Electronic Supplementary Information for Dalton Transactions

Site Specific Ligand Substitution in Cubane-type $Mo_3FeS_4^{4+}$ Clusters Bearing diphosphane Ligands: Kinetics and Mechanism of Reaction and Isolation of Mixed Ligand Cl/SPh Complexes

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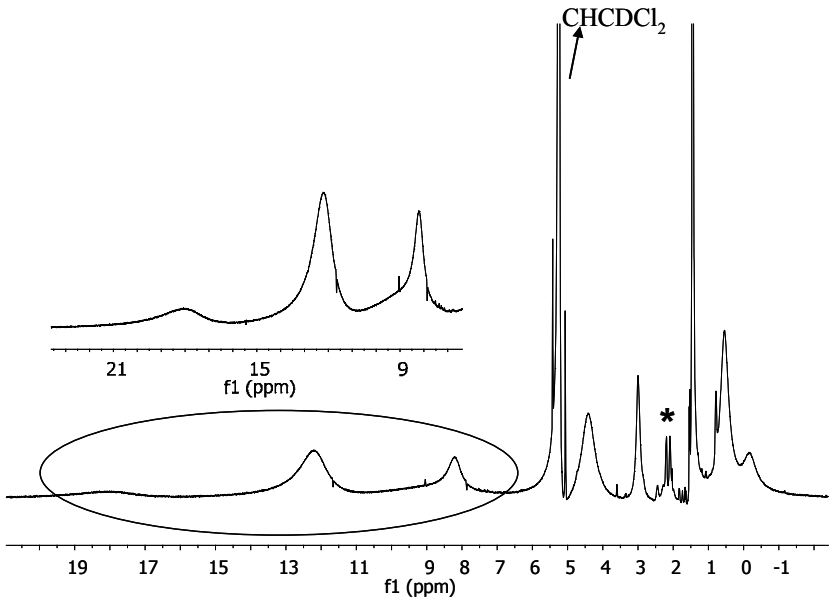

Figure S1. ^{1}H NMR spectra of the open-shell 14 metal electrons cluster **1** (top) together with the diamagnetic starting $[Mo_3S_4(dmpe)_3Cl_3]^+$ complex (bottom). * impurity

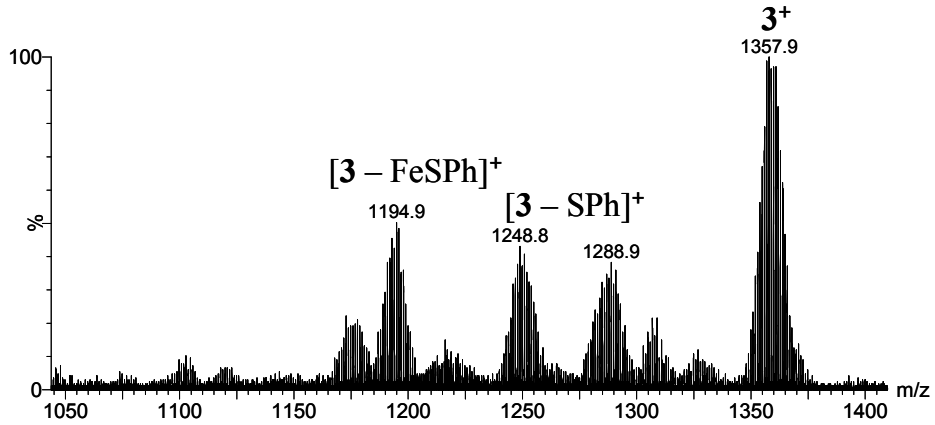

Figure S2. ESI mass spectrum of CH_3CN solutions of **1** after prolonged reaction with an excess of NaSPh. Note that identical ionization mechanisms to that observed for **1**, that is, losses of anionic SPh^- and $FeSPh^-$ fragments are also observed.

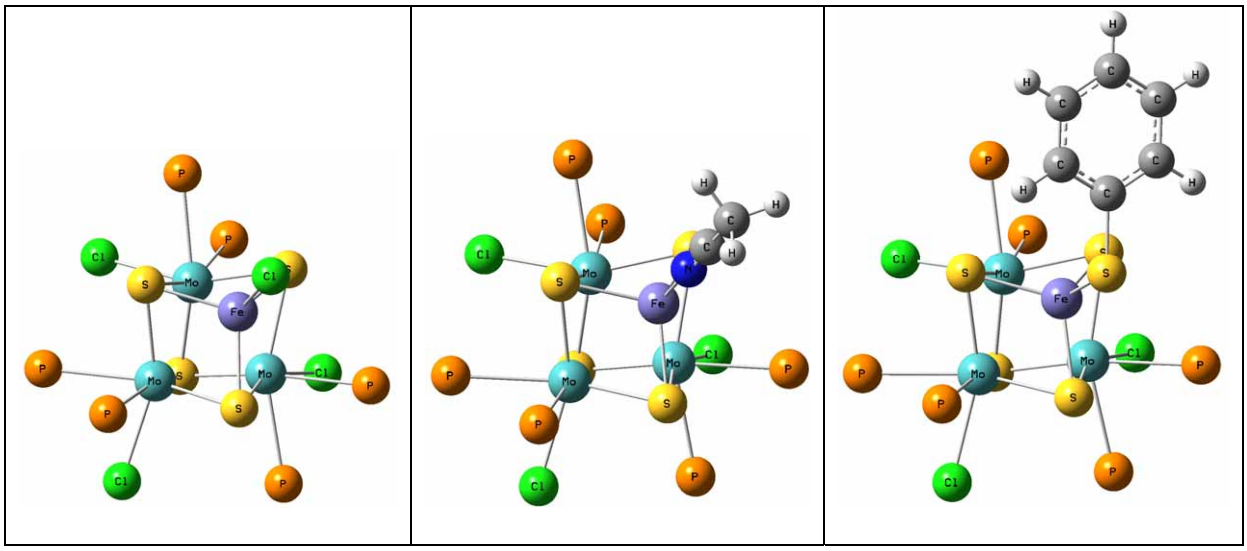

Figure S3. Optimized geometries for the $[Mo_3(FeX)S_4(dmpe)_3Cl_3]$ cluster with different X ligands coordinated at the Fe site: Cl^- (**1**), CH_3CN an PhS^- (**2**). Although the complete dmpe ($Me_2PCH_2CH_2PMe_2$) ligand was used in the calculations, for simplicity only the P atoms of the three dmpe ligands are shown in the Figure.

Table S1. Summary of kinetic data at 25.0 º C for the reaction of cluster **1** with $(Et_4N)(PhS)$, $(Hlut)(BPh_4)$, HCl and HBF_4.

$(ET_4N)(PHS)$				
	$[PhS^-]$	**k_{1obs}/s^{-1}**	**k_{2obs}/s^{-1}**	**k_{3obs}/s^{-1}**
	0.05	0.061	$3.7\cdot10^{-3}$	$6.2\cdot10^{-4}$
	0.04	0.043	$3.0\cdot10^{-3}$	$8.6\cdot10^{-4}$
	0.03	0.052	$3.1\cdot10^{-3}$	$8.5\cdot10^{-4}$
	0.02	0.060	$4.2\cdot10^{-3}$	$10.0\cdot10^{-4}$
	0.01	0.082	$3.7\cdot10^{-3}$	$9.7\cdot10^{-4}$
$(Hlut)BPh_4$				
	$[Hlut^+]$	**k_{1obs}/s^{-1}**		
	0.05	$3.6\cdot10^{-3}$		
	0.04	$1.9\cdot10^{-3}$		
	0.03	$2.3\cdot10^{-3}$		
	0.02	$1.5\cdot10^{-3}$		
	0.01	$3.3\cdot10^{-3}$		
HCl				
	[HCl]	**k_{1obs}/s^{-1}**		
	0.04	$3.9\cdot10^{-4}$		
	0.02	$5.8\cdot10^{-4}$		
	0.01	$4.0\cdot10^{-4}$		
HBF_4				
	$[HBF_4]$	**k_{1obs}/s^{-1}**		
	0.04	$4.6\cdot10^{-4}$		
	0.02	$5.3\cdot10^{-4}$		

	0.01	$5.0 \cdot 10^{-4}$		

DFT Calculations: Cartesian coordinates and solution energies (acetonitrile, CPCM method) of the species discussed in the text.

