

ESI for manuscript:

Supramolecular network of a framework material supported by the anion- π linkage of Keggin-type heteropolyoxotungstates: Experimental and theoretical insights

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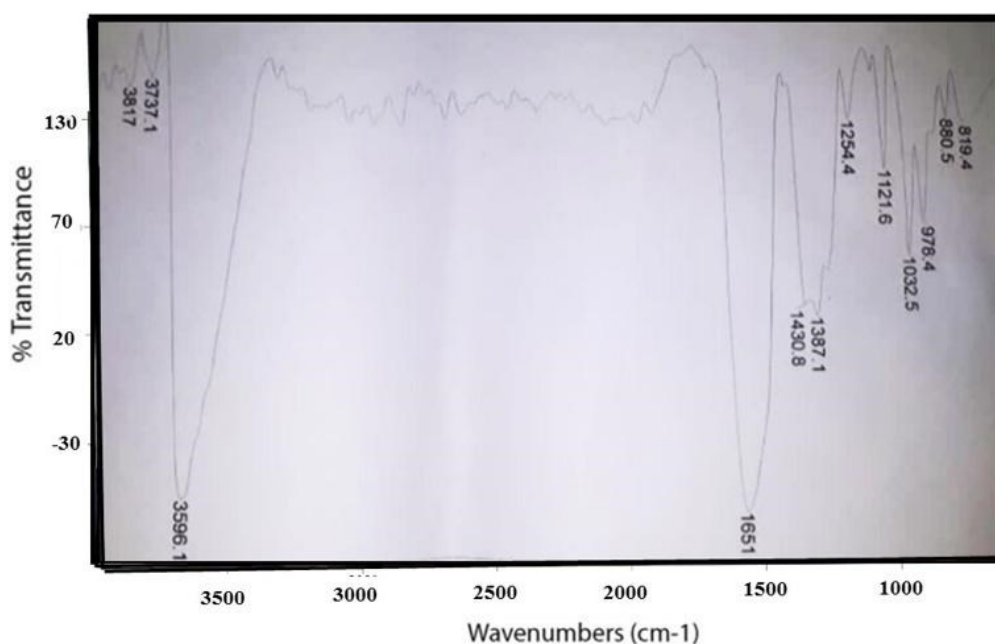
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IR of compound 1



X-ray coordinates of the complexes:

1·HFB

W	-2.13786603	-0.08942831	-0.07876327
Na	0.00000000	0.00000000	5.18383674
W	-2.87501047	-1.97495141	-2.73897011
W	-0.86641080	-1.73540715	-5.81507005
W	0.45716258	-3.53368744	-2.85667659
La	-3.73409587	-0.76078702	3.70023540
Si	0.00000000	0.00000000	-2.85406352
O	-2.61789171	1.28480743	3.79994245
O	-0.44136452	1.86523973	3.86894399
O	1.33832842	5.43884355	2.12335599

O	0.38691959	6.80609204	0.63496137
O	-4.06963658	4.31813874	-0.16574625
H	-4.12484246	5.11609411	-0.42304334
O	-5.90048720	-1.23927332	4.83263450
H	-6.17824545	-0.52423526	5.24313687
H	-5.78867469	-1.88051179	5.40933186
O	-3.43355758	-2.78097673	5.20682790
H	-2.93812491	-3.36931070	4.79902539
H	-4.21159578	-3.12847314	5.38102670
O	-3.51156254	-0.13127035	6.02843749
H	-3.04111497	0.59869685	6.08184047
H	-3.10671126	-0.76860561	6.46143519
O	-5.27399531	1.10449875	3.37554282
H	-6.02226676	0.80887494	3.04514148
H	-4.91899199	1.67689550	2.82624467
O	-2.85550923	-0.13557839	1.49413725
O	-0.65288090	-1.34633540	0.11443193
O	0.07909930	-2.88210462	-4.57247456
O	0.30758428	-5.22963068	-3.03178293
O	-1.52109566	-0.10650433	-6.56686370
O	-3.35560501	1.11739269	-0.94545824
O	-3.07612164	-1.57160457	-0.89116835
O	-4.07200941	-3.18002506	-2.95237407
O	-3.99018484	-0.37019282	-3.06736375
O	-1.37844217	-3.00375982	-2.43597433
O	-1.44080095	-2.83402569	-6.96817374
O	-2.24839528	-1.77395454	-4.52236941
O	0.00000000	0.00000000	-4.50346402
O	-1.52745478	-0.12099902	-2.30216340
N	-0.82557948	3.99025893	2.32615153
C	-1.65638882	2.01850640	3.40064488
C	-1.82792745	3.09702255	2.43484877
C	-2.98420355	3.18089661	1.61334925
H	-3.69089860	2.55064916	1.69474729
C	-3.04847107	4.19779008	0.70395285
C	-1.99239891	5.13743477	0.63495608
H	-2.03218034	5.86642141	0.02655888
C	-0.91209467	4.97662733	1.45865539
C	0.36712307	5.83348542	1.39795770
O	0.86851533	-1.26231529	-2.30216340
O	0.65893945	1.38331378	-2.30216340
W	1.14637996	-1.80673178	-0.07876327
W	3.14786325	-1.50235591	-2.73897011
W	1.93611244	0.11736993	-5.81507005
W	2.83168144	2.16275800	-2.85667659
La	2.52590853	-2.85342850	3.70023540
O	0.19627025	-2.90956416	3.79994245
O	-1.39466252	-1.31485306	3.86894399
O	-5.37934074	-1.56039554	2.12335599
O	-6.08770799	-3.06796384	0.63496137
O	-1.70479954	-5.68347796	-0.16574625
H	-2.36824652	-6.13026548	-0.42304334
O	4.02348544	-4.49033513	4.83263450
H	3.54312373	-5.08840015	5.24313687
H	4.52290811	-4.07288308	5.40933186
O	4.12517531	-1.58305967	5.20682790
H	4.38697147	-0.85983577	4.79902539
H	4.81513513	-2.08311259	5.38102670
O	1.86946469	-2.97546683	6.02843749
H	1.00207121	-2.93303105	6.08184047
H	2.21898785	-2.30618832	6.46143519
O	1.68047379	-5.11966341	3.37554282
H	2.31062706	-5.61987350	3.04514148
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O	1.54516899	-2.40515399	1.49413725
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O	2.45642650	1.50955430	-4.57247456
O	4.37520098	2.88119126	-3.03178293
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O	0.71011195	-3.46473565	-0.94545824
O	2.89911026	-1.87819717	-0.89116835

