.0665
Absolute structure parameter	0.012(5)
Largest diff. peak and hole	0.198 and -0.250 e.Å^{-3}

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)for [Mn(BQA)$_2$]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	5082(1)	739(1)	783(1)	17(1)
N(1)	5903(1)	391(1)	314(1)	21(1)
N(2)	5903(1)	1076(1)	1948(1)	19(1)
N(3)	4740(1)	1308(1)	1885(1)	19(1)
N(21)	5568(1)	1722(1)	-250(1)	17(1)
N(22)	4241(1)	481(1)	-323(1)	18(1)
N(23)	4101(1)	-381(1)	1195(1)	20(1)
C(1)	5880(1)	57(1)	-515(2)	29(1)
C(2)	6451(1)	-83(1)	-811(2)	36(1)
C(3)	7052(2)	127(1)	-220(2)	35(1)
C(4)	7111(1)	495(1)	659(2)	27(1)
C(5)	6512(1)	622(1)	908(2)	21(1)
C(6)	6528(1)	1013(1)	1782(2)	20(1)
C(7)	7194(1)	1309(1)	2326(2)	26(1)
C(8)	7783(1)	1180(2)	2064(2)	31(1)
C(9)	7747(2)	773(2)	1270(2)	33(1)
C(10)	5746(1)	1321(1)	2790(2)	17(1)
C(11)	6064(1)	1401(1)	3710(2)	21(1)
C(12)	5843(1)	1673(1)	4501(2)	23(1)

C(13)	5308(1)	1886(1)	4419(2)	24(1)
C(14)	4943(1)	1784(1)	3528(2)	20(1)
C(15)	5135(1)	1478(1)	2733(2)	18(1)
C(16)	4360(1)	1957(1)	3384(2)	26(1)
C(17)	3983(1)	1793(1)	2530(2)	27(1)
C(18)	4179(1)	1444(1)	1796(2)	25(1)
C(21)	6223(1)	2346(1)	-158(2)	21(1)
C(22)	6531(1)	2899(1)	-882(2)	23(1)
C(23)	6148(1)	2775(1)	-1729(2)	23(1)
C(24)	5453(1)	2106(1)	-1871(2)	20(1)
C(25)	5174(1)	1596(1)	-1084(2)	17(1)
C(26)	5055(1)	1924(1)	-2747(2)	25(1)
C(27)	4407(1)	1244(1)	-2836(2)	25(1)
C(28)	4108(1)	739(1)	-2060(2)	22(1)
C(29)	4454(1)	902(1)	-1148(2)	18(1)
C(30)	3529(1)	-113(1)	-154(2)	20(1)
C(31)	2863(1)	-286(1)	-619(2)	29(1)
C(32)	2179(1)	-937(2)	-372(2)	37(1)
C(33)	2132(2)	-1421(2)	334(2)	39(1)
C(34)	2775(1)	-1248(1)	876(2)	29(1)
C(35)	3470(1)	-585(1)	655(2)	22(1)
C(36)	2775(2)	-1684(1)	1655(2)	35(1)
C(37)	3408(2)	-1464(1)	2197(2)	37(1)
C(38)	4065(2)	-800(1)	1941(2)	28(1)

Table S16. Bond lengths [Å] and angles [°] for [Mn(BQA)$_2$].

Mn(1)-N(22)	2.1663(19)	N(2)-C(6)	1.372(3)
Mn(1)-N(2)	2.1806(19)	N(3)-C(18)	1.320(3)
Mn(1)-N(1)	2.2321(19)	N(3)-C(15)	1.370(3)
Mn(1)-N(3)	2.2366(19)	N(21)-C(21)	1.321(3)
Mn(1)-N(23)	2.2454(18)	N(21)-C(25)	1.357(3)
Mn(1)-N(21)	2.2589(18)	N(22)-C(29)	1.366(3)
N(1)-C(1)	1.325(3)	N(22)-C(30)	1.378(3)
N(1)-C(5)	1.369(3)	N(23)-C(38)	1.323(3)
N(2)-C(10)	1.369(3)	N(23)-C(35)	1.368(3)

C(1)-C(2)	1.400(4)	C(26)-C(27)	1.370(3)
C(1)-H(1)	0.9500	C(26)-H(26)	0.9500
C(2)-C(3)	1.358(4)	C(27)-C(28)	1.403(3)
C(2)-H(2)	0.9500	C(27)-H(27)	0.9500
C(3)-C(4)	1.404(4)	C(28)-C(29)	1.404(3)
C(3)-H(3)	0.9500	C(28)-H(28)	0.9500
C(4)-C(9)	1.414(4)	C(30)-C(31)	1.387(3)
C(4)-C(5)	1.422(3)	C(30)-C(35)	1.445(3)
C(5)-C(6)	1.443(3)	C(31)-C(32)	1.413(4)
C(6)-C(7)	1.407(3)	C(31)-H(31)	0.9500
C(7)-C(8)	1.409(3)	C(32)-C(33)	1.363(4)
C(7)-H(7)	0.9500	C(32)-H(32)	0.9500
C(8)-C(9)	1.360(4)	C(33)-C(34)	1.402(4)
C(8)-H(8)	0.9500	C(33)-H(33)	0.9500
C(9)-H(9)	0.9500	C(34)-C(36)	1.401(4)
C(10)-C(11)	1.403(3)	C(34)-C(35)	1.429(3)
C(10)-C(15)	1.445(3)	C(36)-C(37)	1.368(4)
C(11)-C(12)	1.404(3)	C(36)-H(36)	0.9500
C(11)-H(11)	0.9500	C(37)-C(38)	1.402(4)
C(12)-C(13)	1.375(3)	C(37)-H(37)	0.9500
C(12)-H(12)	0.9500	C(38)-H(38)	0.9500
C(13)-C(14)	1.404(3)		
C(13)-H(13)	0.9500	N(22)-Mn(1)-N(2)	174.66(7)
C(14)-C(15)	1.417(3)	N(22)-Mn(1)-N(1)	110.72(7)
C(14)-C(16)	1.423(3)	N(2)-Mn(1)-N(1)	74.24(7)
C(16)-C(17)	1.359(3)	N(22)-Mn(1)-N(3)	100.89(7)
C(16)-H(16)	0.9500	N(2)-Mn(1)-N(3)	74.08(7)
C(17)-C(18)	1.412(3)	N(1)-Mn(1)-N(3)	148.27(7)
C(17)-H(17)	0.9500	N(22)-Mn(1)-N(23)	74.38(7)
C(18)-H(18)	0.9500	N(2)-Mn(1)-N(23)	107.06(7)
C(21)-C(22)	1.406(3)	N(1)-Mn(1)-N(23)	100.40(7)
C(21)-H(21)	0.9500	N(3)-Mn(1)-N(23)	90.41(7)
C(22)-C(23)	1.363(3)	N(22)-Mn(1)-N(21)	73.39(7)
C(22)-H(22)	0.9500	N(2)-Mn(1)-N(21)	104.93(7)
C(23)-C(24)	1.415(3)	N(1)-Mn(1)-N(21)	91.98(7)
C(23)-H(23)	0.9500	N(3)-Mn(1)-N(21)	94.49(6)
C(24)-C(26)	1.404(3)	N(23)-Mn(1)-N(21)	147.75(7)
C(24)-C(25)	1.418(3)	C(1)-N(1)-C(5)	119.2(2)
C(25)-C(29)	1.457(3)	C(1)-N(1)-Mn(1)	125.53(17)

C(5)-N(1)-Mn(1)	114.90(15)	C(7)-C(8)-H(8)	118.8
C(10)-N(2)-C(6)	125.46(19)	C(8)-C(9)-C(4)	119.2(2)
C(10)-N(2)-Mn(1)	117.29(14)	C(8)-C(9)-H(9)	120.4
C(6)-N(2)-Mn(1)	117.24(15)	C(4)-C(9)-H(9)	120.4
C(18)-N(3)-C(15)	119.7(2)	N(2)-C(10)-C(11)	129.3(2)
C(18)-N(3)-Mn(1)	125.64(16)	N(2)-C(10)-C(15)	115.21(18)
C(15)-N(3)-Mn(1)	114.55(14)	C(11)-C(10)-C(15)	115.40(19)
C(21)-N(21)-C(25)	119.20(19)	C(10)-C(11)-C(12)	121.9(2)
C(21)-N(21)-Mn(1)	125.94(15)	C(10)-C(11)-H(11)	119.0
C(25)-N(21)-Mn(1)	114.36(14)	C(12)-C(11)-H(11)	119.0
C(29)-N(22)-C(30)	124.42(19)	C(13)-C(12)-C(11)	122.2(2)
C(29)-N(22)-Mn(1)	118.14(14)	C(13)-C(12)-H(12)	118.9
C(30)-N(22)-Mn(1)	117.43(15)	C(11)-C(12)-H(12)	118.9
C(38)-N(23)-C(35)	119.4(2)	C(12)-C(13)-C(14)	118.5(2)
C(38)-N(23)-Mn(1)	126.47(17)	C(12)-C(13)-H(13)	120.7
C(35)-N(23)-Mn(1)	113.79(14)	C(14)-C(13)-H(13)	120.7
N(1)-C(1)-C(2)	122.9(3)	C(13)-C(14)-C(15)	120.0(2)
N(1)-C(1)-H(1)	118.6	C(13)-C(14)-C(16)	122.6(2)
C(2)-C(1)-H(1)	118.6	C(15)-C(14)-C(16)	117.3(2)
C(3)-C(2)-C(1)	118.7(2)	N(3)-C(15)-C(14)	121.0(2)
C(3)-C(2)-H(2)	120.6	N(3)-C(15)-C(10)	117.40(19)
C(1)-C(2)-H(2)	120.6	C(14)-C(15)-C(10)	121.6(2)
C(2)-C(3)-C(4)	120.8(2)	C(17)-C(16)-C(14)	120.3(2)
C(2)-C(3)-H(3)	119.6	C(17)-C(16)-H(16)	119.8
C(4)-C(3)-H(3)	119.6	C(14)-C(16)-H(16)	119.8
C(3)-C(4)-C(9)	123.3(2)	C(16)-C(17)-C(18)	118.7(2)
C(3)-C(4)-C(5)	117.3(2)	C(16)-C(17)-H(17)	120.7
C(9)-C(4)-C(5)	119.3(2)	C(18)-C(17)-H(17)	120.7
N(1)-C(5)-C(4)	121.1(2)	N(3)-C(18)-C(17)	122.7(2)
N(1)-C(5)-C(6)	117.2(2)	N(3)-C(18)-H(18)	118.6
C(4)-C(5)-C(6)	121.7(2)	C(17)-C(18)-H(18)	118.6
N(2)-C(6)-C(7)	128.6(2)	N(21)-C(21)-C(22)	122.9(2)
N(2)-C(6)-C(5)	115.6(2)	N(21)-C(21)-H(21)	118.5
C(7)-C(6)-C(5)	115.7(2)	C(22)-C(21)-H(21)	118.5
C(6)-C(7)-C(8)	121.5(2)	C(23)-C(22)-C(21)	118.5(2)
C(6)-C(7)-H(7)	119.2	C(23)-C(22)-H(22)	120.7
C(8)-C(7)-H(7)	119.2	C(21)-C(22)-H(22)	120.7
C(9)-C(8)-C(7)	122.4(2)	C(22)-C(23)-C(24)	120.6(2)
C(9)-C(8)-H(8)	118.8	C(22)-C(23)-H(23)	119.7

C(24)-C(23)-H(23)	119.7	C(30)-C(31)-H(31)	119.4
C(26)-C(24)-C(23)	123.3(2)	C(32)-C(31)-H(31)	119.4
C(26)-C(24)-C(25)	120.0(2)	C(33)-C(32)-C(31)	122.5(3)
C(23)-C(24)-C(25)	116.7(2)	C(33)-C(32)-H(32)	118.8
N(21)-C(25)-C(24)	122.01(19)	C(31)-C(32)-H(32)	118.8
N(21)-C(25)-C(29)	117.12(18)	C(32)-C(33)-C(34)	118.9(2)
C(24)-C(25)-C(29)	120.86(19)	C(32)-C(33)-H(33)	120.5
C(27)-C(26)-C(24)	119.3(2)	C(34)-C(33)-H(33)	120.5
C(27)-C(26)-H(26)	120.4	C(36)-C(34)-C(33)	123.4(2)
C(24)-C(26)-H(26)	120.4	C(36)-C(34)-C(35)	117.1(2)
C(26)-C(27)-C(28)	121.9(2)	C(33)-C(34)-C(35)	119.5(2)
C(26)-C(27)-H(27)	119.1	N(23)-C(35)-C(34)	121.2(2)
C(28)-C(27)-H(27)	119.1	N(23)-C(35)-C(30)	117.92(19)
C(27)-C(28)-C(29)	121.9(2)	C(34)-C(35)-C(30)	120.9(2)
C(27)-C(28)-H(28)	119.1	C(37)-C(36)-C(34)	120.9(2)
C(29)-C(28)-H(28)	119.1	C(37)-C(36)-H(36)	119.5
N(22)-C(29)-C(28)	129.5(2)	C(34)-C(36)-H(36)	119.5
N(22)-C(29)-C(25)	114.58(18)	C(36)-C(37)-C(38)	118.5(2)
C(28)-C(29)-C(25)	115.77(19)	C(36)-C(37)-H(37)	120.7
N(22)-C(30)-C(31)	128.5(2)	C(38)-C(37)-H(37)	120.7
N(22)-C(30)-C(35)	114.9(2)	N(23)-C(38)-C(37)	122.9(3)
C(31)-C(30)-C(35)	116.4(2)	N(23)-C(38)-H(38)	118.5
C(30)-C(31)-C(32)	121.2(2)	C(37)-C(38)-H(38)	118.5