Cl^-
E(CH_3CN)= -15.1245437 a. u.

$Cl \cdots H \cdots Cl^-$
E(CH_3CN)= -30.6939541 a. u.

Cl	-0.000025	1.616262	0.000000
H	0.000856	-0.000442	0.000000
Cl	-0.000025	-1.616236	0.000000

CH_3CN
E(CH_3CN)= -132.7371901 a. u.

C	1.191565	0.000429	-0.000198
H	1.573895	-0.405375	0.942984
H	1.569432	1.021844	-0.120319
H	1.572242	-0.612688	-0.824604
C	-0.277128	-0.002080	0.001005
N	-1.457456	0.000875	-0.000415

Hsph
E(CH_3CN)= -242.3143622 a. u.

S	2.338746	-0.085005	-0.000425
H	2.574220	1.270773	0.001601
C	0.494296	0.001202	0.000768
C	-0.211205	-1.219634	0.000518
C	-0.208427	1.222061	0.000199
C	-1.618096	-1.213537	-0.000228
H	0.327538	-2.163939	0.000935
C	-1.616697	1.218503	-0.000053
H	0.326035	2.169524	-0.000055
C	-2.327518	0.003598	-0.000239
H	-2.155286	-2.158913	-0.000510
H	-2.152126	2.164957	-0.000237
H	-3.414435	0.004509	-0.000719

sph^-
E(CH_3CN)= -241.8580585 a. u.

S	-2.390399	-0.000039	-0.000497
C	-0.592302	0.000172	0.000204
C	0.174556	-1.212444	-0.000025
C	0.174185	1.212309	0.000135
C	1.580328	-1.212066	0.000139
H	-0.370359	-2.155137	-0.000259
C	1.580458	1.211891	0.000311

H	-0.369658	2.155588	0.000026
C	2.309203	0.000150	0.000422
H	2.114640	-2.164580	0.000095
H	2.114216	2.164731	0.000407
H	3.398981	-0.000044	0.000573

1 (mofecl)

E(CH_3CN)= a. u.

C	3.61773400	-3.80916100	-0.75061600
C	4.48981300	-2.83573500	0.05759000
P	3.45681300	-1.72191500	1.19959800
Mo	1.39570500	-0.81875200	-0.15481100
P	1.98982100	-3.07181600	-1.46736200
Mo	-1.39083500	-0.83242600	-0.21946500
P	-3.27806800	-2.09413600	1.09206100
C	-4.76340600	-2.31162900	-0.07387300
C	-5.09336700	-1.02173600	-0.84274500
P	-3.58078500	-0.07105700	-1.56020800
S	-1.98017100	1.12852400	1.20169500
Fe	-0.17965900	-0.07049800	1.96258900
Cl	-0.31828000	-0.09779200	4.21974600
Mo	-0.04094400	1.61894000	-0.21090400
P	-0.29395700	3.89984000	1.06570200
C	0.28357800	5.31521400	-0.06389700
C	1.58579200	5.00835000	-0.82670700
P	1.90089800	3.15751900	-1.27543600
S	0.05074600	-0.02435700	-2.04546600
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C	2.28658900	-2.93120600	-3.32053600
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mofe-vac

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Mo	1.243053	-1.101672	0.021807
P	2.858371	-2.739670	-1.243073
C	4.223462	-3.250717	-0.025805
C	4.809053	-2.041811	0.719651
P	3.525308	-0.772031	1.375947
S	2.185318	0.756103	-1.414143
Fe	0.190752	-0.150700	-2.001498
Mo	0.393258	1.591623	0.062847
P	1.049215	3.798297	-1.212230
C	0.080216	5.292628	-0.530391
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S	-0.040615	-0.033211	1.851337
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S	-1.450189	1.409861	-1.534039
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H	5.472732	-1.471487	0.057418
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H	-1.897976	4.258193	3.436102
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H	-1.853498	-2.200351	3.676871
H	-3.412996	-1.402301	3.367720
H	-2.625184	-5.031765	1.710234
H	-1.632345	-4.607743	0.281444
H	-0.963532	-4.388667	1.905661
Cl	1.871140	2.685526	1.792762
Cl	1.247970	-3.174643	1.507810
Cl	-3.329512	0.591302	1.437731

mofe-ch3cn

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C	2.16264400	-4.56064700	-1.54591100

C	2.53539700	-4.66589100	-0.05246500
P	2.60141700	-2.95199800	0.79095700
Mo	0.99539200	-1.26809300	-0.41633000
P	0.59245400	-3.50524700	-1.77303100
Mo	-1.59897700	-0.23519900	-0.23913200
P	-3.89031300	-0.63720000	1.03811800
C	-5.27107800	-0.66185200	-0.27253800
C	-5.16367700	0.48301400	-1.30445300
P	-3.39343700	1.20024500	-1.55638900
S	-1.26407900	1.70774000	1.25403700
Fe	-0.00647800	-0.05233800	2.07022500
Cl	-1.70071100	-0.44950000	3.75636200
Mo	0.54449200	1.54028800	-0.37788400
P	1.30201400	3.69720600	0.87643900
C	2.83045400	4.47986100	0.03165700
C	2.89368200	4.16568900	-1.47779500
P	2.69018900	2.29582700	-1.80067300
S	-0.12901100	0.00992500	-2.17326600
S	-0.64345100	-2.06836400	1.14204700
S	2.13141300	0.36574100	0.98500300
C	2.31407700	-3.37347600	2.60560400
C	4.44019300	-2.53929100	0.78081100
C	-0.72177800	-4.74384600	-1.22959700
C	0.36519900	-3.41025800	-3.63426300
C	4.42427900	1.69844400	-1.35095200
C	2.65216300	2.16372600	-3.67421300
C	0.07102200	5.11826000	0.97067500
C	1.85365400	3.54525300	2.67134500
C	-3.22455900	1.26063500	-3.42935400
C	-3.70997200	3.01050700	-1.11569200
C	-4.56668100	0.64447100	2.24681400
C	-4.16926300	-2.27696300	1.91369500
H	1.98119600	-5.55833700	-1.96693900
H	2.96119900	-4.07772000	-2.11569500
H	3.50995300	-5.15480600	0.07266600
H	1.79333900	-5.26401100	0.49172500
H	3.85620100	4.49122900	-1.89486600
H	2.80525800	5.56398500	0.20133000
H	2.08971000	4.67394400	-2.01733000
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H	-5.18569000	-1.62738900	-0.77474100
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H	3.48501900	2.72139600	-4.11962800
H	2.72744800	1.10613700	-3.94096700
H	1.69884600	2.56178600	-4.03079600
H	5.16435200	2.20413100	-1.98350800
H	4.62887900	1.91922900	-0.29867400
H	4.47462700	0.61903800	-1.50401500
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H	1.00465500	3.20021200	3.26858500
H	2.65178600	2.80107700	2.74279200
H	0.51565000	5.97213100	1.49585800
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H	-3.97452900	3.08874100	-0.05670600

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H	3.00299200	-4.16301400	2.92913100
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H	4.59621400	-1.60361100	1.32622400
H	0.41128800	-4.41148300	-4.07927800
H	-0.61123900	-2.96001900	-3.83282900
H	1.15120400	-2.77538100	-4.05037100
H	-0.60065500	-5.67712900	-1.79368100
H	-0.62409800	-4.94059900	-0.15806800
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Cl	-0.34529800	3.37185900	-1.97614800
Cl	-2.74990700	-2.03727600	-1.76726200
Cl	2.97143700	-1.33533800	-2.14245000
C	2.12583600	0.12294500	6.05106500
H	3.16697000	0.46487200	6.03266700
H	1.54228400	0.80701300	6.67864800
H	2.09179200	-0.87322800	6.50810600
C	1.56209100	0.08174800	4.70062100
N	1.04607000	0.04046100	3.64772400

mofecl-hcl1

E(CH_3CN)= -1196.1778888 a. u.

