Dimolybdenum Cyclopentadienyl Complexes with Bridging Chalcogenophosphinidene Ligands.

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SUPPORTING INFORMATION

DFT Analysis of *syn*-8b

(*syn*-[$Mo_2Cp_2(\mu\text{-}\kappa^2_{P,S}\text{:}\kappa^1_P,\eta^4\text{-SPMes*})(CO)_3$])

Optimized Geometry

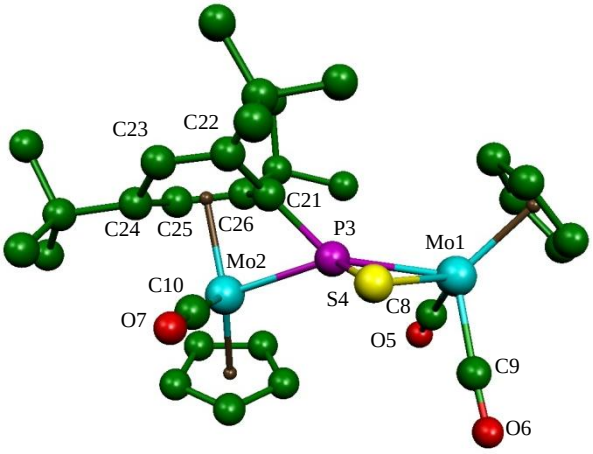
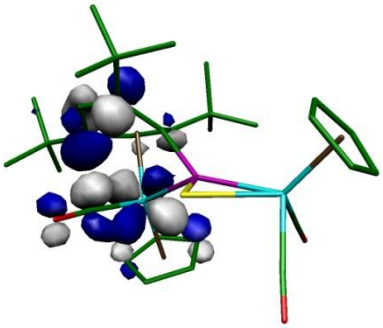
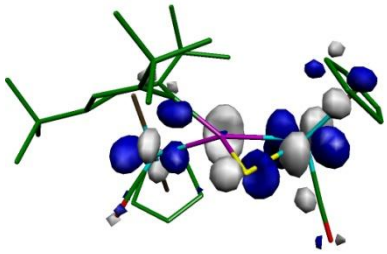
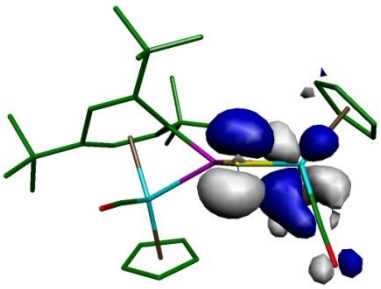
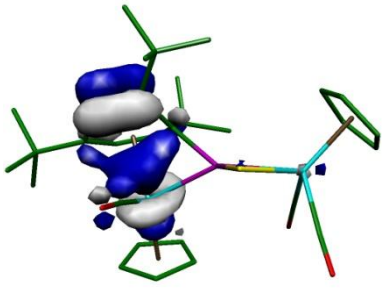


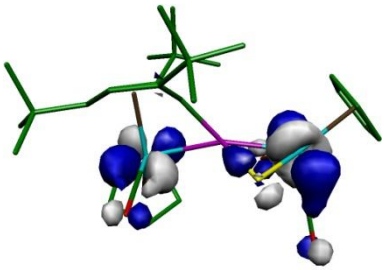
Table S1: Selected distances (Å) and angles (deg.)

Parameter	(Xray)	DFT
Mo1-P	2.434	2.499
Mo1-S	2.565	2.631
S-P	2.036	2.059
Mo1-CO	1.951	1.969
	1.960	1.979
Mo2-P	2.415	2.460
Mo2-CO	2.002	1.982
Mo2-C21	2.289	2.337
Mo2-C26	2.229	2.272
Mo2-C25	2.275	2.335
Mo2-C24	2.499	2.632
Mo2-C23	3.237	3.306
Mo2-C22	3.221	3.274
P-C21	1.783	1.815
C9-O6	1.148	1.162
C8-O5	1.159	1.168
C10-O7	1.100	1.158
C21-C26	1.476	1.480
C26-C25	1.429	1.436
C25-C24	1.420	1.416
C24-C23	1.490	1.476
C23-C22	1.336	1.343
C22-C21	1.498	1.503

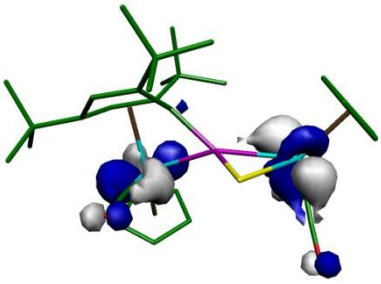
Table S2: Molecular Orbitals of ***syn*-8b**.