Table S17. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Mn(BQA)_2]$. The anisotropic displacement factor exponent takes the form:
$-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	21(1)	17(1)	13(1)	0(1)	-1(1)	9(1)
N(1)	24(1)	15(1)	22(1)	0(1)	2(1)	7(1)
N(2)	21(1)	20(1)	14(1)	2(1)	0(1)	10(1)
N(3)	25(1)	18(1)	16(1)	2(1)	0(1)	12(1)
N(21)	22(1)	16(1)	14(1)	-3(1)	-1(1)	9(1)
N(22)	20(1)	17(1)	15(1)	0(1)	0(1)	7(1)

N(23)	26(1)	17(1)	17(1)	1(1)	4(1)	11(1)
C(1)	28(1)	20(1)	31(1)	-7(1)	4(1)	6(1)
C(2)	32(1)	25(1)	42(2)	-13(1)	9(1)	8(1)
C(3)	31(1)	22(1)	50(2)	-4(1)	13(1)	13(1)
C(4)	29(1)	20(1)	32(1)	6(1)	6(1)	13(1)
C(5)	23(1)	14(1)	24(1)	4(1)	2(1)	8(1)
C(6)	21(1)	16(1)	21(1)	6(1)	3(1)	8(1)
C(7)	24(1)	28(1)	23(1)	5(1)	2(1)	11(1)
C(8)	20(1)	38(1)	33(1)	8(1)	0(1)	14(1)
C(9)	28(1)	36(1)	42(2)	10(1)	8(1)	20(1)
C(10)	21(1)	11(1)	16(1)	2(1)	-1(1)	5(1)
C(11)	24(1)	20(1)	16(1)	2(1)	-2(1)	9(1)
C(12)	29(1)	22(1)	13(1)	0(1)	-2(1)	8(1)
C(13)	29(1)	20(1)	19(1)	-1(1)	3(1)	10(1)
C(14)	26(1)	15(1)	16(1)	3(1)	4(1)	9(1)
C(15)	26(1)	13(1)	14(1)	3(1)	1(1)	7(1)
C(16)	37(1)	24(1)	22(1)	-1(1)	4(1)	19(1)
C(17)	38(1)	30(1)	24(1)	1(1)	0(1)	24(1)
C(18)	34(1)	28(1)	20(1)	2(1)	-3(1)	19(1)
C(21)	21(1)	19(1)	19(1)	-2(1)	-2(1)	9(1)
C(22)	21(1)	16(1)	28(1)	1(1)	2(1)	6(1)
C(23)	28(1)	18(1)	25(1)	6(1)	6(1)	13(1)
C(24)	26(1)	16(1)	18(1)	3(1)	4(1)	12(1)
C(25)	22(1)	16(1)	15(1)	-1(1)	1(1)	11(1)
C(26)	35(1)	25(1)	16(1)	6(1)	2(1)	16(1)
C(27)	33(1)	29(1)	15(1)	-2(1)	-4(1)	16(1)
C(28)	26(1)	20(1)	18(1)	-4(1)	-4(1)	10(1)
C(29)	22(1)	15(1)	18(1)	-2(1)	0(1)	10(1)
C(30)	22(1)	17(1)	19(1)	-3(1)	2(1)	8(1)
C(31)	25(1)	32(1)	24(1)	0(1)	0(1)	10(1)
C(32)	20(1)	43(2)	32(1)	-6(1)	-3(1)	3(1)
C(33)	25(1)	30(1)	40(2)	-3(1)	7(1)	-2(1)
C(34)	32(1)	20(1)	27(1)	-1(1)	10(1)	6(1)
C(35)	23(1)	18(1)	22(1)	-1(1)	7(1)	9(1)
C(36)	41(2)	23(1)	37(2)	8(1)	19(1)	13(1)
C(37)	48(2)	31(1)	37(2)	17(1)	20(1)	25(1)
C(38)	36(1)	30(1)	24(1)	9(1)	10(1)	22(1)

Table S18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Mn(BQA)_2]$.

	x	y	z	U(eq)
H(1)	5458	-94	-927	35
H(2)	6418	-320	-1413	44
H(3)	7437	24	-404	42
H(7)	7249	1604	2882	31
H(8)	8220	1383	2457	37
H(9)	8144	677	1127	40
H(11)	6441	1266	3801	25
H(12)	6070	1712	5112	28
H(13)	5189	2097	4954	28
H(16)	4234	2189	3887	31
H(17)	3596	1910	2429	33
H(18)	3896	1302	1214	31
H(21)	6499	2424	424	25
H(22)	6995	3349	-783	27
H(23)	6348	3141	-2228	28
H(26)	5232	2268	-3271	30
H(27)	4153	1112	-3440	30
H(28)	3658	273	-2154	26
H(31)	2867	37	-1112	35
H(32)	1735	-1040	-711	45
H(33)	1670	-1869	457	46
H(36)	2328	-2139	1808	42
H(37)	3402	-1754	2734	44
H(38)	4503	-644	2321	33

[Cr(BQA)$_2$]

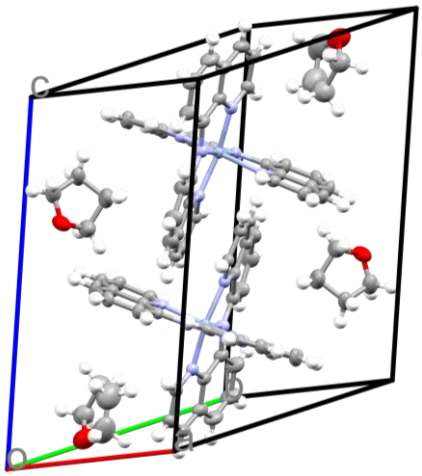

Fig. S24 Unit cell with complete molecules of Cr(BQA)$_2$

The unit cell of [Cr(BQA)$_2$] was determined using 9872 reflections and the structure was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of [Cr(BQA)$_2$] and two solvent molecules. One of the ligands and both solvent molecules were found to be disordered. The disorder was refined with the help of same distance restraints and similarity restraints on the anisotropic displacement parameters of the solvent atoms. Disordered atoms with very similar coordinates were set to the same anisotropic displacement parameters. The disorder ratios were allowed to refine freely and converged to 0.54(2) (ligand), 0.508(7) and 0.545(9) (solvent molecules).

Table S29. Crystal data and structure refinement for [Cr(BQA)$_2$].

CCDC No	2057276	
Empirical formula	C_{44} H_{40} Cr N_6 O_2	
Formula weight	736.82	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.0724(5) Å	α= 81.026(4)°.
	b = 12.7579(7) Å	β= 75.685(4)°.
	c = 16.0711(9) Å	γ = 79.295(4)°.
Volume	1759.15(17) Å^3	
Z	2	
Density (calculated)	1.391 Mg/m^3	
Absorption coefficient	3.061 mm^{-1}	
F(000)	772	
Crystal size	0.096 x 0.077 x 0.054 mm^3	
Theta range for data collection	3.549 to 66.586°.	

Index ranges	$-10 \leq h \leq 10, -15 \leq k \leq 15, -19 \leq l \leq 19$
Reflections collected	47080
Independent reflections	6152 [R(int) = 0.1039]
Completeness to theta = 66.586°	99.2 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6152 / 2210 / 724
Goodness-of-fit on F^2	1.034
Final R indices [I>2σ(I)]	R1 = 0.0570, wR2 = 0.1444
R indices (all data)	R1 = 0.0714, wR2 = 0.1548
Largest diff. peak and hole	0.691 and -0.544 e.Å^{-3}

Table S30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for [Cr(BQA)$_2$]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	3523(1)	6099(1)	2548(1)	29(1)
N(1)	1599(15)	5510(11)	3297(15)	28(3)
N(2)	4434(13)	4594(13)	2800(20)	33(3)
N(3)	5707(15)	6224(14)	1980(20)	30(2)
C(1)	162(18)	6031(13)	3489(17)	34(3)
C(2)	-1078(17)	5521(14)	3991(15)	41(3)
C(3)	-796(18)	4448(13)	4258(15)	41(3)
C(4)	675(16)	3854(11)	4032(17)	37(2)
C(5)	1056(18)	2742(10)	4290(12)	45(3)
C(6)	2506(18)	2246(11)	4021(12)	43(3)
C(7)	3698(18)	2799(11)	3531(18)	39(3)
C(8)	3439(13)	3895(10)	3286(10)	32(1)
C(9)	1876(14)	4416(9)	3532(10)	32(1)
C(10)	6293(17)	7093(12)	1524(15)	36(3)
C(11)	7895(17)	7093(13)	1255(14)	42(3)
C(12)	8881(16)	6211(13)	1407(13)	40(3)
C(13)	8326(14)	5260(12)	1853(16)	32(2)
C(14)	9279(14)	4288(12)	2027(12)	37(3)
C(15)	8645(12)	3411(12)	2443(13)	36(3)
C(16)	7049(11)	3458(10)	2760(8)	32(2)

C(17)	6029(13)	4387(12)	2604(16)	32(2)
C(18)	6697(14)	5306(14)	2130(20)	30(2)
N(1A)	1514(19)	5608(13)	3150(18)	29(3)
N(2A)	4322(15)	4552(14)	2900(20)	29(3)
N(3A)	5818(18)	6090(17)	2060(30)	31(4)
C(1A)	150(20)	6226(17)	3340(20)	37(4)
C(2A)	-1170(20)	5826(17)	3848(18)	44(4)
C(3A)	-1030(18)	4770(17)	4192(17)	41(4)
C(4A)	390(20)	4100(14)	4040(20)	38(3)
C(5A)	640(20)	2993(14)	4352(13)	42(3)
C(6A)	2050(20)	2427(13)	4183(14)	48(4)
C(7A)	3340(20)	2864(13)	3680(19)	42(3)
C(8A)	3196(16)	3939(12)	3346(12)	32(1)
C(9A)	1686(17)	4560(11)	3524(12)	32(1)
C(10A)	6510(20)	6946(15)	1684(17)	33(3)
C(11A)	8130(20)	6836(15)	1394(17)	44(4)
C(12A)	8999(19)	5880(14)	1518(15)	40(3)
C(13A)	8339(17)	4970(14)	1940(20)	35(3)
C(14A)	9181(17)	3954(14)	2101(14)	35(3)
C(15A)	8403(16)	3132(14)	2507(15)	40(3)
C(16A)	6803(14)	3247(11)	2730(10)	32(2)
C(17A)	5886(15)	4239(13)	2610(20)	32(2)
C(18A)	6697(17)	5112(16)	2200(30)	31(3)
N(21)	3077(3)	5982(2)	1391(2)	34(1)
N(22)	2625(3)	7616(2)	2261(2)	36(1)
N(23)	3723(3)	6723(2)	3579(2)	31(1)
C(21)	3283(3)	5110(3)	992(2)	39(1)
C(22)	3009(4)	5156(3)	163(2)	47(1)
C(23)	2527(4)	6121(3)	-259(2)	50(1)
C(24)	2304(4)	7064(3)	137(2)	46(1)
C(25)	1827(5)	8098(4)	-253(2)	58(1)
C(26)	1656(5)	8964(4)	174(3)	62(1)
C(27)	1899(5)	8881(3)	1014(2)	54(1)
C(28)	2318(4)	7879(3)	1442(2)	41(1)
C(29)	2570(3)	6962(3)	981(2)	37(1)
C(30)	4443(4)	6256(2)	4203(2)	35(1)
C(31)	4429(4)	6769(3)	4914(2)	40(1)
C(32)	3606(4)	7771(3)	5008(2)	44(1)
C(33)	2831(4)	8303(2)	4357(2)	40(1)

C(34)	1920(5)	9332(3)	4400(2)	53(1)
C(35)	1244(5)	9781(3)	3734(3)	59(1)
C(36)	1437(5)	9271(3)	2994(2)	51(1)
C(37)	2318(4)	8260(2)	2912(2)	38(1)
C(38)	2955(3)	7758(2)	3635(2)	34(1)
O(41)	2876(13)	9555(7)	6556(6)	69(2)
C(41)	3043(16)	10644(9)	6196(6)	81(3)
C(42)	3523(16)	11076(11)	6908(7)	90(3)
C(43)	2362(10)	10601(6)	7638(5)	59(2)
C(44)	2319(12)	9517(9)	7400(8)	64(2)
O(41A)	3421(14)	9351(8)	6637(8)	71(3)
C(41A)	4083(16)	10273(7)	6254(7)	73(3)
C(42A)	2922(16)	11229(9)	6730(8)	77(3)
C(43A)	3380(20)	10579(9)	7555(8)	95(3)
C(44A)	2820(20)	9559(11)	7466(9)	85(4)
O(51)	2899(9)	11280(6)	428(4)	85(2)
C(51)	1885(15)	11953(16)	992(9)	76(3)
C(52)	2633(16)	12051(13)	1718(8)	87(3)
C(53)	4116(15)	11333(15)	1507(10)	119(4)
C(54)	4289(12)	11078(12)	636(9)	110(3)
O(51A)	1646(7)	11502(5)	1554(4)	67(2)
C(51A)	2683(16)	11770(14)	1953(8)	83(3)
C(52A)	4207(12)	11900(11)	1327(8)	81(3)
C(53A)	3822(12)	11880(13)	491(7)	98(3)
C(54A)	2115(14)	11938(16)	706(8)	74(3)

Table S31. Bond lengths [Å] and angles [°] for $[Cr(BQA)_2]$.

