

Supporting Information

Trinuclear molybdenum clusters with sulfide bridges as potential anionic receptors via chalcogen bonding

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Table S1. Cartesian atomic coordinates for model supramolecular associates.

Atom	X	Y	Z
SAQBOB			
I	15.623812	13.246100	16.431629
Mo	17.460406	14.556395	12.430017
Mo	17.394981	11.847809	12.437739
Mo	19.398110	13.163459	13.735958
S	17.750851	15.903281	10.387564
S	16.007933	16.611886	12.568185
S	17.610585	10.482896	10.400543
S	15.854037	9.855325	12.581492
S	21.800725	13.074214	13.130385
S	20.808950	13.141326	15.834599
S	15.775230	13.241102	11.180756
S	19.418680	15.647683	13.504967
S	19.291052	10.672274	13.541603
S	15.592339	13.240924	13.231752
S	18.008088	14.845013	14.767535
S	17.919864	11.568651	14.774600
S	19.068510	13.160782	11.384476
N	16.160342	18.061403	10.330555
N	15.962086	8.372966	10.351913
N	23.421468	12.822722	15.237897
C	22.197237	12.992287	14.814029
C	24.541615	12.647801	14.331017
C	16.591549	17.013667	10.994287
C	15.278103	19.080581	10.925285
C	16.415597	9.424272	11.009073
C	16.348685	8.194476	8.886446
C	15.503619	9.076216	7.986137
C	23.723809	12.735262	16.705007
C	16.569245	18.245248	8.876589
C	15.726657	17.370647	7.966422
C	24.063322	14.104280	17.276736
C	13.853138	18.903876	10.632849

C	15.144280	7.303811	10.958143
C	13.776314	7.257403	10.537561
C	24.856346	11.212742	14.045152
H	25.324726	13.070823	14.715455
H	24.340880	13.099381	13.496423
H	15.553183	19.953397	10.603277
H	15.399535	19.071657	11.886381
H	17.285445	8.419373	8.769800
H	16.229732	7.266328	8.631797
H	15.756396	8.936994	7.071042
H	15.639920	9.997225	8.219429
H	14.576772	8.851319	8.097854
H	24.469747	12.131965	16.844654
H	22.953088	12.372927	17.169948
H	17.506005	18.013211	8.771443
H	16.460204	19.175181	8.625225
H	15.999259	17.500944	7.054613
H	14.799810	17.609823	8.060067
H	15.843133	16.449638	8.206285
H	24.256622	14.020390	18.213189
H	23.317384	14.695082	17.155162
H	24.831564	14.457690	16.821653
H	13.350063	19.596417	11.066574
H	13.563189	18.047124	10.956500
H	13.711881	18.952068	9.684895
H	15.558140	6.448844	10.752780
H	15.166584	7.410905	11.922525
H	13.307934	6.548798	10.999215
H	13.736663	7.100332	9.591250
H	13.350063	8.094522	10.739637
H	25.599806	11.162765	13.438922
H	24.090582	10.789721	13.647570
H	25.079384	10.764732	14.863316
SAQBUH			
Mo	7.576996	11.700947	11.483875
Mo	7.540854	14.400619	11.483875
Mo	5.573674	13.024141	12.754625
S	7.398866	10.333350	9.444500
S	9.128538	9.740132	11.649625
S	7.313673	15.775320	9.460750
S	9.058834	16.384522	11.651250
S	3.188276	12.967306	12.132250
S	4.153794	13.015261	14.846000
S	9.244710	13.070320	10.278125
S	5.661449	10.537601	12.559625
S	5.591746	15.510681	12.545000
S	9.376371	13.075648	12.293125
S	7.006462	11.402562	13.806000