C	1.681103	4.769282	-1.466524
C	0.661972	5.218981	-0.408922
P	0.325147	3.861691	0.877780
Mo	0.000769	1.574999	-0.392293
P	1.424520	2.994713	-2.155561
Mo	1.090962	-0.985271	-0.617593
P	3.277849	-2.162317	0.246937
C	3.767660	-3.486944	-1.026225
C	2.569272	-4.334100	-1.481585
P	0.959102	-3.353541	-1.862467
S	-0.101201	-2.240991	1.194090
Fe	0.450127	-0.080442	1.721970
Cl	0.930979	-0.007865	3.974072
Mo	-1.611894	-0.712090	0.003723
P	-3.229498	-1.727935	1.804900
C	-5.020142	-1.120889	1.531025
C	-5.295044	-0.783190	0.051734
P	-3.967246	0.403964	-0.630544
S	-0.604028	-0.038057	-2.137626
S	2.122286	1.013765	0.586549
S	-1.462064	1.156164	1.568410
C	1.718497	4.031033	2.136096
C	-1.141761	4.575852	1.815145
C	3.224066	2.629541	-2.580718
C	0.670584	3.235154	-3.863942
C	-4.567671	2.017859	0.145503
C	-4.414021	0.591950	-2.445090
C	-3.397194	-3.602507	1.823167
C	-2.906053	-1.332562	3.616939
C	0.847770	-3.322027	-3.741753

C	-0.266199	-4.721185	-1.426122
C	3.262982	-3.083728	1.892500
C	4.848158	-1.134405	0.365057
H	2.693382	4.772225	-1.042416
H	1.683096	5.461796	-2.318204
H	-0.305782	5.440799	-0.868058
H	1.017943	6.119144	0.109894
H	-6.276564	-0.302665	-0.055519
H	-5.709916	-1.896192	1.887122
H	-5.277256	-1.683929	-0.567615
H	-5.163224	-0.237300	2.166145
H	4.201764	-2.940593	-1.868189
H	4.545008	-4.126185	-0.586027
H	2.293792	-5.051964	-0.698170
H	2.827193	-4.913419	-2.377592
H	-5.482015	0.815818	-2.554771
H	-3.818018	1.408612	-2.860430
H	-4.169568	-0.338622	-2.962949
H	-5.620830	2.175037	-0.118541
H	-4.464570	1.969036	1.233773
H	-3.960627	2.842023	-0.230415
H	-3.634262	-1.845792	4.255990
H	-1.892458	-1.646578	3.881870
H	-2.969987	-0.252514	3.774282
H	-4.145598	-3.904939	2.565167
H	-3.684681	-3.947537	0.827824
H	-2.427968	-4.038799	2.081002
H	0.937603	-4.337018	-4.147170
H	-0.122604	-2.900120	-4.020680
H	1.638619	-2.679348	-4.133579
H	0.065772	-5.657590	-1.891609
H	-0.304144	-4.843343	-0.339900
H	-1.262375	-4.455132	-1.778724
H	5.716683	-1.795490	0.473998
H	4.941815	-0.540586	-0.547228
H	4.788337	-0.471420	1.232191
H	4.242796	-3.538041	2.080223
H	3.033987	-2.378564	2.696702
H	2.488141	-3.855663	1.884077
H	1.725141	5.041237	2.562270
H	1.565961	3.296606	2.932827
H	2.682511	3.818344	1.666068
H	-0.934100	5.615248	2.096586
H	-2.024746	4.533058	1.173353
H	-1.320875	3.982706	2.715894
H	1.303949	3.897669	-4.465773
H	0.600266	2.256380	-4.348112
H	-0.333752	3.650021	-3.761965
H	3.641095	3.495759	-3.109803
H	3.787388	2.448221	-1.661290
H	3.289727	1.734909	-3.199552
Cl	-2.803564	-2.474122	-1.424571
Cl	2.755418	-0.670601	-2.566759
Cl	-1.778952	3.115768	-1.481613
Cl	4.318818	0.466467	3.997252
H	2.959783	0.340025	4.016022

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E(CH_3CN)= -1196.172491 a. u.

C	3.379478	-3.947581	0.257137

C	4.074888	-3.009775	1.256600
P	2.841940	-1.840340	2.105333
Mo	1.212641	-0.858914	0.278801
P	2.074039	-3.115901	-0.883243
Mo	-1.482951	-0.781962	-0.439609
P	-3.662622	-1.997409	0.367006
C	-4.811865	-2.202684	-1.131935
C	-4.924564	-0.911764	-1.959936
P	-3.279120	0.049737	-2.242841
S	-2.334467	1.172479	0.862015
Fe	-0.777054	-0.097649	1.968984
Cl	-1.445192	-0.199749	4.127924
Mo	-0.114664	1.621583	-0.072500
P	-0.571349	3.824354	1.281879
C	0.815098	5.100467	0.980741
C	1.440254	4.942823	-0.419069
P	1.996187	3.143607	-0.726998
S	0.369661	-0.004502	-1.865591
S	-0.418926	-2.273327	1.327725
S	1.204748	1.026055	1.889894
C	2.119232	-2.848794	3.523204
C	3.986487	-0.648132	3.005083
C	0.976304	-4.627101	-1.142052
C	2.931596	-2.985923	-2.555011
C	3.601974	3.145669	0.267757
C	2.577027	3.180759	-2.512959
C	-2.141180	4.768212	0.849638
C	-0.667534	3.705872	3.157978
C	-2.846251	-0.243717	-4.051479
C	-4.023430	1.783403	-2.301235
C	-4.741325	-1.191606	1.687278
C	-3.513044	-3.765698	0.990004
H	2.839005	-4.738886	0.791706
H	4.119646	-4.438273	-0.388053
H	4.798351	-2.364701	0.749298
H	4.604662	-3.589143	2.024847
H	2.317163	5.595412	-0.522700
H	0.400284	6.107920	1.111380
H	0.722427	5.198969	-1.203452
H	1.569609	4.952914	1.764106
H	-4.376128	-3.010379	-1.726639
H	-5.802978	-2.519852	-0.780448
H	-5.591995	-0.199424	-1.457809
H	-5.358968	-1.125650	-2.944844
H	3.247303	4.033320	-2.675662
H	3.107040	2.255774	-2.747880
H	1.700125	3.264490	-3.159247
H	4.238356	3.969902	-0.076638
H	3.377880	3.274044	1.331097
H	4.117196	2.194693	0.131141
H	-0.970869	4.667907	3.587041
H	-1.386206	2.928965	3.434507
H	0.306980	3.413040	3.558458
H	-2.168672	5.721249	1.391206
H	-2.170251	4.939298	-0.228476
H	-3.005632	4.161078	1.133136
H	-3.711435	-0.035325	-4.692291
H	-2.023117	0.426446	-4.317491
H	-2.515327	-1.276847	-4.173756
H	-4.926570	1.759808	-2.923701
H	-4.281158	2.104402	-1.287857