Cr(1)-N(2)	1.967(14)	N(1)-C(9)	1.380(10)
Cr(1)-N(22)	1.986(3)	N(2)-C(17)	1.386(9)
Cr(1)-N(3)	1.991(13)	N(2)-C(8)	1.397(9)
Cr(1)-N(1A)	2.003(15)	N(3)-C(10)	1.349(10)
Cr(1)-N(23)	2.007(2)	N(3)-C(18)	1.368(10)
Cr(1)-N(2A)	2.014(14)	C(1)-C(2)	1.414(10)
Cr(1)-N(21)	2.030(3)	C(1)-H(1)	0.9500
Cr(1)-N(3A)	2.034(15)	C(2)-C(3)	1.365(10)
Cr(1)-N(1)	2.056(12)	C(2)-H(2)	0.9500
N(1)-C(1)	1.334(10)	C(3)-C(4)	1.400(10)

C(3)-H(3)	0.9500	C(5A)-C(6A)	1.333(12)
C(4)-C(5)	1.418(10)	C(5A)-H(5A)	0.9500
C(4)-C(9)	1.423(9)	C(6A)-C(7A)	1.405(12)
C(5)-C(6)	1.346(10)	C(6A)-H(6A)	0.9500
C(5)-H(5)	0.9500	C(7A)-C(8A)	1.388(11)
C(6)-C(7)	1.406(10)	C(7A)-H(7A)	0.9500
C(6)-H(6)	0.9500	C(8A)-C(9A)	1.435(9)
C(7)-C(8)	1.385(10)	C(10A)-C(11A)	1.412(12)
C(7)-H(7)	0.9500	C(10A)-H(10A)	0.9500
C(8)-C(9)	1.437(8)	C(11A)-C(12A)	1.339(12)
C(10)-C(11)	1.410(10)	C(11A)-H(11A)	0.9500
C(10)-H(10)	0.9500	C(12A)-C(13A)	1.406(11)
C(11)-C(12)	1.332(10)	C(12A)-H(12A)	0.9500
C(11)-H(11)	0.9500	C(13A)-C(14A)	1.399(11)
C(12)-C(13)	1.420(9)	C(13A)-C(18A)	1.429(11)
C(12)-H(12)	0.9500	C(14A)-C(15A)	1.362(11)
C(13)-C(14)	1.406(10)	C(14A)-H(14A)	0.9500
C(13)-C(18)	1.427(9)	C(15A)-C(16A)	1.392(11)
C(14)-C(15)	1.358(10)	C(15A)-H(15A)	0.9500
C(14)-H(14)	0.9500	C(16A)-C(17A)	1.394(9)
C(15)-C(16)	1.404(9)	C(16A)-H(16A)	0.9500
C(15)-H(15)	0.9500	C(17A)-C(18A)	1.433(11)
C(16)-C(17)	1.392(8)	N(21)-C(21)	1.331(4)
C(16)-H(16)	0.9500	N(21)-C(29)	1.375(4)
C(17)-C(18)	1.441(9)	N(22)-C(37)	1.373(4)
N(1A)-C(1A)	1.334(11)	N(22)-C(28)	1.390(4)
N(1A)-C(9A)	1.376(10)	N(23)-C(30)	1.333(4)
N(2A)-C(17A)	1.381(11)	N(23)-C(38)	1.379(4)
N(2A)-C(8A)	1.390(10)	C(21)-C(22)	1.404(5)
N(3A)-C(10A)	1.348(11)	C(21)-H(21)	0.9500
N(3A)-C(18A)	1.370(11)	C(22)-C(23)	1.362(5)
C(1A)-C(2A)	1.403(12)	C(22)-H(22)	0.9500
C(1A)-H(1A)	0.9500	C(23)-C(24)	1.406(5)
C(2A)-C(3A)	1.369(12)	C(23)-H(23)	0.9500
C(2A)-H(2A)	0.9500	C(24)-C(25)	1.408(5)
C(3A)-C(4A)	1.395(11)	C(24)-C(29)	1.419(4)
C(3A)-H(3A)	0.9500	C(25)-C(26)	1.355(6)
C(4A)-C(5A)	1.421(11)	C(25)-H(25)	0.9500
C(4A)-C(9A)	1.428(10)	C(26)-C(27)	1.406(5)

C(26)-H(26)	0.9500	C(42A)-H(42D)	0.9900
C(27)-C(28)	1.388(5)	C(43A)-C(44A)	1.523(14)
C(27)-H(27)	0.9500	C(43A)-H(43C)	0.9900
C(28)-C(29)	1.433(5)	C(43A)-H(43D)	0.9900
C(30)-C(31)	1.400(4)	C(44A)-H(44C)	0.9900
C(30)-H(30)	0.9500	C(44A)-H(44D)	0.9900
C(31)-C(32)	1.365(5)	O(51)-C(54)	1.353(12)
C(31)-H(31)	0.9500	O(51)-C(51)	1.393(12)
C(32)-C(33)	1.419(5)	C(51)-C(52)	1.519(14)
C(32)-H(32)	0.9500	C(51)-H(51A)	0.9900
C(33)-C(38)	1.415(4)	C(51)-H(51B)	0.9900
C(33)-C(34)	1.417(5)	C(52)-C(53)	1.476(14)
C(34)-C(35)	1.361(5)	C(52)-H(52A)	0.9900
C(34)-H(34)	0.9500	C(52)-H(52B)	0.9900
C(35)-C(36)	1.402(5)	C(53)-C(54)	1.450(14)
C(35)-H(35)	0.9500	C(53)-H(53A)	0.9900
C(36)-C(37)	1.393(5)	C(53)-H(53B)	0.9900
C(36)-H(36)	0.9500	C(54)-H(54A)	0.9900
C(37)-C(38)	1.434(4)	C(54)-H(54B)	0.9900
O(41)-C(44)	1.322(10)	O(51A)-C(51A)	1.378(13)
O(41)-C(41)	1.439(10)	O(51A)-C(54A)	1.383(12)
C(41)-C(42)	1.528(12)	C(51A)-C(52A)	1.515(14)
C(41)-H(41A)	0.9900	C(51A)-H(51C)	0.9900
C(41)-H(41B)	0.9900	C(51A)-H(51D)	0.9900
C(42)-C(43)	1.503(11)	C(52A)-C(53A)	1.474(13)
C(42)-H(42A)	0.9900	C(52A)-H(52C)	0.9900
C(42)-H(42B)	0.9900	C(52A)-H(52D)	0.9900
C(43)-C(44)	1.501(11)	C(53A)-C(54A)	1.492(13)
C(43)-H(43A)	0.9900	C(53A)-H(53C)	0.9900
C(43)-H(43B)	0.9900	C(53A)-H(53D)	0.9900
C(44)-H(44A)	0.9900	C(54A)-H(54C)	0.9900
C(44)-H(44B)	0.9900	C(54A)-H(54D)	0.9900
O(41A)-C(44A)	1.358(12)		
O(41A)-C(41A)	1.406(10)	N(2)-Cr(1)-N(22)	178.5(9)
C(41A)-C(42A)	1.612(13)	N(2)-Cr(1)-N(3)	81.6(5)
C(41A)-H(41C)	0.9900	N(22)-Cr(1)-N(3)	97.6(4)
C(41A)-H(41D)	0.9900	N(22)-Cr(1)-N(1A)	95.5(4)
C(42A)-C(43A)	1.556(13)	N(2)-Cr(1)-N(23)	100.8(10)
C(42A)-H(42C)	0.9900	N(22)-Cr(1)-N(23)	80.44(10)

N(3)-Cr(1)-N(23)	90.5(13)	C(3)-C(4)-C(5)	124.5(9)
N(1A)-Cr(1)-N(23)	93.7(10)	C(3)-C(4)-C(9)	117.5(8)
N(22)-Cr(1)-N(2A)	176.6(6)	C(5)-C(4)-C(9)	118.0(8)
N(1A)-Cr(1)-N(2A)	81.3(5)	C(6)-C(5)-C(4)	119.4(9)
N(23)-Cr(1)-N(2A)	98.4(12)	C(6)-C(5)-H(5)	120.3
N(2)-Cr(1)-N(21)	98.0(10)	C(4)-C(5)-H(5)	120.3
N(22)-Cr(1)-N(21)	80.79(10)	C(5)-C(6)-C(7)	122.7(9)
N(3)-Cr(1)-N(21)	90.5(12)	C(5)-C(6)-H(6)	118.7
N(1A)-Cr(1)-N(21)	89.6(9)	C(7)-C(6)-H(6)	118.7
N(23)-Cr(1)-N(21)	161.17(10)	C(8)-C(7)-C(6)	121.5(9)
N(2A)-Cr(1)-N(21)	100.5(12)	C(8)-C(7)-H(7)	119.3
N(22)-Cr(1)-N(3A)	103.2(5)	C(6)-C(7)-H(7)	119.3
N(1A)-Cr(1)-N(3A)	161.3(6)	C(7)-C(8)-N(2)	131.0(9)
N(23)-Cr(1)-N(3A)	88.7(15)	C(7)-C(8)-C(9)	115.9(7)
N(2A)-Cr(1)-N(3A)	79.9(5)	N(2)-C(8)-C(9)	113.0(8)
N(21)-Cr(1)-N(3A)	94.1(15)	N(1)-C(9)-C(4)	121.0(8)
N(2)-Cr(1)-N(1)	80.6(4)	N(1)-C(9)-C(8)	116.7(8)
N(22)-Cr(1)-N(1)	100.3(3)	C(4)-C(9)-C(8)	122.3(7)
N(3)-Cr(1)-N(1)	161.7(5)	N(3)-C(10)-C(11)	121.4(10)
N(23)-Cr(1)-N(1)	88.7(8)	N(3)-C(10)-H(10)	119.3
N(21)-Cr(1)-N(1)	96.1(8)	C(11)-C(10)-H(10)	119.3
C(1)-N(1)-C(9)	119.3(10)	C(12)-C(11)-C(10)	120.8(10)
C(1)-N(1)-Cr(1)	127.8(8)	C(12)-C(11)-H(11)	119.6
C(9)-N(1)-Cr(1)	112.5(7)	C(10)-C(11)-H(11)	119.6
C(17)-N(2)-C(8)	126.5(11)	C(11)-C(12)-C(13)	120.1(9)
C(17)-N(2)-Cr(1)	115.6(8)	C(11)-C(12)-H(12)	119.9
C(8)-N(2)-Cr(1)	117.0(7)	C(13)-C(12)-H(12)	119.9
C(10)-N(3)-C(18)	118.8(9)	C(14)-C(13)-C(12)	124.0(8)
C(10)-N(3)-Cr(1)	128.4(9)	C(14)-C(13)-C(18)	118.7(8)
C(18)-N(3)-Cr(1)	112.7(8)	C(12)-C(13)-C(18)	117.2(8)
N(1)-C(1)-C(2)	122.3(10)	C(15)-C(14)-C(13)	120.0(9)
N(1)-C(1)-H(1)	118.8	C(15)-C(14)-H(14)	120.0
C(2)-C(1)-H(1)	118.8	C(13)-C(14)-H(14)	120.0
C(3)-C(2)-C(1)	118.5(9)	C(14)-C(15)-C(16)	121.8(9)
C(3)-C(2)-H(2)	120.8	C(14)-C(15)-H(15)	119.1
C(1)-C(2)-H(2)	120.8	C(16)-C(15)-H(15)	119.1
C(2)-C(3)-C(4)	121.3(9)	C(17)-C(16)-C(15)	121.5(7)
C(2)-C(3)-H(3)	119.3	C(17)-C(16)-H(16)	119.3
C(4)-C(3)-H(3)	119.3	C(15)-C(16)-H(16)	119.3