S	6.959994	14.688347	13.806000
S	5.924772	13.025917	10.406500
N	9.115630	8.285507	9.386000
C	8.612218	9.317421	10.076625
C	8.756787	8.047509	8.012875
C	10.050169	7.337069	10.047375
C	9.544175	8.885828	7.068750
C	11.482957	7.553753	9.628125
N	8.965897	17.887103	9.418500
C	8.519280	16.819667	10.075000
C	8.612218	18.116220	8.035625
C	9.895273	18.810675	10.042500
C	9.353137	17.253035	7.049250
C	11.320316	18.597543	9.633000
N	1.543797	12.780816	14.239875
C	2.788128	12.903367	13.801125
C	1.226260	12.747070	15.707250
C	0.423382	12.612086	13.316875
C	1.019732	14.082697	16.267875
C	0.054214	11.191206	13.089375
H	7.793850	8.241104	7.891000
H	8.903938	7.093743	7.798375
H	9.784264	6.411721	9.823125
H	9.980466	7.445411	11.028875
H	9.267944	8.690457	6.149000
H	10.496786	8.685129	7.171125
H	9.386698	9.832490	7.262125
H	12.058654	6.909029	10.088000
H	11.759188	8.464893	9.863750
H	11.562986	7.429426	8.658000
H	8.785185	19.064657	7.817875
H	7.641536	17.956371	7.926750
H	9.825570	18.716542	11.025625
H	9.629368	19.736023	9.808500
H	9.058834	17.467944	6.139250
H	9.169843	16.309926	7.237750
H	10.316074	17.421765	7.127250
H	11.890850	19.251148	10.086375
H	11.400346	18.711213	8.662875
H	11.596547	17.691732	9.880000
H	0.410474	12.205359	15.850250
H	1.969761	12.306597	16.188250
H	0.660890	13.024141	12.447500
H	-0.364006	13.095185	13.674375
H	0.815786	14.008101	17.225000
H	0.271068	14.517841	15.809625
H	1.830354	14.617303	16.147625
H	-0.699614	11.145027	12.463750

H	-0.203946	10.780927	13.940875
H	0.820949	10.709883	12.712375
Cl	10.099219	13.072096	15.652000
O	10.383195	13.034798	17.033250
O	10.625866	14.286948	15.065375
O	10.690406	11.940720	15.019875
O	8.689666	13.025917	15.470000
SAQCAO			
Mo	13.568384	9.830755	2.697187
Mo	13.675880	12.408431	3.579266
Mo	15.031524	11.678159	1.331079
S	11.523571	8.676386	1.920193
S	13.618549	7.426854	3.420046
S	13.847874	13.782089	5.680970
S	11.760062	13.976553	3.716195
S	14.596762	12.443600	-0.955320
S	17.213693	12.056742	0.127376
S	15.911797	9.619741	2.213158
S	14.767562	9.325977	0.563639
S	14.298162	10.490689	4.900792
S	12.296348	10.660328	4.652408
S	16.031237	12.722883	3.254457
S	14.947916	14.019997	2.159023
S	12.660640	11.700915	1.544434
N	11.431602	6.088365	2.623946
N	11.828143	15.534330	5.993041
N	16.833874	12.958722	-2.343718
C	12.127938	7.257215	2.662158
C	12.354874	14.564081	5.231969
C	16.314310	12.571864	-1.114540
C	10.060431	5.980789	2.031647
C	12.059857	4.847108	3.219428
C	10.161955	5.507043	0.652802
C	11.657344	4.675401	4.802075
C	12.262905	15.943945	7.324120
C	10.663603	16.363903	5.359345
C	13.316366	17.077626	6.957914
C	9.567144	15.821888	5.665048
C	15.831772	13.018716	-3.668429
C	18.480951	13.287655	-2.369194
C	15.235766	11.667815	-4.353075
C	18.915713	11.988473	-3.037918
H	9.533701	5.403605	2.553889
H	9.657918	6.872426	2.015725
H	12.955657	4.929859	3.136634
H	11.669288	4.129248	2.741768
H	9.254211	5.432568	0.289780
H	10.550135	4.623682	0.649618