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O	2.31568864	-3.27050484	-3.06736375
O	3.29055325	0.30811398	-2.43597433
O	3.17473911	0.16924253	-6.96817374
O	2.66048730	-1.06019021	-4.52236941
N	-3.04287608	-2.71010243	2.32615153
C	-0.91988363	-2.44372836	3.40064488
C	-1.76813624	-3.13154290	2.43484877
C	-1.26263544	-4.17484442	1.61334925
H	-0.36347809	-4.47173614	1.69474729
C	-2.11115740	-4.73894896	0.70395285
C	-3.45294981	-4.29418553	0.63495608
H	-4.06437973	-4.69313067	0.02655888
C	-3.85383862	-3.27821125	1.45865539
C	-5.23550825	-2.59880482	1.39795770
W	0.99148554	1.89616009	-0.07876327
W	-0.27285331	3.47730784	-2.73897011
W	-1.06970112	1.61803776	-5.81507005
W	-3.28884454	1.37092892	-2.85667659
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O	2.42162146	1.62475672	3.79994245
O	1.83602756	-0.55038667	3.86894399
O	4.04101232	-3.87844801	2.12335599
O	5.70078893	-3.73812767	0.63496137
O	5.77443612	1.36533922	-0.16574625
H	6.49308898	1.01417137	-0.42304334
O	1.87700123	5.72960845	4.83263450
H	2.63512172	5.61263541	5.24313687
H	1.26576658	5.95339487	5.40933186
O	-0.69161773	4.36403640	5.20682790
H	-1.44884603	4.22914647	4.79902539
H	-0.60353935	5.21158573	5.38102670
O	1.64209786	3.10673719	6.02843749
H	2.03904430	2.33433473	6.08184047
H	0.88772394	3.07479393	6.46143519
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H	3.71163970	4.81099855	3.04514148
H	3.91173008	3.42152409	2.82624467
O	1.31034024	2.54073238	1.49413725
O	-0.83952013	1.23857904	0.11443193
O	-2.53552580	1.37255031	-4.57247456
O	-4.68278526	2.34843995	-3.03178293
O	0.66831224	1.37055955	-6.56686370
O	2.64549307	2.34734296	-0.94545824
O	0.17701138	3.44980174	-0.89116835
O	-0.71797764	5.11647618	-2.95237407
O	1.67449621	3.64069767	-3.06736375
O	-1.91211108	2.69564584	-2.43597433
O	-1.73393763	2.66478316	-6.96817374
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N	3.86845556	-1.28015650	2.32615153
C	2.57627245	0.42522144	3.40064488
C	3.59606368	0.03452035	2.43484877
C	4.24683899	0.99394781	1.61334925
H	4.05437616	1.92108698	1.69474729
C	5.15962846	0.54115835	0.70395285
C	5.44534819	-0.84324924	0.63495608
H	6.09656007	-1.17329074	0.02655888
C	4.76593329	-1.69841661	1.45865539
C	4.86838518	-3.23468060	1.39795770
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W	-0.86641080	-1.73540715	-6.02228898
W	0.45716258	-3.53368744	-3.06389605
La	-3.73409587	-0.76078702	3.49301594
Si	0.00000000	0.00000000	-3.06128298
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O	-0.44136505	1.86523973	3.66172453
O	1.33832842	5.43884355	1.91613706
O	0.38691959	6.80609204	0.42774191
O	-4.06963658	4.31813874	-0.37296571
H	-4.12484246	5.11609411	-0.63026280
O	-5.90048720	-1.23927332	4.62541504
H	-6.17824545	-0.52423526	5.03591794
H	-5.78867469	-1.88051179	5.20211240
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H	-2.93812544	-3.36931070	4.59180646
H	-4.21159578	-3.12847314	5.17380777
O	-3.51156254	-0.13127035	5.82121856
H	-3.04111497	0.59869685	5.87462101
H	-3.10671126	-0.76860561	6.25421573
O	-5.27399584	1.10449875	3.16832336
H	-6.02226676	0.80887494	2.83792255
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O	-0.65288090	-1.34633540	-0.09278753
O	0.07909930	-2.88210462	-4.77969349
O	0.30758428	-5.22963068	-3.23900239
O	-1.52109566	-0.10650433	-6.77408316
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O	-3.07612164	-1.57160457	-1.09838782
O	-4.07200941	-3.18002453	-3.15959353
O	-3.99018484	-0.37019282	-3.27458321
O	-1.37844217	-3.00375982	-2.64319326
O	-1.44080095	-2.83402569	-7.17539320
O	-2.24839528	-1.77395454	-4.72958887
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N	-0.82557948	3.99025893	2.11893260
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C	-1.82792745	3.09702255	2.22762931
C	-2.98420355	3.18089661	1.40612979
H	-3.69089860	2.55064916	1.48752783
C	-3.04847160	4.19779008	0.49673392
C	-1.99239891	5.13743477	0.42773662
H	-2.03218034	5.86642141	-0.18066058
C	-0.91209467	4.97662733	1.25143593
C	0.36712307	5.83348542	1.19073877
O	0.86851533	-1.26231529	-2.50938286
O	0.65893945	1.38331378	-2.50938286
W	1.14637996	-1.80673178	-0.28598220
W	3.14786325	-1.50235591	-2.94618904
W	1.93611244	0.11736993	-6.02228898
W	2.83168144	2.16275800	-3.06389605
La	2.52590906	-2.85342850	3.49301594
O	0.19627025	-2.90956416	3.59272299
O	-1.39466252	-1.31485306	3.66172453
O	-5.37934074	-1.56039554	1.91613706
O	-6.08770799	-3.06796384	0.42774191