N(2)-C(17)-C(16)	131.4(8)	N(1A)-C(9A)-C(4A)	120.7(10)
N(2)-C(17)-C(18)	112.0(9)	N(1A)-C(9A)-C(8A)	117.6(9)
C(16)-C(17)-C(18)	116.6(7)	C(4A)-C(9A)-C(8A)	121.7(8)
N(3)-C(18)-C(13)	121.6(8)	N(3A)-C(10A)-C(11A)	120.8(12)
N(3)-C(18)-C(17)	117.2(8)	N(3A)-C(10A)-H(10A)	119.6
C(13)-C(18)-C(17)	121.2(9)	C(11A)-C(10A)-H(10A)	119.6
C(1A)-N(1A)-C(9A)	119.3(11)	C(12A)-C(11A)-C(10A)	120.2(11)
C(1A)-N(1A)-Cr(1)	126.6(11)	C(12A)-C(11A)-H(11A)	119.9
C(9A)-N(1A)-Cr(1)	113.0(8)	C(10A)-C(11A)-H(11A)	119.9
C(17A)-N(2A)-C(8A)	129.4(11)	C(11A)-C(12A)-C(13A)	121.4(11)
C(17A)-N(2A)-Cr(1)	115.7(8)	C(11A)-C(12A)-H(12A)	119.3
C(8A)-N(2A)-Cr(1)	114.8(8)	C(13A)-C(12A)-H(12A)	119.3
C(10A)-N(3A)-C(18A)	119.5(11)	C(14A)-C(13A)-C(12A)	124.3(10)
C(10A)-N(3A)-Cr(1)	126.5(11)	C(14A)-C(13A)-C(18A)	119.1(10)
C(18A)-N(3A)-Cr(1)	113.9(8)	C(12A)-C(13A)-C(18A)	116.6(10)
N(1A)-C(1A)-C(2A)	122.5(13)	C(15A)-C(14A)-C(13A)	118.7(10)
N(1A)-C(1A)-H(1A)	118.8	C(15A)-C(14A)-H(14A)	120.7
C(2A)-C(1A)-H(1A)	118.8	C(13A)-C(14A)-H(14A)	120.7
C(3A)-C(2A)-C(1A)	118.8(12)	C(14A)-C(15A)-C(16A)	122.8(11)
C(3A)-C(2A)-H(2A)	120.6	C(14A)-C(15A)-H(15A)	118.6
C(1A)-C(2A)-H(2A)	120.6	C(16A)-C(15A)-H(15A)	118.6
C(2A)-C(3A)-C(4A)	120.9(11)	C(15A)-C(16A)-C(17A)	121.8(8)
C(2A)-C(3A)-H(3A)	119.6	C(15A)-C(16A)-H(16A)	119.1
C(4A)-C(3A)-H(3A)	119.6	C(17A)-C(16A)-H(16A)	119.1
C(3A)-C(4A)-C(5A)	125.0(10)	N(2A)-C(17A)-C(16A)	130.7(9)
C(3A)-C(4A)-C(9A)	117.7(10)	N(2A)-C(17A)-C(18A)	113.4(10)
C(5A)-C(4A)-C(9A)	117.3(10)	C(16A)-C(17A)-C(18A)	115.6(8)
C(6A)-C(5A)-C(4A)	120.4(11)	N(3A)-C(18A)-C(13A)	121.5(10)
C(6A)-C(5A)-H(5A)	119.8	N(3A)-C(18A)-C(17A)	116.6(10)
C(4A)-C(5A)-H(5A)	119.8	C(13A)-C(18A)-C(17A)	121.9(10)
C(5A)-C(6A)-C(7A)	123.2(12)	C(21)-N(21)-C(29)	118.9(3)
C(5A)-C(6A)-H(6A)	118.4	C(21)-N(21)-Cr(1)	128.4(2)
C(7A)-C(6A)-H(6A)	118.4	C(29)-N(21)-Cr(1)	112.6(2)
C(8A)-C(7A)-C(6A)	120.2(11)	C(37)-N(22)-C(28)	128.2(3)
C(8A)-C(7A)-H(7A)	119.9	C(37)-N(22)-Cr(1)	115.8(2)
C(6A)-C(7A)-H(7A)	119.9	C(28)-N(22)-Cr(1)	115.9(2)
C(7A)-C(8A)-N(2A)	129.8(11)	C(30)-N(23)-C(38)	118.4(3)
C(7A)-C(8A)-C(9A)	117.2(9)	C(30)-N(23)-Cr(1)	128.5(2)
N(2A)-C(8A)-C(9A)	112.8(10)	C(38)-N(23)-Cr(1)	113.08(19)

N(21)-C(21)-C(22)	122.3(3)	C(35)-C(34)-C(33)	119.3(3)
N(21)-C(21)-H(21)	118.8	C(35)-C(34)-H(34)	120.3
C(22)-C(21)-H(21)	118.8	C(33)-C(34)-H(34)	120.3
C(23)-C(22)-C(21)	119.6(3)	C(34)-C(35)-C(36)	122.4(3)
C(23)-C(22)-H(22)	120.2	C(34)-C(35)-H(35)	118.8
C(21)-C(22)-H(22)	120.2	C(36)-C(35)-H(35)	118.8
C(22)-C(23)-C(24)	119.9(3)	C(37)-C(36)-C(35)	121.2(3)
C(22)-C(23)-H(23)	120.0	C(37)-C(36)-H(36)	119.4
C(24)-C(23)-H(23)	120.0	C(35)-C(36)-H(36)	119.4
C(23)-C(24)-C(25)	124.0(3)	N(22)-C(37)-C(36)	130.6(3)
C(23)-C(24)-C(29)	117.7(3)	N(22)-C(37)-C(38)	112.9(3)
C(25)-C(24)-C(29)	118.3(3)	C(36)-C(37)-C(38)	116.5(3)
C(26)-C(25)-C(24)	120.0(3)	N(23)-C(38)-C(33)	121.8(3)
C(26)-C(25)-H(25)	120.0	N(23)-C(38)-C(37)	116.3(3)
C(24)-C(25)-H(25)	120.0	C(33)-C(38)-C(37)	121.9(3)
C(25)-C(26)-C(27)	122.7(4)	C(44)-O(41)-C(41)	109.6(8)
C(25)-C(26)-H(26)	118.7	O(41)-C(41)-C(42)	102.5(8)
C(27)-C(26)-H(26)	118.7	O(41)-C(41)-H(41A)	111.3
C(28)-C(27)-C(26)	119.9(4)	C(42)-C(41)-H(41A)	111.3
C(28)-C(27)-H(27)	120.1	O(41)-C(41)-H(41B)	111.3
C(26)-C(27)-H(27)	120.1	C(42)-C(41)-H(41B)	111.3
C(27)-C(28)-N(22)	129.3(3)	H(41A)-C(41)-H(41B)	109.2
C(27)-C(28)-C(29)	117.8(3)	C(43)-C(42)-C(41)	95.4(7)
N(22)-C(28)-C(29)	112.8(3)	C(43)-C(42)-H(42A)	112.7
N(21)-C(29)-C(24)	121.4(3)	C(41)-C(42)-H(42A)	112.7
N(21)-C(29)-C(28)	117.3(3)	C(43)-C(42)-H(42B)	112.7
C(24)-C(29)-C(28)	121.3(3)	C(41)-C(42)-H(42B)	112.7
N(23)-C(30)-C(31)	122.6(3)	H(42A)-C(42)-H(42B)	110.2
N(23)-C(30)-H(30)	118.7	C(44)-C(43)-C(42)	104.7(7)
C(31)-C(30)-H(30)	118.7	C(44)-C(43)-H(43A)	110.8
C(32)-C(31)-C(30)	120.1(3)	C(42)-C(43)-H(43A)	110.8
C(32)-C(31)-H(31)	120.0	C(44)-C(43)-H(43B)	110.8
C(30)-C(31)-H(31)	120.0	C(42)-C(43)-H(43B)	110.8
C(31)-C(32)-C(33)	119.3(3)	H(43A)-C(43)-H(43B)	108.9
C(31)-C(32)-H(32)	120.4	O(41)-C(44)-C(43)	106.3(8)
C(33)-C(32)-H(32)	120.4	O(41)-C(44)-H(44A)	110.5
C(38)-C(33)-C(34)	118.5(3)	C(43)-C(44)-H(44A)	110.5
C(38)-C(33)-C(32)	117.6(3)	O(41)-C(44)-H(44B)	110.5
C(34)-C(33)-C(32)	123.8(3)	C(43)-C(44)-H(44B)	110.5

H(44A)-C(44)-H(44B)	108.7	H(52A)-C(52)-H(52B)	109.2
C(44A)-O(41A)-C(41A)	102.9(9)	C(54)-C(53)-C(52)	106.7(10)
O(41A)-C(41A)-C(42A)	103.7(9)	C(54)-C(53)-H(53A)	110.4
O(41A)-C(41A)-H(41C)	111.0	C(52)-C(53)-H(53A)	110.4
C(42A)-C(41A)-H(41C)	111.0	C(54)-C(53)-H(53B)	110.4
O(41A)-C(41A)-H(41D)	111.0	C(52)-C(53)-H(53B)	110.4
C(42A)-C(41A)-H(41D)	111.0	H(53A)-C(53)-H(53B)	108.6
H(41C)-C(41A)-H(41D)	109.0	O(51)-C(54)-C(53)	109.5(9)
C(43A)-C(42A)-C(41A)	83.3(9)	O(51)-C(54)-H(54A)	109.8
C(43A)-C(42A)-H(42C)	114.8	C(53)-C(54)-H(54A)	109.8
C(41A)-C(42A)-H(42C)	114.8	O(51)-C(54)-H(54B)	109.8
C(43A)-C(42A)-H(42D)	114.8	C(53)-C(54)-H(54B)	109.8
C(41A)-C(42A)-H(42D)	114.8	H(54A)-C(54)-H(54B)	108.2
H(42C)-C(42A)-H(42D)	111.8	C(51A)-O(51A)-C(54A)	102.9(9)
C(44A)-C(43A)-C(42A)	95.4(10)	O(51A)-C(51A)-C(52A)	111.9(9)
C(44A)-C(43A)-H(43C)	112.7	O(51A)-C(51A)-H(51C)	109.2
C(42A)-C(43A)-H(43C)	112.7	C(52A)-C(51A)-H(51C)	109.2
C(44A)-C(43A)-H(43D)	112.7	O(51A)-C(51A)-H(51D)	109.2
C(42A)-C(43A)-H(43D)	112.7	C(52A)-C(51A)-H(51D)	109.2
H(43C)-C(43A)-H(43D)	110.1	H(51C)-C(51A)-H(51D)	107.9
O(41A)-C(44A)-C(43A)	106.1(10)	C(53A)-C(52A)-C(51A)	101.4(8)
O(41A)-C(44A)-H(44C)	110.5	C(53A)-C(52A)-H(52C)	111.5
C(43A)-C(44A)-H(44C)	110.5	C(51A)-C(52A)-H(52C)	111.5
O(41A)-C(44A)-H(44D)	110.5	C(53A)-C(52A)-H(52D)	111.5
C(43A)-C(44A)-H(44D)	110.5	C(51A)-C(52A)-H(52D)	111.5
H(44C)-C(44A)-H(44D)	108.7	H(52C)-C(52A)-H(52D)	109.3
C(54)-O(51)-C(51)	109.2(9)	C(52A)-C(53A)-C(54A)	104.4(8)
O(51)-C(51)-C(52)	109.0(10)	C(52A)-C(53A)-H(53C)	110.9
O(51)-C(51)-H(51A)	109.9	C(54A)-C(53A)-H(53C)	110.9
C(52)-C(51)-H(51A)	109.9	C(52A)-C(53A)-H(53D)	110.9
O(51)-C(51)-H(51B)	109.9	C(54A)-C(53A)-H(53D)	110.9
C(52)-C(51)-H(51B)	109.9	H(53C)-C(53A)-H(53D)	108.9
H(51A)-C(51)-H(51B)	108.3	O(51A)-C(54A)-C(53A)	108.9(9)
C(53)-C(52)-C(51)	102.3(10)	O(51A)-C(54A)-H(54C)	109.9
C(53)-C(52)-H(52A)	111.3	C(53A)-C(54A)-H(54C)	109.9
C(51)-C(52)-H(52A)	111.3	O(51A)-C(54A)-H(54D)	109.9
C(53)-C(52)-H(52B)	111.3	C(53A)-C(54A)-H(54D)	109.9
C(51)-C(52)-H(52B)	111.3	H(54C)-C(54A)-H(54D)	108.3

Table S32. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cr(BQA)_2]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	26(1)	32(1)	29(1)	-4(1)	-5(1)	-5(1)
N(1)	27(3)	41(4)	17(7)	-4(3)	-7(3)	-4(3)
N(2)	29(3)	42(5)	28(7)	-6(3)	-2(3)	-12(3)
N(3)	31(4)	31(5)	29(5)	-3(4)	-8(4)	-3(3)
C(1)	32(4)	40(5)	29(8)	-5(5)	-5(4)	-4(3)
C(2)	29(4)	49(8)	40(8)	-6(6)	0(4)	-5(5)
C(3)	38(6)	44(6)	40(6)	-8(5)	2(5)	-14(4)
C(4)	35(5)	42(6)	36(4)	-7(5)	-7(4)	-11(4)
C(5)	42(7)	37(5)	49(5)	-1(5)	6(6)	-15(5)
C(6)	48(6)	32(4)	49(7)	-1(4)	-11(5)	-14(4)
C(7)	33(5)	39(4)	44(8)	-3(3)	-3(4)	-9(3)
C(8)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(9)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(10)	32(4)	33(5)	40(8)	1(4)	-7(4)	-7(4)
C(11)	32(5)	33(6)	55(7)	-1(4)	-1(4)	-6(4)
C(12)	28(4)	35(7)	55(5)	-4(6)	-2(4)	-11(5)
C(13)	32(3)	33(6)	33(5)	-8(6)	-9(3)	-4(3)
C(14)	30(4)	34(6)	47(5)	-9(5)	-9(3)	-4(4)
C(15)	32(4)	33(7)	47(6)	-3(5)	-15(4)	-2(3)
C(16)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(17)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(18)	28(4)	35(6)	27(5)	-4(6)	-7(4)	-8(3)
N(1A)	34(4)	38(4)	19(8)	-4(3)	-10(4)	-7(3)
N(2A)	34(4)	24(5)	25(7)	-2(4)	-7(4)	1(3)
N(3A)	28(4)	31(5)	35(9)	-5(5)	-6(5)	-5(4)
C(1A)	25(4)	48(7)	33(10)	-2(5)	1(4)	-6(4)
C(2A)	35(5)	56(8)	37(8)	-10(7)	2(5)	-9(5)
C(3A)	29(5)	55(10)	37(6)	0(9)	-2(4)	-12(5)
C(4A)	39(6)	46(7)	31(5)	-2(6)	-5(6)	-15(5)
C(5A)	43(7)	50(7)	37(6)	2(6)	-12(5)	-18(5)
C(6A)	49(9)	40(7)	52(8)	2(6)	-4(7)	-16(6)
C(7A)	47(8)	41(5)	44(10)	2(5)	-18(7)	-15(5)