	E (eV)	**IA254**
LUMO+1	-1.46	
LUMO	-1.72	
HOMO (154)	-4.91	
HOMO-1	-5.25	

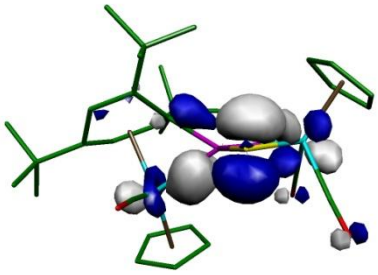
HOMO-2 -5.50



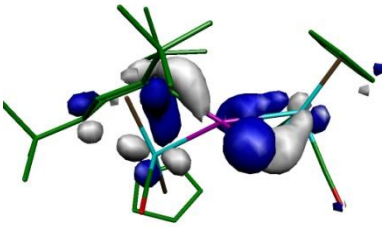
HOMO-3 -5.62



HOMO-4 -6.01



HOMO-5 -6.30



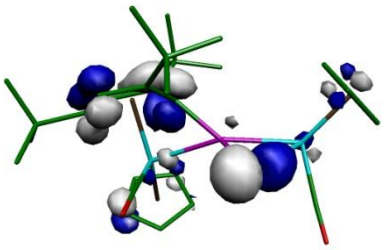
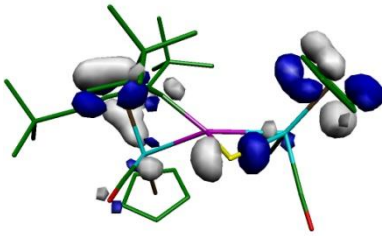
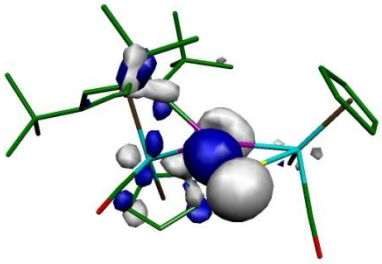
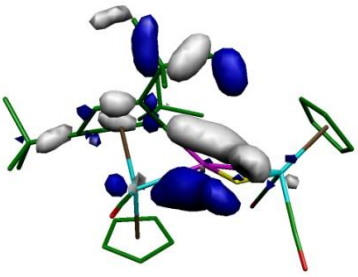
HOMO-6	-6.78	
HOMO-7	-7.08	
142	-8.09	
141	-8.23	
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Table S3: Cartesian Coordinates for ***syn*-8b**.

Mo	-3.22833	-0.10519	-0.17433
Mo	1.39108	-1.19332	-0.31852
P	-0.73747	0.04084	-0.32019
S	-1.59672	0.78982	-2.03466
O	-2.80535	-2.83228	1.31559
O	-4.13088	-2.05965	-2.45657
O	1.92297	0.04472	-3.15259
C	-2.95080	-1.82189	0.74856
C	-3.76420	-1.34184	-1.61994
C	1.73102	-0.36352	-2.08555
C	-5.21979	1.17707	-0.35969
C	-5.31895	0.29855	0.76402
C	-4.35093	0.72271	1.72975
C	-3.68234	1.87286	1.21365
C	-4.21758	2.14770	-0.07028
C	1.01668	-3.19529	-1.55088
C	2.28888	-3.28919	-0.90638
C	2.05478	-3.31971	0.50468
C	0.64731	-3.25590	0.72421
C	0.01331	-3.17092	-0.54752
C	0.68696	0.92430	0.37506
C	1.46057	2.07761	-0.20035
C	2.77048	1.81082	-0.38195
C	3.34602	0.52651	0.06424
C	2.73089	-0.04096	1.20707
C	1.34127	0.19218	1.48196
C	0.87328	3.48366	-0.44814
C	-0.51839	3.64805	0.19171
H	-1.24466	2.96156	-0.24810
H	-0.87794	4.67112	0.02750
H	-0.48322	3.47848	1.27508
C	0.76704	3.74975	-1.96941
H	0.09322	3.03612	-2.45115
H	1.74825	3.67178	-2.45100
H	0.38067	4.76143	-2.14887
C	1.80252	4.55372	0.17563
H	1.36793	5.55153	0.03742
H	2.79380	4.56354	-0.28907
H	1.93567	4.38619	1.25065
C	4.82963	0.25044	-0.25852
C	5.68792	1.31678	0.47572
H	6.75278	1.13173	0.28998
H	5.52101	1.28097	1.55848
H	5.46462	2.33270	0.13517
C	5.30306	-1.13691	0.21636
H	4.70131	-1.93815	-0.22329
H	5.27126	-1.24113	1.30658
H	6.34385	-1.29283	-0.08948
C	5.09322	0.35479	-1.77596
H	6.16791	0.26948	-1.97622
H	4.75142	1.30828	-2.19076
H	4.58116	-0.44363	-2.32189
C	0.81463	0.02877	2.92799
C	1.54787	-1.08443	3.70773
H	1.11035	-1.17586	4.70830
H	2.61272	-0.86843	3.84455
H	1.45341	-2.05707	3.21430
C	-0.69527	-0.23386	3.02436
H	-1.27401	0.53867	2.51358
H	-0.99642	-0.23733	4.07912
H	-0.97151	-1.20022	2.59528
C	1.11321	1.38163	3.62939
H	0.57183	2.20259	3.14696
H	2.18283	1.61847	3.59971
H	0.80240	1.34080	4.68075
H	0.84272	-3.16154	-2.61841
H	3.30522	-0.66884	1.87674
H	-5.82371	1.13660	-1.25643
H	3.45114	2.55907	-0.77387
H	-3.89099	2.93415	-0.73730
H	-1.04990	-3.10254	-0.72366
H	2.81545	-3.40962	1.26934
H	-4.19411	0.28134	2.70514
H	-2.90287	2.43415	1.70993
H	0.13652	-3.28438	1.67597
H	3.24540	-3.37621	-1.40350
H	-6.02927	-0.50842	0.88318