H	-3.299365	2.486836	-2.711212
H	-4.507505	-4.219299	1.080595
H	-2.906187	-4.333027	0.280270
H	-3.020561	-3.766643	1.966280
H	-5.591789	-1.838728	1.932117
H	-4.136894	-1.019083	2.583566
H	-5.103024	-0.222062	1.332468
H	2.905920	-3.124158	4.235340
H	1.353344	-2.250627	4.026677
H	1.639190	-3.751702	3.135155
H	4.762219	-1.206922	3.542099
H	4.448000	0.018875	2.273418
H	3.404289	-0.055007	3.715456
H	3.138339	-3.990053	-2.943449
H	2.274681	-2.454371	-3.248738
H	3.863892	-2.427769	-2.458876
H	1.619329	-5.495244	-1.334124
H	0.373104	-4.799458	-0.246737
H	0.299326	-4.460664	-1.979498
Cl	-0.949952	3.120015	-1.978823
Cl	-1.642696	-2.808603	-2.041695
Cl	3.602551	-0.176253	-0.599110
Cl	4.896002	0.147669	-3.804810
H	4.325930	0.016227	-2.587862

mofecl-hcl3

E(CH_3CN)= -1196.1693599 a. u.

C	-0.696105	5.176450	-0.897641
C	-2.060794	4.835162	-0.281403
P	-1.959765	3.332061	0.875470
Mo	-0.546359	1.462569	-0.330842
P	0.307578	3.673825	-1.552033
Mo	1.806888	-0.035572	-0.044309
P	3.821853	-0.014206	1.634918
C	5.374469	-0.589060	0.700974
C	5.110642	-1.837165	-0.156766
P	3.458894	-1.837147	-1.145563
S	1.015214	-2.029075	1.247667
Fe	0.057998	-0.039372	1.873431
Cl	-0.123385	-0.086999	4.127661
Mo	-0.609922	-1.362669	-0.457834
P	-1.821314	-3.419200	0.651759
C	-3.440215	-3.829184	-0.274654
C	-3.363465	-3.434150	-1.763822
P	-2.819472	-1.615163	-1.956964
S	0.463710	0.110463	-2.110948
S	1.081038	1.958937	1.361930
S	-2.038521	-0.015576	0.999695
C	-1.353005	4.031924	2.517068
C	-3.777382	3.004046	1.233812
C	2.030152	4.396587	-1.307186
C	0.120076	3.743798	-3.423396
C	-4.452980	-0.761537	-1.547133
C	-2.651956	-1.376043	-3.812231
C	-0.877332	-5.047833	0.627168
C	-2.340811	-3.285621	2.457838
C	3.966311	-1.540546	-2.934487
C	3.174390	-3.703757	-1.137053
C	3.768756	-1.103029	3.173677
C	4.375803	1.643443	2.329918

H	-0.050300	5.654080	-0.149474
H	-0.812847	5.885761	-1.727131
H	-2.784421	4.565325	-1.055969
H	-2.454756	5.691962	0.281931
H	-4.345622	-3.552110	-2.240503
H	-3.641993	-4.902448	-0.168099
H	-2.639084	-4.052485	-2.300919
H	-4.251447	-3.291598	0.231829
H	5.672804	0.257403	0.076128
H	6.172863	-0.786282	1.429204
H	5.066459	-2.730449	0.479649
H	5.929094	-1.988365	-0.872454
H	-3.541780	-1.753569	-4.330388
H	-2.533497	-0.306968	-4.007762
H	-1.761850	-1.909738	-4.153781
H	-5.222017	-1.108870	-2.248059
H	-4.762286	-1.000519	-0.525772
H	-4.328002	0.317397	-1.640014
H	-2.595551	-4.275460	2.853526
H	-1.520566	-2.853081	3.038364
H	-3.209256	-2.628666	2.552526
H	-1.514694	-5.851687	1.014223
H	-0.561306	-5.267771	-0.394328
H	0.010510	-4.948257	1.258244
H	4.743840	-2.253329	-3.234410
H	3.082865	-1.674084	-3.566305
H	4.324158	-0.514358	-3.037838
H	4.109363	-4.205691	-1.416341
H	2.870979	-4.022919	-0.135664
H	2.381974	-3.962886	-1.839212
H	5.362870	1.544324	2.797650
H	4.419871	2.365984	1.511627
H	3.651442	1.985353	3.074271
H	4.658891	-0.934224	3.791225
H	2.868292	-0.864529	3.748671
H	3.715569	-2.156287	2.882760
H	-2.077584	4.751972	2.915007
H	-1.221046	3.208328	3.225751
H	-0.382833	4.518599	2.382691
H	-4.292361	3.952434	1.428518
H	-4.228667	2.509993	0.370769
H	-3.872361	2.361859	2.112934
H	0.436999	4.724822	-3.796738
H	0.749242	2.963250	-3.861535
H	-0.919974	3.547552	-3.689793
H	2.030235	5.433821	-1.665325
H	2.288690	4.365971	-0.245162
H	2.766394	3.803480	-1.849062
Cl	-0.018505	-3.187137	-2.152576
Cl	3.547528	1.459860	-1.238802
Cl	-2.446006	1.954176	-2.025538
Cl	-5.265470	-0.504663	2.483182
H	-4.020451	-0.229601	2.058554

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E(CH_3CN)= -1196.1666654 a. u.

C	-3.229725	-4.152497	0.349337
C	-4.199648	-3.222345	-0.393890
P	-3.279108	-1.953659	-1.465359
Mo	-1.317973	-0.932379	-0.053397

P	-1.721961	-3.289146	1.175846
Mo	1.467332	-0.702537	0.034762
P	3.453912	-1.752347	-1.316121
C	4.957655	-1.854836	-0.158679
C	5.166549	-0.551274	0.628247
P	3.581563	0.195529	1.420211
S	1.891147	1.346715	-1.312338
Fe	0.204949	0.022890	-2.130391
Cl	0.349566	0.079246	-4.384670
Mo	-0.099818	1.630444	0.085871
P	-0.018556	3.952333	-1.135879
C	-0.777891	5.276599	-0.006691
C	-2.099787	4.824891	0.634257
P	-2.203106	2.968823	1.151957
S	-0.053647	-0.073269	1.861853
S	0.106375	-2.191859	-1.521741
S	-1.773533	0.986629	-1.564879
C	-2.882858	-2.864620	-3.066426
C	-4.673680	-0.807151	-1.995650
C	-0.531780	-4.748238	1.071889
C	-2.129302	-3.263467	3.013979
C	-4.001933	2.699952	0.636434
C	-2.321792	2.996802	3.029503
C	1.669365	4.701312	-1.495106
C	-0.905332	4.135619	-2.788497
C	3.691528	-0.276893	3.240179
C	4.150542	1.994020	1.462015
C	4.103727	-0.880640	-2.856749
C	3.279270	-3.531095	-1.901557
H	-2.798374	-4.884054	-0.346014
H	-3.758216	-4.716666	1.128446
H	-4.798508	-2.638236	0.310606
H	-4.878382	-3.802538	-1.033568
H	-2.927294	4.974301	-0.070116
H	-0.022235	5.470188	0.759088
H	-2.316748	5.428962	1.523965
H	-0.927032	6.195666	-0.589515
H	4.756648	-2.691193	0.517194
H	5.849814	-2.092389	-0.753979
H	5.560295	0.232128	-0.032489
H	5.901774	-0.700537	1.429668
H	-3.101507	3.696973	3.352704
H	-2.572732	1.988538	3.370066
H	-1.354159	3.287580	3.443865
H	-4.606612	3.533373	1.015089
H	-4.063567	2.669406	-0.455994
H	-4.365819	1.755818	1.039310
H	-0.735064	5.134542	-3.206886
H	-0.523919	3.375283	-3.477413
H	-1.978562	3.967763	-2.659673
H	1.555274	5.752898	-1.784724
H	2.283346	4.628290	-0.594057
H	2.151595	4.148045	-2.305001
H	4.670133	0.005419	3.646962
H	2.905640	0.252538	3.787295
H	3.529046	-1.351211	3.343988
H	5.188672	2.030363	1.815057
H	4.086680	2.421463	0.457272
H	3.506616	2.573316	2.123649
H	4.254321	-3.920286	-2.218678
H	2.886091	-4.129661	-1.076572