C(8A)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(9A)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(10A)	32(5)	34(5)	34(8)	2(4)	-11(5)	-5(4)
C(11A)	31(6)	36(8)	63(9)	-4(7)	-5(6)	-8(5)
C(12A)	32(5)	32(8)	54(8)	-19(6)	-4(4)	1(5)
C(13A)	35(4)	33(7)	41(7)	-13(6)	-9(4)	-5(4)
C(14A)	32(5)	33(8)	46(7)	-13(6)	-18(4)	-2(4)
C(15A)	48(5)	36(7)	34(5)	-2(5)	-10(5)	1(4)
C(16A)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(17A)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(18A)	30(4)	30(5)	34(9)	-11(5)	-10(4)	2(3)
N(21)	27(1)	42(1)	32(1)	-6(1)	-3(1)	-6(1)
N(22)	39(1)	34(1)	35(1)	-2(1)	-8(1)	-2(1)
N(23)	31(1)	32(1)	29(1)	-2(1)	-4(1)	-8(1)
C(21)	30(2)	49(2)	38(2)	-12(1)	-3(1)	-6(1)
C(22)	36(2)	67(2)	42(2)	-19(2)	-3(2)	-10(2)
C(23)	39(2)	81(2)	32(2)	-10(2)	-6(1)	-11(2)
C(24)	34(2)	67(2)	35(2)	-3(2)	-6(1)	-6(2)
C(25)	53(2)	80(3)	36(2)	8(2)	-15(2)	-3(2)
C(26)	67(3)	64(2)	46(2)	12(2)	-14(2)	5(2)
C(27)	61(2)	47(2)	46(2)	4(2)	-10(2)	4(2)
C(28)	38(2)	46(2)	34(2)	1(1)	-5(1)	-4(1)
C(29)	28(2)	50(2)	31(2)	1(1)	-4(1)	-5(1)
C(30)	35(2)	36(2)	34(2)	-1(1)	-6(1)	-10(1)
C(31)	48(2)	44(2)	32(2)	2(1)	-10(1)	-17(1)
C(32)	61(2)	44(2)	31(2)	-6(1)	-6(2)	-21(2)
C(33)	51(2)	35(2)	35(2)	-5(1)	-2(1)	-16(1)
C(34)	74(3)	36(2)	46(2)	-10(2)	-3(2)	-12(2)
C(35)	76(3)	34(2)	61(2)	-8(2)	-9(2)	1(2)
C(36)	66(2)	34(2)	48(2)	-2(2)	-13(2)	4(2)
C(37)	42(2)	33(2)	38(2)	-1(1)	-7(1)	-7(1)
C(38)	35(2)	31(2)	34(2)	-2(1)	-3(1)	-9(1)
O(41)	102(6)	66(4)	52(3)	-4(3)	-33(4)	-27(4)
C(41)	103(6)	90(5)	58(4)	-6(4)	-10(5)	-47(5)
C(42)	105(7)	95(6)	78(6)	-18(5)	5(5)	-61(5)
C(43)	45(4)	63(4)	70(4)	-25(3)	5(4)	-18(3)
C(44)	46(4)	60(4)	81(4)	-20(4)	3(4)	-12(4)
O(41A)	83(6)	44(4)	70(5)	-2(3)	12(5)	-13(4)
C(41A)	89(6)	48(5)	75(5)	-9(4)	8(5)	-29(4)

C(42A)	82(7)	55(5)	93(6)	13(5)	-26(5)	-16(5)
C(43A)	128(8)	70(5)	83(6)	-7(5)	-19(6)	-10(6)
C(44A)	114(9)	61(5)	71(5)	6(4)	-21(6)	-2(6)
O(51)	95(5)	64(4)	79(4)	-5(3)	-3(4)	8(4)
C(51)	69(5)	74(6)	77(6)	-6(6)	-14(5)	2(5)
C(52)	70(5)	98(7)	91(6)	-12(6)	-29(5)	2(5)
C(53)	71(6)	148(9)	128(7)	7(7)	-31(6)	-2(6)
C(54)	70(5)	101(7)	137(7)	-27(6)	13(5)	1(5)
O(51A)	65(4)	61(4)	70(4)	1(3)	-11(3)	-12(3)
C(51A)	72(5)	100(8)	80(6)	-2(6)	-17(4)	-24(5)
C(52A)	58(4)	82(6)	101(6)	-1(5)	-25(4)	-3(5)
C(53A)	73(5)	121(7)	81(5)	12(6)	-8(4)	-2(6)
C(54A)	67(5)	69(6)	79(6)	1(6)	-15(5)	-6(5)

Table S33. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Cr(BQA)_2]$.

	x	y	z	U(eq)
H(1)	-34	6771	3281	41
H(2)	-2084	5916	4138	49
H(3)	-1615	4099	4605	49
H(5)	294	2350	4650	54
H(6)	2732	1493	4169	51
H(7)	4704	2411	3363	47
H(10)	5611	7719	1381	43
H(11)	8275	7729	963	50
H(12)	9958	6218	1216	48
H(14)	10366	4245	1854	44
H(15)	9300	2747	2522	44
H(16)	6657	2843	3088	38
H(1A)	59	6965	3118	44
H(2A)	-2137	6279	3954	52
H(3A)	-1912	4490	4540	49
H(5A)	-200	2654	4686	51
H(6A)	2186	1692	4413	58
H(7A)	4318	2422	3568	51

H(10A)	5908	7632	1613	40
H(11A)	8601	7441	1112	53
H(12A)	10085	5816	1318	48
H(14A)	10273	3839	1934	42
H(15A)	8977	2452	2644	49
H(16A)	6323	2632	2968	38
H(21)	3628	4432	1277	47
H(22)	3159	4516	-102	57
H(23)	2343	6158	-820	60
H(25)	1625	8188	-814	70
H(26)	1360	9657	-107	75
H(27)	1776	9509	1289	65
H(30)	4986	5547	4163	42
H(31)	4993	6421	5332	48
H(32)	3552	8109	5504	53
H(34)	1782	9704	4888	63
H(35)	618	10465	3773	70
H(36)	959	9622	2540	62
H(41A)	2059	11055	6084	97
H(41B)	3845	10667	5652	97
H(42A)	4598	10785	6947	109
H(42B)	3364	11870	6852	109
H(43A)	2683	10532	8193	71
H(43B)	1338	11054	7693	71
H(44A)	2955	8950	7710	77
H(44B)	1250	9361	7551	77
H(41C)	4145	10388	5624	87
H(41D)	5128	10216	6357	87
H(42C)	3262	11942	6572	92
H(42D)	1830	11268	6713	92
H(43C)	4502	10472	7517	114
H(43D)	2815	10898	8090	114
H(44C)	3170	8956	7874	102
H(44D)	1677	9666	7589	102
H(51A)	915	11653	1233	91
H(51B)	1636	12671	677	91
H(52A)	2789	12799	1715	104
H(52B)	2008	11806	2289	104
H(53A)	4973	11695	1538	143

H(53B)	4115	10670	1920	143
H(54A)	5003	11517	224	132
H(54B)	4728	10311	600	132
H(51C)	2860	11202	2429	100
H(51D)	2243	12450	2207	100
H(52C)	4534	12590	1356	97
H(52D)	5027	11301	1437	97
H(53C)	4335	11209	239	117
H(53D)	4139	12501	77	117
H(54C)	1617	12695	629	89
H(54D)	1808	11534	314	89

[Cr(BQA)$_2$]Cl

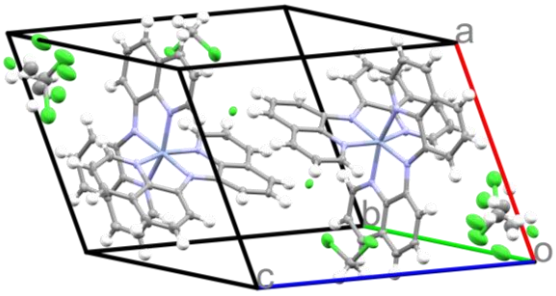

Fig. S25 Unit cell with complete molecules of [Cr(BQA)$_2$]Cl

The unit cell of [Cr(BQA)$_2$]Cl was determined using 9988 reflections and the structure was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one [Cr(BQA)$_2$], the chloride anion and two dichloromethane molecules. One of the solvent molecules was found to be disordered over three positions. The disorder was refined with the help of similarity restraints on 1,2- and 1,3 distances and ADP similarity restraints. The thermal displacement parameters of equivalent atoms of the disordered solvent molecule were set to the same parameters. [7,8] The disorder ratio was allowed to refine and converged to 0.593(2), 0.337(2) and 0.071(2).

Table S19. Crystal data and structure refinement for [Cr(BQA)$_2$]Cl.

CCDC No.	1897893	
Empirical formula	C_{38} H_{28} Cl_5 Cr N_6	
Formula weight	797.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.7738(4) Å	α= 80.5576(14)°.
	b = 11.6879(5) Å	β= 78.3853(14)°.
	c = 15.3294(6) Å	γ = 68.2652(14)°.
Volume	1747.86(12) Å^3	
Z	2	
Density (calculated)	1.516 Mg/m^3	
Absorption coefficient	0.749 mm^{-1}	
F(000)	814	
Crystal size	0.982 x 0.032 x 0.028 mm^3	
Theta range for data collection	2.215 to 27.103°.	
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19	
Reflections collected	89998	
Independent reflections	7699 [R(int) = 0.1164]	

Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7699 / 157 / 478
Goodness-of-fit on F^2	1.045
Final R indices [I>2σ(I)]	R1 = 0.0543, wR2 = 0.1228
R indices (all data)	R1 = 0.0766, wR2 = 0.1323
Largest diff. peak and hole	0.942 and -1.309 e.Å^{-3}

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)for [Cr(BQA)$_2$]Cl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	4635(1)	7507(1)	7468(1)	11(1)
N(1)	6637(2)	6448(2)	7278(2)	14(1)
N(2)	5425(2)	8789(2)	7464(2)	14(1)
N(3)	2899(2)	9010(2)	7651(2)	16(1)
N(21)	4601(2)	7630(2)	6126(2)	14(1)
N(22)	3761(2)	6277(2)	7475(2)	14(1)
N(23)	4379(3)	6968(2)	8808(2)	16(1)
C(1)	7180(3)	5244(3)	7196(2)	16(1)
C(2)	8569(3)	4633(3)	7001(2)	22(1)
C(3)	9412(3)	5300(3)	6867(2)	24(1)
C(4)	8883(3)	6589(3)	6936(2)	19(1)
C(5)	9671(3)	7360(3)	6761(2)	24(1)
C(6)	9034(3)	8610(3)	6794(2)	24(1)
C(7)	7626(3)	9156(3)	7029(2)	19(1)
C(8)	6811(3)	8438(3)	7236(2)	14(1)
C(9)	7466(3)	7136(3)	7155(2)	15(1)
C(10)	4523(3)	9949(3)	7664(2)	14(1)
C(11)	4768(3)	10984(3)	7813(2)	18(1)
C(12)	3693(3)	12095(3)	7990(2)	21(1)
C(13)	2376(3)	12212(3)	8037(2)	22(1)
C(14)	2063(3)	11180(3)	7924(2)	19(1)

C(15)	739(3)	11192(3)	7974(2)	26(1)
C(16)	524(3)	10144(3)	7867(2)	26(1)
C(17)	1635(3)	9058(3)	7717(2)	21(1)
C(18)	3134(3)	10058(3)	7745(2)	15(1)
C(21)	5097(3)	8315(3)	5475(2)	19(1)
C(22)	4992(3)	8331(3)	4575(2)	22(1)
C(23)	4360(3)	7622(3)	4355(2)	21(1)
C(24)	3853(3)	6853(3)	5028(2)	18(1)
C(25)	3279(3)	6025(3)	4846(2)	21(1)
C(26)	2968(3)	5218(3)	5523(2)	22(1)
C(27)	3137(3)	5219(3)	6415(2)	18(1)
C(28)	3589(3)	6078(3)	6645(2)	15(1)
C(29)	4007(3)	6873(3)	5920(2)	14(1)
C(30)	3201(3)	5881(3)	8309(2)	16(1)
C(31)	2305(3)	5243(3)	8535(2)	23(1)
C(32)	1836(4)	4935(3)	9437(2)	30(1)
C(33)	2221(4)	5263(3)	10129(2)	31(1)
C(34)	3096(3)	5957(3)	9938(2)	23(1)
C(35)	3506(4)	6402(3)	10594(2)	32(1)
C(36)	4337(4)	7075(3)	10355(2)	31(1)
C(37)	4763(3)	7345(3)	9447(2)	24(1)
C(38)	3569(3)	6261(3)	9033(2)	18(1)
Cl(41)	1542(1)	10044(1)	5440(1)	41(1)
Cl(42)	1192(1)	12615(1)	5515(1)	57(1)
C(41)	353(4)	11565(3)	5563(3)	33(1)
Cl(51)	869(3)	11889(3)	10629(2)	67(1)
Cl(52)	3701(2)	10448(2)	10131(1)	56(1)
C(51)	2120(9)	10339(10)	10520(8)	51(2)
Cl(53)	1451(3)	9502(3)	9963(2)	32(1)
Cl(54)	1595(5)	11692(5)	10614(4)	67(1)
C(51A)	2511(16)	10165(16)	10339(16)	51(2)
Cl(55)	166(18)	11637(17)	10149(13)	67(1)
Cl(56)	2755(19)	10723(17)	10593(12)	56(1)
C(51B)	1620(30)	10230(30)	10220(50)	51(2)
Cl(1)	-2585(1)	12180(1)	7434(1)	19(1)

Table S21. Bond lengths [Å] and angles [°] for $[Cr(BQA)_2]Cl$.