Table S4: Atomic Charges for ***syn*-8b**.

Atom		Mulliken	NPA
1	Mo	-0.369947	-0.30270
2	Mo	-0.256831	-0.03763
3	P	0.471062	0.75173
4	S	-0.147643	-0.35134
5	O	-0.312657	-0.49326
6	O	-0.289428	-0.46977
7	O	-0.271086	-0.44890
8	C	0.216012	0.55782
9	C	0.268088	0.59629
10	C	0.260768	0.60088
11	C	-0.160998	-0.29610
12	C	-0.160553	-0.29649
13	C	-0.167498	-0.28873
14	C	-0.131051	-0.30211
15	C	-0.113619	-0.26192
16	C	-0.148976	-0.26724
17	C	-0.149473	-0.29694
18	C	-0.157614	-0.28737
19	C	-0.130537	-0.29017
20	C	-0.103096	-0.23332
21	C	-0.304654	-0.39716
22	C	0.211079	0.00890
23	C	-0.203682	-0.23507
24	C	0.176872	-0.02688
25	C	-0.254425	-0.25080
26	C	0.068712	-0.04719
27	C	0.049414	-0.06698
28	C	-0.481518	-0.66685
29	H	0.189300	0.23948
30	H	0.136003	0.23068
31	H	0.137796	0.21993
32	C	-0.453738	-0.65879
33	H	0.189338	0.24904
34	H	0.139462	0.22774
35	H	0.131759	0.22497
36	C	-0.441345	-0.65710
37	H	0.136962	0.22994
38	H	0.137347	0.22446
39	H	0.141447	0.23029
40	C	0.045777	-0.06374
41	C	-0.447477	-0.65790
42	H	0.145692	0.23395
43	H	0.147335	0.23177
44	H	0.151041	0.23240
45	C	-0.476602	-0.66237
46	H	0.165226	0.22794
47	H	0.146608	0.22527
48	H	0.149640	0.23867
49	C	-0.461657	-0.66183
50	H	0.139938	0.23065
51	H	0.156926	0.23617
52	H	0.172295	0.23674
53	C	0.070340	-0.05705
54	C	-0.471157	-0.66505
55	H	0.148527	0.23922
56	H	0.145529	0.22606
57	H	0.158412	0.22799
58	C	-0.480284	-0.66376
59	H	0.175233	0.23444
60	H	0.137878	0.23142
61	H	0.173941	0.23627
62	C	-0.452501	-0.65552
63	H	0.158261	0.23271
64	H	0.149232	0.23232
65	H	0.142486	0.23227
66	H	0.188631	0.28129
67	H	0.154584	0.25877
68	H	0.175856	0.27483
69	H	0.133092	0.23648
70	H	0.179690	0.27578
71	H	0.198834	0.28166
72	H	0.168359	0.26914
73	H	0.168746	0.27182
74	H	0.165171	0.26833
75	H	0.178273	0.27486
76	H	0.174142	0.27195
77	H	0.172928	0.27473
Sum		0.00000	0.00000