H	2.579315	-3.569725	-2.740771
H	4.916676	-1.461510	-3.308170
H	3.285689	-0.768919	-3.575593
H	4.462068	0.119737	-2.597312
H	-3.806498	-3.196162	-3.555264
H	-2.333404	-2.188994	-3.729457
H	-2.242140	-3.726424	-2.859992
H	-5.517232	-1.395894	-2.375944
H	-4.991040	-0.216826	-1.132915
H	-4.313658	-0.135891	-2.779968
H	-2.428944	-4.265577	3.343557
H	-1.238268	-2.952970	3.567407
H	-2.928959	-2.544511	3.199749
H	-1.059164	-5.653288	1.398974
H	-0.192594	-4.867733	0.038908
H	0.340925	-4.567083	1.698425
Cl	0.986621	3.143454	1.838160
Cl	2.110030	-2.763351	1.450839
Cl	-3.390990	-0.491892	1.431698
Cl	-0.097200	-0.387248	5.436547
H	-0.091969	-0.246430	4.099548

mofecl-hcl2sinhcl

E(CH_3CN)= -1180.9950267 a. u.

C	-2.612008	-2.859262	-3.467774
P	-3.099390	-1.717447	-2.048469
C	-4.188456	-0.444823	-2.903447
C	-4.356877	-2.723936	-1.043276
C	-3.682038	-3.704295	-0.070013
P	-2.106253	-3.049772	0.814691
C	-2.573407	-2.903527	2.629382
Mo	-1.238538	-0.830633	-0.392466
S	-1.232583	1.104303	-1.947143
Mo	0.242947	1.643518	-0.074466
S	-0.217517	-0.017395	1.675685
Mo	1.545721	-0.862717	0.155573
S	0.253316	-2.292289	-1.576351
Fe	0.727368	-0.124636	-2.058895
C	-1.093112	-4.638845	0.782432
P	3.636697	-2.194436	-0.712297
C	3.353944	-3.934943	-1.363861
P	3.435918	-0.129799	1.891679
C	4.288261	1.552157	1.855848
S	2.393266	1.120972	-1.161342
C	4.784941	-2.490558	0.770216
C	4.994580	-1.222218	1.613148
C	4.755853	-1.428093	-2.022438
C	2.994740	-0.337738	3.707243
P	0.722600	3.894882	-1.347951
C	0.741646	3.855324	-3.230477
P	-1.790129	3.209816	0.710726
C	-2.292724	3.157450	2.518087
C	-0.601041	5.201803	-0.941022
C	-1.182630	4.998007	0.470172
C	2.346110	4.751303	-0.938582
C	-3.413866	3.282694	-0.244986
Cl	1.200521	3.000469	1.821243
Cl	1.617504	-2.886493	1.709892
Cl	-3.456314	-0.021406	0.676199
Cl	-4.620798	0.226107	4.026942

H	-3.364790	-4.609378	-0.601633
H	-4.391294	-4.016189	0.705876
H	-4.963421	-1.992385	-0.503862
H	-5.009060	-3.266056	-1.740137
H	-2.032948	5.671742	0.634476
H	-0.147343	6.195872	-1.034171
H	-0.432873	5.197385	1.240558
H	-1.385232	5.126757	-1.704497
H	4.310939	-3.278157	1.360853
H	5.747502	-2.865695	0.399104
H	5.729644	-0.564403	1.133327
H	5.392915	-1.487769	2.599786
H	-2.965249	3.992914	2.743795
H	-2.801100	2.216946	2.735007
H	-1.392543	3.228091	3.132923
H	-4.037236	4.081502	0.173204
H	-3.215815	3.489438	-1.300740
H	-3.934148	2.328825	-0.161752
H	0.885407	4.865884	-3.629135
H	1.563693	3.217880	-3.569770
H	-0.200623	3.445389	-3.604359
H	2.425928	5.686366	-1.504451
H	2.389312	4.954684	0.133140
H	3.176187	4.090867	-1.204025
H	3.878256	-0.167148	4.332813
H	2.221037	0.391595	3.963810
H	2.604135	-1.344459	3.868039
H	5.163797	1.514407	2.514923
H	4.611004	1.780092	0.835770
H	3.605171	2.330997	2.193085
H	4.313893	-4.450126	-1.483054
H	2.729714	-4.477407	-0.649947
H	2.841375	-3.893753	-2.328910
H	5.625201	-2.070739	-2.201272
H	4.197630	-1.313468	-2.956997
H	5.090445	-0.437761	-1.701385
H	-3.504775	-3.163431	-4.025851
H	-1.928097	-2.334655	-4.141623
H	-2.099546	-3.745691	-3.084275
H	-5.036594	-0.946512	-3.383078
H	-4.554128	0.267560	-2.160516
H	-3.608768	0.091590	-3.659488
H	-2.856259	-3.888992	3.016142
H	-1.710381	-2.529500	3.186814
H	-3.405106	-2.208979	2.754430
H	-1.733544	-5.463851	1.116786
H	-0.741228	-4.833956	-0.234683
H	-0.228709	-4.546054	1.438929
H	-4.153773	0.134576	2.778509

mofecl-hcl3sinhcl

E(CH_3CN)= -1180.9913293 a. u.

C	1.317121	4.240950	-2.550817
P	1.953750	3.428059	-0.973096
C	3.751792	3.074873	-1.396687
C	2.102932	4.855925	0.267126
C	0.763070	5.192505	0.938466
P	-0.332657	3.687962	1.413058
C	-0.307523	3.615738	3.290706
Mo	0.540508	1.504617	0.160851

S	2.038578	0.010270	-1.145922
Mo	0.645178	-1.392556	0.299757
S	-0.425955	0.107516	1.917615
Mo	-1.823818	-0.069808	-0.123355
S	-1.096900	1.981173	-1.527835
Fe	-0.136738	-0.045072	-1.919051
C	-2.017409	4.444573	1.043833
P	-3.910812	-0.067925	-1.716466
C	-4.472054	1.585850	-2.411898
P	-3.410662	-1.876076	1.049358
C	-3.109626	-3.737783	1.012114
S	-0.989476	-2.083475	-1.408407
C	-5.412778	-0.621416	-0.695534
C	-5.110140	-1.867480	0.150944
C	-3.944800	-1.195738	-3.227631
C	-3.803978	-1.566878	2.862613
P	1.874489	-3.470637	-0.763281
C	2.372470	-3.390630	-2.577084
P	2.877544	-1.581195	1.780079
C	2.705270	-1.297113	3.627477
C	3.509806	-3.825883	0.149305
C	3.444738	-3.392386	1.626163
C	0.947854	-5.106210	-0.680615
C	4.476478	-0.696708	1.314601
Cl	0.086676	-3.149799	2.012474
Cl	-3.484963	1.428521	1.102886
Cl	2.398840	1.953419	1.856878
Cl	5.261240	-0.520043	-2.716251
H	0.145104	5.805169	0.270904
H	0.933220	5.777580	1.850197
H	2.841658	4.535518	1.005862
H	2.497892	5.734553	-0.259253
H	4.434633	-3.479066	2.091686
H	3.722403	-4.898894	0.070665
H	2.743022	-4.010327	2.192832
H	4.308311	-3.295574	-0.383850
H	-5.676383	0.229594	-0.062360
H	-6.248775	-0.818236	-1.379209
H	-5.112052	-2.765512	-0.479580
H	-5.887309	-2.006052	0.912488
H	3.605840	-1.645394	4.146351
H	2.568511	-0.227695	3.804196
H	1.831525	-1.843161	3.990442
H	5.252432	-0.971167	2.038869
H	4.800946	-0.994886	0.313928
H	4.321073	0.381735	1.340000
H	2.878851	-4.317810	-2.867999
H	1.474746	-3.266960	-3.190290
H	3.044852	-2.548154	-2.754608
H	1.578036	-5.904900	-1.088101
H	0.683568	-5.326111	0.355196
H	0.030364	-5.029917	-1.270795
H	-4.561196	-2.279249	3.209433
H	-2.887324	-1.698383	3.444919
H	-4.161111	-0.542824	2.986146
H	-4.029875	-4.245299	1.325493
H	-2.848915	-4.052478	-0.002413
H	-2.294535	-4.002562	1.684740
H	-5.472363	1.488322	-2.849067
H	-4.492792	2.316825	-1.600349
H	-3.771744	1.923676	-3.180865