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H	3.54312373	-5.08840015	5.03591794
H	4.52290811	-4.07288308	5.20211240
O	4.12517531	-1.58305967	4.99960844
H	4.38697147	-0.85983577	4.59180646
H	4.81513513	-2.08311259	5.17380777
O	1.86946469	-2.97546683	5.82121856
H	1.00207121	-2.93303105	5.87462101
H	2.21898785	-2.30618832	6.25421573
O	1.68047379	-5.11966341	3.16832336
H	2.31062706	-5.61987350	2.83792255
H	1.00726191	-5.09841959	2.61902521
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O	1.49240102	0.10775636	-0.09278753
O	2.45642650	1.50955430	-4.77969349
O	4.37520098	2.88119126	-3.23900239
O	0.85278290	-1.26405522	-6.77408316
O	0.71011195	-3.46473565	-1.15267770
O	2.89911026	-1.87819717	-1.09838782
O	4.78998704	-1.93645112	-3.15959353
O	2.31568864	-3.27050484	-3.27458321
O	3.29055325	0.30811398	-2.64319326
O	3.17473858	0.16924253	-7.17539320
O	2.66048730	-1.06019021	-4.72958887
N	-3.04287608	-2.71010243	2.11893260
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C	-1.26263544	-4.17484442	1.40612979
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C	-2.11115740	-4.73894896	0.49673392
C	-3.45294981	-4.29418553	0.42773662
H	-4.06437973	-4.69313067	-0.18066058
C	-3.85383862	-3.27821125	1.25143593
C	-5.23550825	-2.59880482	1.19073877
W	0.99148554	1.89616009	-0.28598220
W	-0.27285331	3.47730784	-2.94618904
W	-1.06970112	1.61803776	-6.02228898
W	-3.28884454	1.37092892	-3.06389605
La	1.20818680	3.61421552	3.49301594
O	2.42162146	1.62475672	3.59272299
O	1.83602756	-0.55038667	3.66172453
O	4.04101232	-3.87844801	1.91613706
O	5.70078893	-3.73812767	0.42774191
O	5.77443612	1.36533922	-0.37296571
H	6.49308898	1.01417137	-0.63026280
O	1.87700123	5.72960845	4.62541504
H	2.63512172	5.61263541	5.03591794
H	1.26576658	5.95339487	5.20211240
O	-0.69161773	4.36403640	4.99960844
H	-1.44884603	4.22914647	4.59180646
H	-0.60353935	5.21158573	5.17380777
O	1.64209786	3.10673719	5.82121856
H	2.03904377	2.33433473	5.87462101
H	0.88772394	3.07479393	6.25421573
O	3.59352152	4.01516466	3.16832336
H	3.71163970	4.81099855	2.83792255
H	3.91173008	3.42152409	2.61902521
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O	-0.71797764	5.11647618	-3.15959353
O	1.67449621	3.64069767	-3.27458321
O	-1.91211108	2.69564584	-2.64319326
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C	-1.14137765	-0.65897437	-9.77338361
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