Cr(1)-N(2)	1.978(2)	C(12)-H(12)	0.9500
Cr(1)-N(22)	1.986(2)	C(13)-C(14)	1.412(4)
Cr(1)-N(1)	2.039(2)	C(13)-H(13)	0.9500
Cr(1)-N(23)	2.042(2)	C(14)-C(15)	1.408(5)
Cr(1)-N(3)	2.045(2)	C(14)-C(18)	1.413(4)
Cr(1)-N(21)	2.045(2)	C(15)-C(16)	1.369(5)
N(1)-C(1)	1.325(4)	C(15)-H(15)	0.9500
N(1)-C(9)	1.377(4)	C(16)-C(17)	1.399(4)
N(2)-C(8)	1.380(4)	C(16)-H(16)	0.9500
N(2)-C(10)	1.384(4)	C(17)-H(17)	0.9500
N(3)-C(17)	1.325(4)	C(21)-C(22)	1.403(4)
N(3)-C(18)	1.374(4)	C(21)-H(21)	0.9500
N(21)-C(21)	1.328(4)	C(22)-C(23)	1.366(5)
N(21)-C(29)	1.373(4)	C(22)-H(22)	0.9500
N(22)-C(30)	1.384(4)	C(23)-C(24)	1.415(4)
N(22)-C(28)	1.390(4)	C(23)-H(23)	0.9500
N(23)-C(37)	1.328(4)	C(24)-C(25)	1.413(4)
N(23)-C(38)	1.372(4)	C(24)-C(29)	1.415(4)
C(1)-C(2)	1.392(4)	C(25)-C(26)	1.362(5)
C(1)-H(1)	0.9500	C(25)-H(25)	0.9500
C(2)-C(3)	1.368(4)	C(26)-C(27)	1.415(4)
C(2)-H(2)	0.9500	C(26)-H(26)	0.9500
C(3)-C(4)	1.414(4)	C(27)-C(28)	1.385(4)
C(3)-H(3)	0.9500	C(27)-H(27)	0.9500
C(4)-C(9)	1.412(4)	C(28)-C(29)	1.439(4)
C(4)-C(5)	1.414(4)	C(30)-C(31)	1.386(4)
C(5)-C(6)	1.370(5)	C(30)-C(38)	1.434(4)
C(5)-H(5)	0.9500	C(31)-C(32)	1.409(5)
C(6)-C(7)	1.406(4)	C(31)-H(31)	0.9500
C(6)-H(6)	0.9500	C(32)-C(33)	1.369(5)
C(7)-C(8)	1.387(4)	C(32)-H(32)	0.9500
C(7)-H(7)	0.9500	C(33)-C(34)	1.417(5)
C(8)-C(9)	1.436(4)	C(33)-H(33)	0.9500
C(10)-C(11)	1.392(4)	C(34)-C(35)	1.413(5)
C(10)-C(18)	1.436(4)	C(34)-C(38)	1.413(4)
C(11)-C(12)	1.406(4)	C(35)-C(36)	1.360(5)
C(11)-H(11)	0.9500	C(35)-H(35)	0.9500
C(12)-C(13)	1.362(5)	C(36)-C(37)	1.397(5)

C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
Cl(41)-C(41)	1.779(4)
Cl(42)-C(41)	1.757(4)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
Cl(51)-C(51)	1.824(10)
Cl(52)-C(51)	1.733(8)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
Cl(53)-C(51A)	1.818(15)
Cl(54)-C(51A)	1.764(14)
C(51A)-H(51C)	0.9900
C(51A)-H(51D)	0.9900
Cl(55)-C(51B)	1.810(18)
Cl(56)-C(51B)	1.755(18)
C(51B)-H(51E)	0.9900
C(51B)-H(51F)	0.9900
N(2)-Cr(1)-N(22)	177.44(10)
N(2)-Cr(1)-N(1)	80.51(10)
N(22)-Cr(1)-N(1)	102.04(10)
N(2)-Cr(1)-N(23)	99.77(10)
N(22)-Cr(1)-N(23)	80.39(10)
N(1)-Cr(1)-N(23)	93.73(10)
N(2)-Cr(1)-N(3)	80.42(10)
N(22)-Cr(1)-N(3)	97.03(10)
N(1)-Cr(1)-N(3)	160.92(10)
N(23)-Cr(1)-N(3)	89.76(10)
N(2)-Cr(1)-N(21)	99.04(10)
N(22)-Cr(1)-N(21)	80.78(10)
N(1)-Cr(1)-N(21)	90.08(9)
N(23)-Cr(1)-N(21)	161.17(10)
N(3)-Cr(1)-N(21)	92.64(10)
C(1)-N(1)-C(9)	119.4(3)
C(1)-N(1)-Cr(1)	127.7(2)
C(9)-N(1)-Cr(1)	112.72(18)
C(8)-N(2)-C(10)	127.2(2)
C(8)-N(2)-Cr(1)	116.31(18)
C(10)-N(2)-Cr(1)	116.46(19)
C(17)-N(3)-C(18)	119.2(3)
C(17)-N(3)-Cr(1)	127.9(2)
C(18)-N(3)-Cr(1)	112.87(19)
C(21)-N(21)-C(29)	119.6(2)
C(21)-N(21)-Cr(1)	127.6(2)
C(29)-N(21)-Cr(1)	112.70(18)
C(30)-N(22)-C(28)	127.4(2)
C(30)-N(22)-Cr(1)	115.49(19)
C(28)-N(22)-Cr(1)	116.12(18)
C(37)-N(23)-C(38)	119.8(3)
C(37)-N(23)-Cr(1)	127.3(2)
C(38)-N(23)-Cr(1)	112.31(19)
N(1)-C(1)-C(2)	122.6(3)
N(1)-C(1)-H(1)	118.7
C(2)-C(1)-H(1)	118.7
C(3)-C(2)-C(1)	119.1(3)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	120.5(3)
C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7
C(9)-C(4)-C(5)	118.7(3)
C(9)-C(4)-C(3)	116.9(3)
C(5)-C(4)-C(3)	124.3(3)
C(6)-C(5)-C(4)	119.0(3)
C(6)-C(5)-H(5)	120.5
C(4)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	122.5(3)
C(5)-C(6)-H(6)	118.7
C(7)-C(6)-H(6)	118.7
C(8)-C(7)-C(6)	120.8(3)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
N(2)-C(8)-C(7)	129.8(3)
N(2)-C(8)-C(9)	113.3(2)
C(7)-C(8)-C(9)	116.8(3)
N(1)-C(9)-C(4)	121.4(3)
N(1)-C(9)-C(8)	116.5(3)

C(4)-C(9)-C(8)	122.0(3)	C(29)-C(24)-C(23)	117.5(3)
N(2)-C(10)-C(11)	129.8(3)	C(26)-C(25)-C(24)	119.1(3)
N(2)-C(10)-C(18)	113.2(2)	C(26)-C(25)-H(25)	120.5
C(11)-C(10)-C(18)	116.9(3)	C(24)-C(25)-H(25)	120.5
C(10)-C(11)-C(12)	120.7(3)	C(25)-C(26)-C(27)	122.2(3)
C(10)-C(11)-H(11)	119.7	C(25)-C(26)-H(26)	118.9
C(12)-C(11)-H(11)	119.7	C(27)-C(26)-H(26)	118.9
C(13)-C(12)-C(11)	122.4(3)	C(28)-C(27)-C(26)	121.1(3)
C(13)-C(12)-H(12)	118.8	C(28)-C(27)-H(27)	119.4
C(11)-C(12)-H(12)	118.8	C(26)-C(27)-H(27)	119.4
C(12)-C(13)-C(14)	119.4(3)	C(27)-C(28)-N(22)	130.3(3)
C(12)-C(13)-H(13)	120.3	C(27)-C(28)-C(29)	116.5(3)
C(14)-C(13)-H(13)	120.3	N(22)-C(28)-C(29)	113.2(2)
C(15)-C(14)-C(13)	124.1(3)	N(21)-C(29)-C(24)	121.2(3)
C(15)-C(14)-C(18)	117.2(3)	N(21)-C(29)-C(28)	117.1(2)
C(13)-C(14)-C(18)	118.7(3)	C(24)-C(29)-C(28)	121.7(3)
C(16)-C(15)-C(14)	120.4(3)	N(22)-C(30)-C(31)	129.8(3)
C(16)-C(15)-H(15)	119.8	N(22)-C(30)-C(38)	113.3(3)
C(14)-C(15)-H(15)	119.8	C(31)-C(30)-C(38)	116.8(3)
C(15)-C(16)-C(17)	119.2(3)	C(30)-C(31)-C(32)	121.1(3)
C(15)-C(16)-H(16)	120.4	C(30)-C(31)-H(31)	119.4
C(17)-C(16)-H(16)	120.4	C(32)-C(31)-H(31)	119.4
N(3)-C(17)-C(16)	122.4(3)	C(33)-C(32)-C(31)	122.0(3)
N(3)-C(17)-H(17)	118.8	C(33)-C(32)-H(32)	119.0
C(16)-C(17)-H(17)	118.8	C(31)-C(32)-H(32)	119.0
N(3)-C(18)-C(14)	121.7(3)	C(32)-C(33)-C(34)	119.3(3)
N(3)-C(18)-C(10)	116.6(3)	C(32)-C(33)-H(33)	120.3
C(14)-C(18)-C(10)	121.7(3)	C(34)-C(33)-H(33)	120.3
N(21)-C(21)-C(22)	122.2(3)	C(35)-C(34)-C(38)	117.0(3)
N(21)-C(21)-H(21)	118.9	C(35)-C(34)-C(33)	124.4(3)
C(22)-C(21)-H(21)	118.9	C(38)-C(34)-C(33)	118.5(3)
C(23)-C(22)-C(21)	119.4(3)	C(36)-C(35)-C(34)	120.9(3)
C(23)-C(22)-H(22)	120.3	C(36)-C(35)-H(35)	119.6
C(21)-C(22)-H(22)	120.3	C(34)-C(35)-H(35)	119.6
C(22)-C(23)-C(24)	120.0(3)	C(35)-C(36)-C(37)	119.0(3)
C(22)-C(23)-H(23)	120.0	C(35)-C(36)-H(36)	120.5
C(24)-C(23)-H(23)	120.0	C(37)-C(36)-H(36)	120.5
C(25)-C(24)-C(29)	119.0(3)	N(23)-C(37)-C(36)	122.1(3)
C(25)-C(24)-C(23)	123.4(3)	N(23)-C(37)-H(37)	118.9

C(36)-C(37)-H(37)	118.9	Cl(51)-C(51)-H(51B)	109.8
N(23)-C(38)-C(34)	121.1(3)	H(51A)-C(51)-H(51B)	108.3
N(23)-C(38)-C(30)	116.8(3)	Cl(54)-C(51A)-Cl(53)	111.5(9)
C(34)-C(38)-C(30)	122.1(3)	Cl(54)-C(51A)-H(51C)	109.3
Cl(42)-C(41)-Cl(41)	110.4(2)	Cl(53)-C(51A)-H(51C)	109.3
Cl(42)-C(41)-H(41A)	109.6	Cl(54)-C(51A)-H(51D)	109.3
Cl(41)-C(41)-H(41A)	109.6	Cl(53)-C(51A)-H(51D)	109.3
Cl(42)-C(41)-H(41B)	109.6	H(51C)-C(51A)-H(51D)	108.0
Cl(41)-C(41)-H(41B)	109.6	Cl(56)-C(51B)-Cl(55)	102.3(15)
H(41A)-C(41)-H(41B)	108.1	Cl(56)-C(51B)-H(51E)	111.3
Cl(52)-C(51)-Cl(51)	109.2(6)	Cl(55)-C(51B)-H(51E)	111.3
Cl(52)-C(51)-H(51A)	109.8	Cl(56)-C(51B)-H(51F)	111.3
Cl(51)-C(51)-H(51A)	109.8	Cl(55)-C(51B)-H(51F)	111.3
Cl(52)-C(51)-H(51B)	109.8	H(51E)-C(51B)-H(51F)	109.2