H	-4.918078	-1.129620	-3.726860
H	-3.162063	-0.892352	-3.930097
H	-3.754606	-2.230711	-2.930553
H	2.005354	5.032425	-2.867892
H	1.242206	3.490360	-3.343486
H	0.322096	4.663410	-2.387427
H	4.277527	4.017992	-1.584487
H	4.223455	2.555109	-0.560108
H	3.811809	2.452756	-2.293520
H	-0.583492	4.592294	3.704480
H	-1.029670	2.863907	3.621503
H	0.689383	3.328855	3.630329
H	-2.055862	5.444229	1.492863
H	-2.156639	4.520849	-0.038477
H	-2.810345	3.818343	1.450652
H	4.078495	-0.182377	-2.194117

mofecl-hcl4sinhcl

E(CH_3CN)= -1180.9883792 a. u.

C	-3.959882	-1.588600	-3.075034
P	-3.876868	-0.545392	-1.507514
C	-4.704724	1.057337	-2.039011
C	-5.172377	-1.314326	-0.354865
C	-4.622552	-2.541295	0.385009
P	-2.861688	-2.340143	1.119900
C	-3.113741	-2.092965	2.966881
Mo	-1.599680	-0.367958	-0.191695
S	-1.273194	1.582998	-1.704763
Mo	0.576256	1.561256	-0.104252
S	-0.043456	-0.031656	1.658082
Mo	1.106785	-1.237181	-0.166835
S	-0.828635	-2.108413	-1.658279
Fe	0.184030	-0.140825	-2.185392
C	-2.329873	-4.145226	1.023157
P	2.522185	-3.026404	-1.464885
C	1.645302	-4.595313	-2.015909
P	3.412457	-1.190215	1.204579
C	4.641791	0.240266	1.184892
S	2.263359	0.511882	-1.561318
C	3.852397	-3.677943	-0.278536
C	4.563510	-2.534616	0.459407
C	3.490329	-2.524502	-3.003900
C	3.307533	-1.596691	3.038747
P	1.555758	3.697264	-1.288518
C	0.768756	4.280633	-2.898278
P	-0.833732	3.603445	0.986017
C	-0.956534	3.590495	2.862398
C	1.405098	5.170998	-0.104539
C	0.016797	5.272690	0.545016
C	3.394076	3.714754	-1.683729
C	-2.579824	4.068413	0.439064
Cl	0.873822	-3.320482	1.276807
Cl	2.151175	2.466775	1.635742
Cl	-3.239311	0.899416	1.292575
Cl	-0.114113	-0.247905	5.337704
H	-4.560815	-3.400651	-0.294403
H	-5.292962	-2.824685	1.205617
H	-5.462040	-0.527512	0.346809
H	-6.052795	-1.588484	-0.950372
H	-0.679245	5.783114	-0.130873

H	2.179355	5.019937	0.651453
H	0.071946	5.867150	1.464500
H	1.637870	6.089769	-0.658207
H	3.338089	-4.341363	0.421862
H	4.575880	-4.271913	-0.851878
H	5.236450	-2.000357	-0.223530
H	5.179172	-2.931986	1.275862
H	-1.430541	4.514943	3.211670
H	-1.565176	2.734197	3.163591
H	0.043155	3.496283	3.291493
H	-2.833664	5.040225	0.879257
H	-2.615851	4.144228	-0.652018
H	-3.291844	3.315038	0.771781
H	1.292529	5.165309	-3.277200
H	0.828839	3.479843	-3.641535
H	-0.286127	4.520350	-2.738329
H	3.704250	4.731135	-1.952311
H	3.948260	3.383675	-0.801896
H	3.606291	3.037913	-2.515185
H	4.316173	-1.701721	3.454585
H	2.790536	-0.782472	3.554555
H	2.742536	-2.519880	3.178147
H	5.616055	-0.134483	1.520667
H	4.735070	0.639714	0.171142
H	4.304169	1.036605	1.847397
H	2.381466	-5.348177	-2.320112
H	1.050818	-4.974480	-1.181649
H	0.982630	-4.374659	-2.857487
H	4.070082	-3.374972	-3.379997
H	2.795069	-2.194841	-3.782496
H	4.163948	-1.694545	-2.772973
H	-4.973008	-1.561128	-3.491499
H	-3.255935	-1.192689	-3.813242
H	-3.680098	-2.622794	-2.857444
H	-5.727646	0.852159	-2.375115
H	-4.728156	1.743431	-1.189628
H	-4.139404	1.514118	-2.855777
H	-3.751543	-2.892019	3.361650
H	-2.141618	-2.132089	3.466322
H	-3.570487	-1.119315	3.151110
H	-3.160853	-4.768240	1.375376
H	-2.086103	-4.405351	-0.010658
H	-1.447744	-4.313293	1.639393
H	-0.097056	-0.133110	4.012729

mofecl-mcn (los dos coordinados)

E(CH_3CN)= -1313.3715231 a. u.

C	2.16264400	-4.56064700	-1.54591100
C	2.53539700	-4.66589100	-0.05246500
P	2.60141700	-2.95199800	0.79095700
Mo	0.99539200	-1.26809300	-0.41633000
P	0.59245400	-3.50524700	-1.77303100
Mo	-1.59897700	-0.23519900	-0.23913200
P	-3.89031300	-0.63720000	1.03811800
C	-5.27107800	-0.66185200	-0.27253800
C	-5.16367700	0.48301400	-1.30445300
P	-3.39343700	1.20024500	-1.55638900
S	-1.26407900	1.70774000	1.25403700
Fe	-0.00647800	-0.05233800	2.07022500
Cl	-1.70071100	-0.44950000	3.75636200