H	10.664798	6.092503	0.111454
H	12.016858	3.924441	5.110962
H	10.665992	4.683676	4.875316
H	11.955944	5.482218	5.270182
H	12.735887	15.277804	7.718986
H	11.564181	16.330803	7.766752
H	10.467722	17.046595	6.040807
H	10.886956	16.684561	4.575983
H	13.611382	17.423109	7.741276
H	12.806357	17.766524	6.438857
H	13.970897	16.717662	6.387906
H	8.895891	16.243915	4.942189
H	9.297210	15.312973	6.139523
H	9.723610	14.938527	5.251076
H	15.043468	13.486256	-3.362726
H	16.294005	13.616588	-4.279834
H	18.673250	13.960002	-2.951939
H	18.817772	13.357993	-1.496668
H	14.829670	11.990542	-5.184203
H	14.912084	11.144418	-3.865862
H	16.169787	11.278888	-4.795706
H	19.922592	11.986404	-3.034733
H	18.577698	11.804353	-3.824464
H	18.726998	11.210618	-2.381931
S	17.916000	10.343807	5.308395
O	16.881650	10.513446	4.391288
O	18.950350	10.174169	4.391288
O	17.545736	9.363214	6.223368
O	18.286264	11.324400	6.223368
VIFXUD			
Mo	2.084387	0.824941	14.175644
Mo	2.083726	0.820599	11.454290
Mo	0.581026	-0.990823	12.815601
S	2.952955	-0.912783	12.812884
S	3.504068	2.338595	12.796941
S	1.500312	2.721600	12.807811
S	0.778854	-0.970351	15.293101
S	-0.294525	0.554593	14.444320
S	0.780015	-0.979160	10.350784
S	-0.300697	0.542062	11.175107
S	3.982025	0.278165	15.671927
S	2.086627	2.373335	16.154202
S	4.066001	0.308934	10.070695
S	2.195624	2.408943	9.492944
S	-1.632731	-2.218496	12.878649
S	0.960277	-3.413538	12.776831
C	3.481956	1.540949	16.720177
N	4.081862	1.844921	17.861185

C	3.576806	2.919367	18.725728
H	3.140883	3.589345	18.176783
H	4.325418	3.343687	19.173218
C	2.613621	2.420606	19.747527
H	2.261452	3.162544	20.243933
H	3.062604	1.818866	20.345388
H	1.894087	1.957825	19.309096
C	5.214317	1.065761	18.377882
H	5.271301	0.232011	17.886911
H	5.046576	0.848639	19.309096
C	6.518701	1.774201	18.278238
H	7.206264	1.239459	18.682247
H	6.460283	2.617877	18.732975
H	6.731515	1.923085	17.354272
C	3.739188	1.743184	9.167201
N	4.625192	2.281647	8.347588
C	4.337686	3.522347	7.621821
H	3.376576	3.620363	7.531236
H	4.714795	3.462794	6.730464
C	4.889860	4.732030	8.308455
H	4.734575	5.507467	7.764945
H	5.834950	4.620367	8.442521
H	4.457518	4.844934	9.158142
C	5.964497	1.707203	8.207000
H	6.347394	2.012415	7.368183
H	5.884550	0.741939	8.156272
C	6.904682	2.052118	9.312137
H	7.759787	1.647650	9.143648
H	6.553780	1.723332	10.143707
H	7.004988	3.004975	9.361052
C	-0.731366	-3.673713	12.935536
N	-1.236012	-4.897043	13.066703
C	-2.656779	-5.127813	13.265265
H	-3.003876	-5.598038	12.489858
H	-3.106121	-4.269249	13.310558
C	-2.999177	-5.911935	14.491786
H	-3.951643	-6.019876	14.546137
H	-2.685526	-5.444192	15.269005
H	-2.580372	-6.775463	14.448305
C	-0.351886	-6.059579	13.006192
H	0.279598	-5.934268	12.281512
H	-0.883971	-6.844942	12.799659
C	0.423886	-6.321366	14.290687
H	0.963417	-7.109211	14.183797
H	-0.191603	-6.451640	15.015367
H	0.989425	-5.569502	14.480916
Cl	-1.529488	2.831029	12.875569