Table S22. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cr(BQA)_2]Cl$. The anisotropic displacement factor exponent takes the form:
$-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	16(1)	10(1)	10(1)	-1(1)	-3(1)	-6(1)
N(1)	19(1)	13(1)	11(1)	-1(1)	-3(1)	-7(1)
N(2)	19(1)	11(1)	14(1)	-1(1)	-4(1)	-6(1)
N(3)	19(1)	12(1)	15(1)	-1(1)	-2(1)	-5(1)
N(21)	17(1)	14(1)	12(1)	-2(1)	-2(1)	-6(1)
N(22)	19(1)	15(1)	12(1)	-1(1)	-1(1)	-8(1)
N(23)	21(1)	13(1)	14(1)	-1(1)	-4(1)	-6(1)
C(1)	24(2)	14(1)	13(1)	1(1)	-4(1)	-10(1)
C(2)	23(2)	13(2)	26(2)	-3(1)	-5(1)	-3(1)
C(3)	20(2)	19(2)	31(2)	-2(1)	-5(1)	-4(1)
C(4)	20(2)	17(2)	21(2)	-2(1)	-6(1)	-6(1)
C(5)	16(2)	23(2)	34(2)	-7(1)	-1(1)	-9(1)
C(6)	21(2)	25(2)	31(2)	-6(1)	-2(1)	-14(1)
C(7)	24(2)	13(1)	22(2)	-4(1)	-4(1)	-7(1)
C(8)	20(2)	14(1)	10(1)	-2(1)	-5(1)	-6(1)
C(9)	19(2)	15(1)	13(1)	-1(1)	-4(1)	-7(1)
C(10)	21(2)	13(1)	7(1)	-1(1)	-2(1)	-6(1)
C(11)	24(2)	16(2)	16(1)	0(1)	-6(1)	-8(1)
C(12)	31(2)	14(2)	21(2)	-2(1)	-6(1)	-11(1)
C(13)	25(2)	13(2)	27(2)	-4(1)	-4(1)	-3(1)
C(14)	24(2)	14(2)	16(1)	-2(1)	-3(1)	-5(1)
C(15)	21(2)	21(2)	30(2)	-3(1)	-2(1)	-2(1)
C(16)	17(2)	28(2)	35(2)	-4(2)	-4(1)	-8(1)
C(17)	21(2)	17(2)	25(2)	-3(1)	-3(1)	-6(1)
C(18)	21(2)	12(1)	11(1)	1(1)	-4(1)	-5(1)
C(21)	23(2)	18(2)	17(2)	1(1)	-3(1)	-9(1)
C(22)	28(2)	22(2)	12(1)	3(1)	-2(1)	-8(1)
C(23)	24(2)	22(2)	13(1)	-2(1)	-4(1)	-2(1)
C(24)	17(2)	16(2)	17(1)	-4(1)	-4(1)	-1(1)
C(25)	20(2)	24(2)	18(2)	-8(1)	-6(1)	-4(1)
C(26)	21(2)	22(2)	27(2)	-12(1)	-4(1)	-8(1)
C(27)	19(2)	17(2)	20(2)	-4(1)	-2(1)	-6(1)
C(28)	15(1)	13(1)	16(1)	-5(1)	-1(1)	-4(1)

C(29)	14(1)	14(1)	13(1)	-2(1)	-2(1)	-3(1)
C(30)	18(1)	12(1)	16(1)	-3(1)	1(1)	-4(1)
C(31)	26(2)	19(2)	25(2)	-7(1)	3(1)	-11(1)
C(32)	34(2)	25(2)	31(2)	-4(1)	10(2)	-19(2)
C(33)	45(2)	26(2)	19(2)	1(1)	7(2)	-17(2)
C(34)	33(2)	16(2)	16(2)	0(1)	1(1)	-6(1)
C(35)	54(2)	25(2)	13(2)	1(1)	-2(2)	-12(2)
C(36)	52(2)	30(2)	16(2)	-2(1)	-12(2)	-16(2)
C(37)	33(2)	23(2)	18(2)	-2(1)	-8(1)	-11(1)
C(38)	22(2)	12(1)	16(1)	-1(1)	-1(1)	-4(1)
Cl(41)	32(1)	42(1)	35(1)	-2(1)	-1(1)	1(1)
Cl(42)	62(1)	69(1)	52(1)	-29(1)	18(1)	-42(1)
C(41)	28(2)	38(2)	33(2)	-8(2)	0(2)	-11(2)
Cl(51)	67(2)	54(1)	62(1)	4(1)	19(2)	-20(2)
Cl(52)	71(1)	52(1)	48(1)	2(1)	-7(1)	-30(1)
C(51)	56(5)	56(4)	48(5)	0(3)	-1(4)	-33(4)
Cl(53)	36(1)	42(2)	14(1)	2(1)	-4(1)	-8(1)
Cl(54)	67(2)	54(1)	62(1)	4(1)	19(2)	-20(2)
C(51A)	56(5)	56(4)	48(5)	0(3)	-1(4)	-33(4)
Cl(55)	67(2)	54(1)	62(1)	4(1)	19(2)	-20(2)
Cl(56)	71(1)	52(1)	48(1)	2(1)	-7(1)	-30(1)
C(51B)	56(5)	56(4)	48(5)	0(3)	-1(4)	-33(4)
Cl(1)	21(1)	17(1)	21(1)	-4(1)	-5(1)	-9(1)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3})for $[Cr(BQA)_2]Cl$.

	x	y	z	U(eq)
H(1)	6598	4779	7275	20
H(2)	8926	3765	6960	26
H(3)	10361	4893	6726	29
H(5)	10628	7016	6622	29
H(6)	9564	9128	6652	28
H(7)	7228	10028	7046	22
H(11)	5671	10940	7795	21
H(12)	3892	12790	8081	25
H(13)	1674	12982	8144	26
H(15)	-9	11932	8084	31
H(16)	-369	10155	7894	32
H(17)	1478	8327	7661	25
H(21)	5537	8810	5623	23
H(22)	5357	8830	4123	26
H(23)	4261	7645	3750	26
H(25)	3112	6033	4259	25
H(26)	2625	4634	5393	26
H(27)	2938	4619	6863	22
H(31)	2001	5010	8074	27
H(32)	1234	4485	9568	36
H(33)	1906	5028	10731	37
H(35)	3196	6229	11209	38
H(36)	4624	7358	10799	37
H(37)	5346	7812	9282	28
H(41A)	-212	11821	5081	40
H(41B)	-249	11573	6144	40
H(51A)	2127	9839	11108	62
H(51B)	1885	9924	10096	62
H(51C)	2882	9647	10870	62
H(51D)	3280	10165	9860	62
H(51E)	1390	9580	10648	62
H(51F)	1993	9907	9624	62

[Fe(BQA)$_2$]

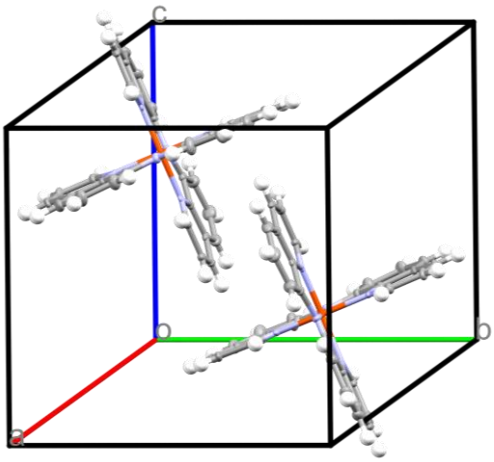

Fig. S26 **Unit cell with complete molecules of Fe(BQA)$_2$**

The unit cell of [Fe(BQA)$_2$] was determined using 9870 reflections and the structure was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of [Fe(BQA)$_2$] and heavily disordered solvent molecules. SQUEEZE was used to include a solvent model in the refinement. SQUEEZE identified one independent void with a size of 289 Å^3 at 0.0 0.5 0.5 in the unit cell. The equivalent of 98 electrons were found in the unit cell, which corresponds to about two molecules of DCM. The obtained model was added as .fab-file to the refinement using SHELXL.

Table S24. Crystal data and structure refinement for [Fe(BQA)$_2$].

CCDC No.	1897891	
Empirical formula	C_{36} H_{24} Fe N_6	
Formula weight	596.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.8578(15) Å	α= 90.362(6)°.
	b = 12.2367(15) Å	β= 101.553(5)°.
	c = 12.2682(15) Å	γ = 116.949(5)°.
Volume	1545.0(3) Å^3	
Z	2	
Density (calculated)	1.282 Mg/m^3	
Absorption coefficient	0.523 mm^{-1}	
F(000)	616	
Crystal size	0.664 x 0.375 x 0.006 mm^3	
Theta range for data collection	2.299 to 26.732°.	

Index ranges	$-15 \leq h \leq 14$, $-15 \leq k \leq 15$, $-15 \leq l \leq 15$
Reflections collected	43004
Independent reflections	6492 [R(int) = 0.0848]
Completeness to theta = 25.242°	99.3 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6492 / 0 / 388
Goodness-of-fit on F^2	1.078
Final R indices [I>2σ(I)]	R1 = 0.0608, wR2 = 0.1245
R indices (all data)	R1 = 0.0816, wR2 = 0.1338
Largest diff. peak and hole	0.693 and -0.908 e.Å^{-3}

Table S25. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)for [Fe(BQA)2]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	4779(1)	2422(1)	7462(1)	14(1)
N(1)	5083(3)	3996(2)	8153(2)	17(1)
N(2)	6637(3)	3127(2)	7937(2)	17(1)
N(3)	4924(3)	1020(2)	6889(2)	15(1)
N(21)	4359(3)	1638(2)	8803(2)	17(1)
N(22)	2917(3)	1727(2)	6977(2)	15(1)
N(23)	4738(3)	3020(2)	5996(2)	16(1)
C(1)	4218(4)	4381(3)	8218(3)	20(1)
C(2)	4571(4)	5563(3)	8728(3)	26(1)
C(3)	5836(4)	6331(3)	9188(3)	26(1)
C(4)	6795(4)	5959(3)	9143(3)	24(1)
C(5)	8133(4)	6698(3)	9593(3)	33(1)
C(6)	8986(4)	6259(4)	9494(4)	42(1)
C(7)	8566(4)	5068(4)	8959(3)	37(1)
C(8)	7267(3)	4300(3)	8497(3)	21(1)
C(9)	6373(3)	4764(3)	8606(2)	20(1)
C(10)	7168(3)	2409(3)	7629(3)	20(1)
C(11)	8442(4)	2633(4)	7780(3)	32(1)
C(12)	8753(4)	1736(4)	7379(3)	34(1)

C(13)	7823(4)	624(3)	6834(3)	28(1)
C(14)	6511(4)	338(3)	6660(2)	21(1)
C(15)	5479(4)	-799(3)	6137(3)	24(1)
C(16)	4230(4)	-1006(3)	6010(3)	25(1)
C(17)	3990(3)	-55(3)	6388(3)	20(1)
C(18)	6194(3)	1239(3)	7045(2)	16(1)
C(21)	5172(4)	1655(3)	9739(3)	22(1)
C(22)	4718(4)	1021(3)	10640(3)	28(1)
C(23)	3417(4)	354(3)	10569(3)	27(1)
C(24)	2529(4)	314(3)	9592(3)	24(1)
C(25)	1167(4)	-339(3)	9448(3)	29(1)
C(26)	393(4)	-324(3)	8471(3)	30(1)
C(27)	889(4)	338(3)	7604(3)	25(1)
C(28)	2220(3)	1022(3)	7704(2)	18(1)
C(29)	3050(3)	986(3)	8720(2)	17(1)
C(30)	2466(3)	2020(3)	5958(2)	18(1)
C(31)	1226(4)	1774(3)	5393(3)	27(1)
C(32)	1008(4)	2171(4)	4329(3)	34(1)
C(33)	1983(4)	2801(3)	3791(3)	31(1)
C(34)	3267(4)	3092(3)	4335(3)	22(1)
C(35)	4357(4)	3753(3)	3865(3)	26(1)
C(36)	5576(4)	4028(3)	4448(3)	24(1)
C(37)	5738(3)	3658(3)	5530(3)	19(1)
C(38)	3501(3)	2726(3)	5409(2)	18(1)

Table S26. Bond lengths [Å] and angles [°] for [Fe(BQA)$_2$].