Mo	0.54449200	1.54028800	-0.37788400
P	1.30201400	3.69720600	0.87643900
C	2.83045400	4.47986100	0.03165700
C	2.89368200	4.16568900	-1.47779500
P	2.69018900	2.29582700	-1.80067300
S	-0.12901100	0.00992500	-2.17326600
S	-0.64345100	-2.06836400	1.14204700
S	2.13141300	0.36574100	0.98500300
C	2.31407700	-3.37347600	2.60560400
C	4.44019300	-2.53929100	0.78081100
C	-0.72177800	-4.74384600	-1.22959700
C	0.36519900	-3.41025800	-3.63426300
C	4.42427900	1.69844400	-1.35095200
C	2.65216300	2.16372600	-3.67421300
C	0.07102200	5.11826000	0.97067500
C	1.85365400	3.54525300	2.67134500
C	-3.22455900	1.26063500	-3.42935400
C	-3.70997200	3.01050700	-1.11569200
C	-4.56668100	0.64447100	2.24681400
C	-4.16926300	-2.27696300	1.91369500
H	1.98119600	-5.55833700	-1.96693900
H	2.96119900	-4.07772000	-2.11569500
H	3.50995300	-5.15480600	0.07266600
H	1.79333900	-5.26401100	0.49172500
H	3.85620100	4.49122900	-1.89486600
H	2.80525800	5.56398500	0.20133000
H	2.08971000	4.67394400	-2.01733000
H	3.71704300	4.08783900	0.54727500
H	-5.18569000	-1.62738900	-0.77474100
H	-6.23661200	-0.62012500	0.24931600
H	-5.79765800	1.32909800	-1.01217000
H	-5.50757800	0.13273800	-2.28389100
H	3.48501900	2.72139600	-4.11962800
H	2.72744800	1.10613700	-3.94096700
H	1.69884600	2.56178600	-4.03079600
H	5.16435200	2.20413100	-1.98350800
H	4.62887900	1.91922900	-0.29867400
H	4.47462700	0.61903800	-1.50401500
H	2.20590200	4.51138600	3.05201100
H	1.00465500	3.20021200	3.26858500
H	2.65178600	2.80107700	2.74279200
H	0.51565000	5.97213100	1.49585800
H	-0.22188200	5.40148600	-0.04232700
H	-0.81782700	4.77380900	1.50725300
H	-4.09888300	1.75027100	-3.87550600
H	-2.31909000	1.81961000	-3.67915100
H	-3.13487400	0.23655900	-3.80070700
H	-4.53408300	3.39770400	-1.72805000
H	-3.97452900	3.08874100	-0.05670600
H	-2.80449100	3.59053200	-1.30220600
H	-5.21866700	-2.36929500	2.22019700
H	-3.90984100	-3.08651500	1.22571600
H	-3.51548400	-2.31251400	2.78797000
H	-5.56487000	0.34118400	2.58663500
H	-3.88136300	0.71514200	3.09327000
H	-4.62883800	1.61924700	1.75246700
H	3.00299200	-4.16301400	2.92913100
H	2.47423700	-2.47457400	3.20753700
H	1.27926900	-3.69569100	2.74859900
H	5.01212100	-3.34481100	1.25717700
H	4.76501300	-2.39798400	-0.25205700

H	4.59621400	-1.60361100	1.32622400
H	0.41128800	-4.41148300	-4.07927800
H	-0.61123900	-2.96001900	-3.83282900
H	1.15120400	-2.77538100	-4.05037100
H	-0.60065500	-5.67712900	-1.79368100
H	-0.62409800	-4.94059900	-0.15806800
H	-1.70710600	-4.31233400	-1.41368300
Cl	-0.34529800	3.37185900	-1.97614800
Cl	-2.74990700	-2.03727600	-1.76726200
Cl	2.97143700	-1.33533800	-2.14245000
C	2.12583600	0.12294500	6.05106500
H	3.16697000	0.46487200	6.03266700
H	1.54228400	0.80701300	6.67864800
H	2.09179200	-0.87322800	6.50810600
C	1.56209100	0.08174800	4.70062100
N	1.04607000	0.04046100	3.64772400

mofe(cl..HCl)(mcn) (los dos grupos coordinados)

E(CH_3CN)= -1328.93086 a. u.

C	-2.92224700	-2.67384100	-3.48853700
C	-3.58763000	-3.15705600	-2.18337000
P	-2.40723000	-3.03640500	-0.68496000
Mo	-0.64273000	-1.13079300	-1.04872600
P	-2.12505700	-0.96286100	-3.23904400
Mo	-0.19475100	1.57807200	-0.45251900
P	-1.48271200	3.72011900	0.45686700
C	-1.11524300	5.15254600	-0.74273200
C	0.38081000	5.27519400	-1.10304900
P	1.38099200	3.63147600	-1.01717700
S	0.92370300	1.44227200	1.75104300
Fe	-0.79278700	-0.09469200	1.73976100
Cl	-2.23138600	1.44290900	3.02220400
Mo	1.75717400	-0.27428400	0.21405600
P	3.26903900	-0.79432400	2.28574600
C	4.53606800	-2.16728000	1.87546700
C	4.91894300	-2.18229000	0.38126500
P	3.36166100	-2.21910300	-0.72138900
S	1.07917900	0.27444400	-2.07326000
S	-2.27299600	0.27801700	-0.01485000
S	0.35840000	-2.08407600	0.95945800
C	-3.58711200	-2.94798900	0.77816400
C	-1.72691100	-4.78645700	-0.52970700
C	-3.65775300	0.13475300	-3.27050300
C	-1.27779800	-0.59351000	-4.87233100
C	2.89795200	-4.04261800	-0.56177700
C	4.04148700	-2.08763300	-2.46764700
C	4.33572000	0.60762200	2.95136500
C	2.46494000	-1.43712000	3.86410100
C	2.27544900	3.58871200	-2.67114700
C	2.74174900	4.15086500	0.18601000
C	-1.01891700	4.51872100	2.10367000
C	-3.36248700	3.71126400	0.46571500
H	-3.66548400	-2.60184500	-4.29357700
H	-2.12935800	-3.35799400	-3.80367800
H	-3.92254400	-4.19770800	-2.27915000
H	-4.46978900	-2.54827300	-1.94752400
H	5.53103600	-3.06530300	0.15333200
H	5.42462200	-2.02219400	2.50329400
H	5.48608100	-1.28667900	0.11292000
H	4.08005600	-3.12262400	2.16705400
H	-1.70334500	4.94869300	-1.63942900

H	-1.47877700	6.08270100	-0.28508400
H	0.88562300	5.97468000	-0.42554500
H	0.48882800	5.66568500	-2.12118800
H	4.85450000	-2.80709400	-2.62321400
H	3.22536500	-2.29073300	-3.16631200
H	4.40598700	-1.06892900	-2.62151600
H	3.74660300	-4.66696900	-0.86723500
H	2.63208300	-4.26646800	0.47594900
H	2.03612100	-4.24471700	-1.19986600
H	3.22656400	-1.65881200	4.62122900
H	1.77917700	-0.67391500	4.24296700
H	1.88875900	-2.33869400	3.63952200
H	4.95740200	0.24654600	3.77929800
H	4.95985500	0.99637600	2.14447200
H	3.67999600	1.40920400	3.30360600
H	2.77555800	4.54670400	-2.85907100
H	3.01386200	2.78316900	-2.64699900
H	1.53980400	3.38612100	-3.45384100
H	3.22350500	5.06755500	-0.17675700
H	2.30303500	4.33225900	1.17224300
H	3.47914100	3.35075800	0.26613300
H	-3.74381200	4.72051000	0.66384900
H	-3.71043400	3.36757800	-0.51223300
H	-3.70671100	3.02227500	1.23953000
H	-1.63623400	5.41124800	2.26444200
H	-1.18189800	3.80164400	2.90897000
H	0.03732700	4.80613700	2.08638600
H	-4.32779400	-3.75480500	0.72356800
H	-3.01632200	-3.04337700	1.70561900
H	-4.09501900	-1.98131300	0.80010000
H	-2.55076400	-5.50422300	-0.43755600
H	-1.11800900	-5.01149200	-1.40775900
H	-1.09131300	-4.83995200	0.35927400
H	-1.96881700	-0.74861300	-5.70958800
H	-0.94716300	0.44850400	-4.85112000
H	-0.40997600	-1.24992700	-4.97275900
H	-4.22532200	-0.05426800	-4.19018400
H	-4.28345600	-0.07518700	-2.39799700
H	-3.34075100	1.17822600	-3.22797200
Cl	3.93812800	0.93688300	-0.45341400
Cl	-1.29161400	2.54228200	-2.63942200
Cl	0.34116900	-2.96218200	-2.62740200
Cl	-4.72785900	-0.65859000	3.79013000
H	-3.72272800	0.23701700	3.43784200
C	-1.85374600	-2.37992600	5.49869600
H	-1.59480700	-3.44481400	5.48646400
H	-1.39534200	-1.91540000	6.37962700
H	-2.94293700	-2.27574200	5.57274200
C	-1.39944800	-1.71813200	4.27525200
N	-1.09228200	-1.14863400	3.29670000