Fe(1)-N(2)	1.922(3)	N(2)-C(10)	1.380(4)
Fe(1)-N(22)	1.928(3)	N(3)-C(17)	1.316(4)
Fe(1)-N(3)	1.942(2)	N(3)-C(18)	1.376(4)
Fe(1)-N(1)	1.946(2)	N(21)-C(21)	1.337(4)
Fe(1)-N(23)	1.946(3)	N(21)-C(29)	1.367(4)
Fe(1)-N(21)	1.947(3)	N(22)-C(28)	1.372(4)
N(1)-C(1)	1.322(4)	N(22)-C(30)	1.374(4)
N(1)-C(9)	1.371(4)	N(23)-C(37)	1.334(4)
N(2)-C(8)	1.378(4)	N(23)-C(38)	1.377(4)

C(1)-C(2)	1.413(4)	C(25)-H(25)	0.9500
C(1)-H(1)	0.9500	C(26)-C(27)	1.401(5)
C(2)-C(3)	1.352(5)	C(26)-H(26)	0.9500
C(2)-H(2)	0.9500	C(27)-C(28)	1.389(5)
C(3)-C(4)	1.414(5)	C(27)-H(27)	0.9500
C(3)-H(3)	0.9500	C(28)-C(29)	1.439(4)
C(4)-C(5)	1.408(5)	C(30)-C(31)	1.386(5)
C(4)-C(9)	1.421(4)	C(30)-C(38)	1.443(5)
C(5)-C(6)	1.367(6)	C(31)-C(32)	1.412(5)
C(5)-H(5)	0.9500	C(31)-H(31)	0.9500
C(6)-C(7)	1.414(5)	C(32)-C(33)	1.368(6)
C(6)-H(6)	0.9500	C(32)-H(32)	0.9500
C(7)-C(8)	1.381(5)	C(33)-C(34)	1.409(5)
C(7)-H(7)	0.9500	C(33)-H(33)	0.9500
C(8)-C(9)	1.436(5)	C(34)-C(38)	1.411(4)
C(10)-C(11)	1.380(5)	C(34)-C(35)	1.419(5)
C(10)-C(18)	1.434(4)	C(35)-C(36)	1.362(5)
C(11)-C(12)	1.419(5)	C(35)-H(35)	0.9500
C(11)-H(11)	0.9500	C(36)-C(37)	1.410(4)
C(12)-C(13)	1.359(5)	C(36)-H(36)	0.9500
C(12)-H(12)	0.9500	C(37)-H(37)	0.9500
C(13)-C(14)	1.400(5)		
C(13)-H(13)	0.9500	N(2)-Fe(1)-N(22)	179.48(12)
C(14)-C(15)	1.405(5)	N(2)-Fe(1)-N(3)	83.29(11)
C(14)-C(18)	1.421(4)	N(22)-Fe(1)-N(3)	96.97(11)
C(15)-C(16)	1.360(5)	N(2)-Fe(1)-N(1)	82.95(11)
C(15)-H(15)	0.9500	N(22)-Fe(1)-N(1)	96.79(11)
C(16)-C(17)	1.412(4)	N(3)-Fe(1)-N(1)	166.24(12)
C(16)-H(16)	0.9500	N(2)-Fe(1)-N(23)	96.58(12)
C(17)-H(17)	0.9500	N(22)-Fe(1)-N(23)	82.97(11)
C(21)-C(22)	1.409(5)	N(3)-Fe(1)-N(23)	90.82(10)
C(21)-H(21)	0.9500	N(1)-Fe(1)-N(23)	90.86(10)
C(22)-C(23)	1.363(6)	N(2)-Fe(1)-N(21)	97.46(12)
C(22)-H(22)	0.9500	N(22)-Fe(1)-N(21)	82.99(11)
C(23)-C(24)	1.411(5)	N(3)-Fe(1)-N(21)	90.31(10)
C(23)-H(23)	0.9500	N(1)-Fe(1)-N(21)	91.37(10)
C(24)-C(25)	1.412(5)	N(23)-Fe(1)-N(21)	165.95(12)
C(24)-C(29)	1.421(4)	C(1)-N(1)-C(9)	119.2(3)
C(25)-C(26)	1.361(5)	C(1)-N(1)-Fe(1)	128.0(2)

C(9)-N(1)-Fe(1)	112.7(2)	C(7)-C(8)-C(9)	116.7(3)
C(8)-N(2)-C(10)	128.5(3)	N(1)-C(9)-C(4)	121.3(3)
C(8)-N(2)-Fe(1)	116.0(2)	N(1)-C(9)-C(8)	116.6(3)
C(10)-N(2)-Fe(1)	115.5(2)	C(4)-C(9)-C(8)	122.1(3)
C(17)-N(3)-C(18)	118.9(3)	C(11)-C(10)-N(2)	131.3(3)
C(17)-N(3)-Fe(1)	128.5(2)	C(11)-C(10)-C(18)	116.5(3)
C(18)-N(3)-Fe(1)	112.55(19)	N(2)-C(10)-C(18)	112.1(3)
C(21)-N(21)-C(29)	119.0(3)	C(10)-C(11)-C(12)	121.0(3)
C(21)-N(21)-Fe(1)	128.4(2)	C(10)-C(11)-H(11)	119.5
C(29)-N(21)-Fe(1)	112.6(2)	C(12)-C(11)-H(11)	119.5
C(28)-N(22)-C(30)	128.6(3)	C(13)-C(12)-C(11)	122.1(4)
C(28)-N(22)-Fe(1)	115.6(2)	C(13)-C(12)-H(12)	118.9
C(30)-N(22)-Fe(1)	115.7(2)	C(11)-C(12)-H(12)	118.9
C(37)-N(23)-C(38)	119.1(3)	C(12)-C(13)-C(14)	119.7(3)
C(37)-N(23)-Fe(1)	128.0(2)	C(12)-C(13)-H(13)	120.2
C(38)-N(23)-Fe(1)	112.9(2)	C(14)-C(13)-H(13)	120.2
N(1)-C(1)-C(2)	122.5(3)	C(13)-C(14)-C(15)	123.9(3)
N(1)-C(1)-H(1)	118.8	C(13)-C(14)-C(18)	118.5(3)
C(2)-C(1)-H(1)	118.8	C(15)-C(14)-C(18)	117.6(3)
C(3)-C(2)-C(1)	119.3(3)	C(16)-C(15)-C(14)	120.2(3)
C(3)-C(2)-H(2)	120.3	C(16)-C(15)-H(15)	119.9
C(1)-C(2)-H(2)	120.3	C(14)-C(15)-H(15)	119.9
C(2)-C(3)-C(4)	120.2(3)	C(15)-C(16)-C(17)	119.1(3)
C(2)-C(3)-H(3)	119.9	C(15)-C(16)-H(16)	120.5
C(4)-C(3)-H(3)	119.9	C(17)-C(16)-H(16)	120.5
C(5)-C(4)-C(3)	124.2(3)	N(3)-C(17)-C(16)	122.9(3)
C(5)-C(4)-C(9)	118.3(3)	N(3)-C(17)-H(17)	118.5
C(3)-C(4)-C(9)	117.5(3)	C(16)-C(17)-H(17)	118.5
C(6)-C(5)-C(4)	119.7(3)	N(3)-C(18)-C(14)	121.3(3)
C(6)-C(5)-H(5)	120.2	N(3)-C(18)-C(10)	116.4(3)
C(4)-C(5)-H(5)	120.2	C(14)-C(18)-C(10)	122.2(3)
C(5)-C(6)-C(7)	122.0(4)	N(21)-C(21)-C(22)	121.9(3)
C(5)-C(6)-H(6)	119.0	N(21)-C(21)-H(21)	119.1
C(7)-C(6)-H(6)	119.0	C(22)-C(21)-H(21)	119.1
C(8)-C(7)-C(6)	121.2(4)	C(23)-C(22)-C(21)	120.1(3)
C(8)-C(7)-H(7)	119.4	C(23)-C(22)-H(22)	120.0
C(6)-C(7)-H(7)	119.4	C(21)-C(22)-H(22)	120.0
N(2)-C(8)-C(7)	131.5(3)	C(22)-C(23)-C(24)	119.6(3)
N(2)-C(8)-C(9)	111.7(3)	C(22)-C(23)-H(23)	120.2

C(24)-C(23)-H(23)	120.2	C(30)-C(31)-H(31)	119.5
C(23)-C(24)-C(25)	123.6(3)	C(32)-C(31)-H(31)	119.5
C(23)-C(24)-C(29)	117.5(3)	C(33)-C(32)-C(31)	122.9(4)
C(25)-C(24)-C(29)	118.8(3)	C(33)-C(32)-H(32)	118.5
C(26)-C(25)-C(24)	119.1(3)	C(31)-C(32)-H(32)	118.5
C(26)-C(25)-H(25)	120.4	C(32)-C(33)-C(34)	118.5(3)
C(24)-C(25)-H(25)	120.4	C(32)-C(33)-H(33)	120.7
C(25)-C(26)-C(27)	122.8(4)	C(34)-C(33)-H(33)	120.7
C(25)-C(26)-H(26)	118.6	C(33)-C(34)-C(38)	119.1(3)
C(27)-C(26)-H(26)	118.6	C(33)-C(34)-C(35)	123.5(3)
C(28)-C(27)-C(26)	120.9(3)	C(38)-C(34)-C(35)	117.4(3)
C(28)-C(27)-H(27)	119.5	C(36)-C(35)-C(34)	120.5(3)
C(26)-C(27)-H(27)	119.5	C(36)-C(35)-H(35)	119.8
N(22)-C(28)-C(27)	131.1(3)	C(34)-C(35)-H(35)	119.8
N(22)-C(28)-C(29)	112.0(3)	C(35)-C(36)-C(37)	119.0(3)
C(27)-C(28)-C(29)	116.9(3)	C(35)-C(36)-H(36)	120.5
N(21)-C(29)-C(24)	121.9(3)	C(37)-C(36)-H(36)	120.5
N(21)-C(29)-C(28)	116.6(3)	N(23)-C(37)-C(36)	122.5(3)
C(24)-C(29)-C(28)	121.4(3)	N(23)-C(37)-H(37)	118.8
N(22)-C(30)-C(31)	131.7(3)	C(36)-C(37)-H(37)	118.8
N(22)-C(30)-C(38)	112.2(3)	N(23)-C(38)-C(34)	121.6(3)
C(31)-C(30)-C(38)	116.1(3)	N(23)-C(38)-C(30)	116.0(3)
C(30)-C(31)-C(32)	121.0(4)	C(34)-C(38)-C(30)	122.4(3)

Table S27. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Fe(BQA)_2]$.
The anisotropicdisplacement factor exponent takes the form:
$-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	26(1)	9(1)	10(1)	1(1)	6(1)	10(1)
N(1)	33(2)	13(1)	10(1)	5(1)	11(1)	13(1)
N(2)	20(2)	14(1)	16(1)	-1(1)	2(1)	7(1)
N(3)	29(2)	9(1)	9(1)	4(1)	7(1)	9(1)
N(21)	35(2)	10(1)	13(1)	1(1)	6(1)	16(1)
N(22)	23(2)	12(1)	12(1)	4(1)	7(1)	9(1)

N(23)	28(2)	9(1)	16(1)	-1(1)	10(1)	9(1)
C(1)	35(2)	15(2)	16(1)	7(1)	14(1)	13(2)
C(2)	51(3)	18(2)	22(2)	7(1)	18(2)	22(2)
C(3)	57(3)	11(2)	16(2)	4(1)	17(2)	17(2)
C(4)	46(2)	14(2)	12(1)	1(1)	10(1)	13(2)
C(5)	50(3)	15(2)	26(2)	-6(1)	2(2)	10(2)
C(6)	40(3)	24(2)	45(2)	-12(2)	-7(2)	8(2)
C(7)	37(2)	23(2)	45(2)	-9(2)	-1(2)	14(2)
C(8)	31(2)	12(2)	16(2)	-1(1)	1(1)	8(2)
C(9)	36(2)	11(2)	12(1)	3(1)	8(1)	9(2)
C(10)	30(2)	17(2)	18(2)	2(1)	6(1)	14(2)
C(11)	31(2)	26(2)	37(2)	-3(2)	4(2)	14(2)
C(12)	31(2)	33(2)	47(2)	1(2)	11(2)	21(2)
C(13)	40(2)	29(2)	28(2)	5(2)	12(2)	25(2)
C(14)	40(2)	21(2)	12(1)	5(1)	8(1)	23(2)
C(15)	46(2)	20(2)	16(2)	0(1)	7(2)	22(2)
C(16)	40(2)	13(2)	20(2)	-2(1)	2(2)	13(2)
C(17)	29(2)	15(2)	17(2)	-1(1)	4(1)	11(2)
C(18)	25(2)	16(2)	11(1)	3(1)	6(1)	12(1)
C(21)	41(2)	20(2)	13(1)	2(1)	5(1)	21(2)
C(22)	57(3)	27(2)	12(2)	4(1)	6(2)	31(2)
C(23)	55(3)	20(2)	18(2)	11(1)	19(2)	23(2)
C(24)	48(2)	17(2)	16(2)	5(1)	16(2)	20(2)
C(25)	42(2)	22(2)	28(2)	6(2)	21(2)	13(2)
C(26)	32(2)	23(2)	34(2)	5(2)	19(2)	9(2)
C(27)	30(2)	23(2)	26(2)	3(1)	10(2)	14(2)
C(28)	30(2)	15(2)	15(1)	4(1)	10(1)	14(2)
C(29)	30(2)	11(2)	14(1)	3(1)	10(1)	12(1)
C(30)	33(2)	13(2)	12(1)	2(1)	4(1)	13(2)
C(31)	30(2)	28(2)	23(2)	4(2)	2(2)	15(2)
C(32)	38(2)	34(2)	27(2)	1(2)	-6(2)	20(2)
C(33)	51(3)	29(2)	16(2)	0(2)	0(2)	24(2)
C(34)	44(2)	13(2)	13(1)	2(1)	6(1)	17(2)
C(35)	59(3)	16(2)	11(1)	5(1)	13(2)	22(2)
C(36)	46(2)	15(2)	19(2)	5(1)	16(2)	16(2)
C(37)	33(2)	13(2)	15(1)	4(1)	12(1)	12(2)
C(38)	32(2)	11(2)	12(1)	0(1)	6(1)	12(1)

Table S28. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Fe(BQA)_2]$.

	x	y	z	U(eq)
H(1)	3325	3841	7909	24
H(2)	3926	5816	8747	32
H(3)	6080	7123	9543	31
H(5)	8442	7499	9963	40
H(6)	9888	6768	9793	51
H(7)	9188	4792	8916	44
H(11)	9122	3399	8157	38
H(12)	9640	1919	7495	41
H(13)	8062	44	6573	33
H(15)	5655	-1424	5872	29
H(16)	3528	-1779	5671	30
H(17)	3116	-198	6277	24
H(21)	6082	2106	9798	26
H(22)	5319	1059	11299	34
H(23)	3109	-81	11172	32
H(25)	795	-782	10025	35
H(26)	-523	-781	8374	36
H(27)	307	319	6939	30
H(31)	513	1331	5726	32
H(32)	146	1993	3971	41
H(33)	1800	3036	3067	38
H(35)	4236	4005	3138	31
H(36)	6305	4461	4130	29
H(37)	6592	3872	5943	23

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