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C	1.669076	-4.554200	-1.909060
C	2.376677	-4.604957	-0.540041
P	2.609012	-2.870555	0.234427
Mo	0.712963	-1.251480	-0.617365
P	0.067558	-3.529680	-1.795082
Mo	-1.772088	-0.268484	0.140508
P	-3.464017	-0.763931	2.081120
C	-5.221276	-0.516746	1.398377

C	-5.349011	0.787120	0.593553
P	-3.904705	1.143774	-0.626979
S	-1.200817	1.821794	1.399696
Fe	0.236913	0.065949	1.752474
Cl	0.757705	0.159458	3.977654
Mo	0.250467	1.528615	-0.554064
P	1.302406	3.687848	0.506892
C	2.631781	4.431706	-0.646666
C	2.356744	4.106458	-2.129298
P	2.081965	2.235122	-2.373009
S	-0.812829	-0.045495	-2.113840
S	-0.443325	-2.089038	1.318200
S	2.139554	0.411115	0.531266
C	2.709865	-3.251027	2.075820
C	4.390881	-2.421786	-0.175170
C	-1.069763	-4.773402	-0.949112
C	-0.590373	-3.459620	-3.551297
C	3.870276	1.636769	-2.290454
C	1.641850	2.078700	-4.192234
C	0.134111	5.128462	0.825075
C	2.199824	3.518173	2.154573
C	-4.611851	0.753228	-2.327988
C	-4.001442	3.026975	-0.593430
C	-3.424617	0.283725	3.649041
C	-3.548550	-2.513268	2.767048
H	1.412814	-5.567107	-2.247285
H	2.304801	-4.082253	-2.662741
H	3.363898	-5.074690	-0.632808
H	1.795469	-5.200438	0.175644
H	3.206012	4.416959	-2.752369
H	2.668679	5.516659	-0.486589
H	1.457076	4.616219	-2.484876
H	3.598854	4.018630	-0.332479
H	-5.417109	-1.386678	0.764700
H	-5.933697	-0.524286	2.234534
H	-5.379550	1.650233	1.271381
H	-6.283875	0.792387	0.018207
H	2.375414	2.608362	-4.812110
H	1.633005	1.016944	-4.451433
H	0.645110	2.499756	-4.344306
H	4.475922	2.203484	-3.008420
H	4.265797	1.778861	-1.280532
H	3.900857	0.573835	-2.532344
H	2.512472	4.501970	2.524351
H	1.533563	3.039000	2.878223
H	3.074499	2.873974	2.025627
H	0.697622	6.003874	1.168877
H	-0.406346	5.357663	-0.095852
H	-0.588054	4.831592	1.590982
H	-5.553997	1.292616	-2.482703
H	-3.881888	1.064828	-3.081273
H	-4.765651	-0.324600	-2.410655
H	-5.048543	3.332996	-0.711474
H	-3.613152	3.394542	0.360824
H	-3.390017	3.443082	-1.394377
H	-4.454197	-2.638024	3.372970
H	-3.557687	-3.214458	1.929427
H	-2.665532	-2.703698	3.383494
H	-4.179450	-0.068139	4.362433
H	-2.429116	0.215769	4.099238
H	-3.610950	1.332485	3.399991

H	3.567087	-3.903082	2.279615
H	2.824600	-2.314766	2.627198
H	1.784774	-3.731169	2.405375
H	5.034995	-3.293830	-0.007788
H	4.449247	-2.103000	-1.217490
H	4.716226	-1.612121	0.484144
H	-0.628453	-4.463581	-3.990716
H	-1.596002	-3.030666	-3.520728
H	0.061668	-2.812979	-4.143220
H	-1.080247	-5.706387	-1.526032
H	-0.715154	-4.968600	0.067044
H	-2.074953	-4.353241	-0.889876
Cl	-0.916877	3.329626	-1.968563
Cl	-3.278474	-2.126409	-0.884708
Cl	2.239341	-1.341890	-2.719349
C	4.334109	0.472955	4.871216
H	4.689577	1.497638	5.029172
H	3.241283	0.484269	4.767800
H	4.599990	-0.131511	5.746094
C	4.931815	-0.094896	3.657902
N	5.378861	-0.557088	2.668446

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C	-1.059824	5.021336	-1.253216
C	-0.817870	5.222764	0.257430
P	-1.161062	3.631214	1.258216
Mo	-0.712380	1.510883	-0.234506
P	-0.115383	3.491602	-1.882523
Mo	1.284323	-0.332831	-0.816102
P	3.868098	-0.651976	-0.320302
C	4.644984	-1.235035	-1.954845
C	3.887158	-2.417602	-2.583613
P	1.971079	-2.334439	-2.422710
S	0.890626	-2.142234	0.890854
Fe	0.569529	-0.021785	1.653810
Cl	4.607518	0.263574	3.618184
Mo	-1.213968	-1.266476	-0.036530
P	-2.123560	-3.028199	1.680360
C	-4.026156	-3.149326	1.579192
C	-4.544005	-2.828056	0.162699
P	-3.861110	-1.154540	-0.448248
S	-0.786346	-0.045729	-2.116445
S	1.524792	1.766211	0.612157
S	-1.706092	0.363933	1.733885
C	-0.147807	3.875641	2.827476
C	-2.916859	3.883280	1.891686
C	1.636330	4.183513	-1.949861
C	-0.610696	3.327538	-3.684586
C	-4.988639	0.015490	0.511900
C	-4.488388	-1.029509	-2.214371
C	-1.558953	-4.809905	1.456110
C	-1.800039	-2.742437	3.513128
C	1.347746	-2.224822	-4.193618
C	1.638695	-4.137506	-1.976605
C	4.432168	-1.949807	0.920444
C	4.886235	0.862855	0.119394
H	-0.716593	5.899885	-1.815189
H	-2.120601	4.861849	-1.465530
H	-1.455518	6.025119	0.649335
H	0.224467	5.506606	0.449760

H	-5.640828	-2.776874	0.157747
H	-4.329725	-4.158591	1.884836
H	-4.228156	-3.591154	-0.554140
H	-4.436840	-2.445511	2.314461
H	4.635523	-0.370719	-2.622187
H	5.688037	-1.514733	-1.754266
H	4.183300	-3.357690	-2.101898
H	4.127464	-2.504108	-3.650389
H	-5.557834	-1.268430	-2.257901
H	-4.320008	-0.008784	-2.567211
H	-3.921574	-1.728063	-2.834492
H	-6.034063	-0.206096	0.264678
H	-4.830254	-0.113820	1.586463
H	-4.750150	1.043727	0.238321
H	-2.272123	-3.529040	4.113258
H	-0.719700	-2.748616	3.684074
H	-2.188375	-1.764210	3.808743
H	-2.029048	-5.450173	2.211854
H	-1.822619	-5.147855	0.451883
H	-0.471335	-4.850419	1.563095
H	1.810062	-3.004481	-4.810755
H	0.262057	-2.356421	-4.186538
H	1.588946	-1.235078	-4.588584
H	2.134468	-4.786057	-2.709589
H	2.039125	-4.341623	-0.978983
H	0.564865	-4.328413	-1.973778
H	5.948876	0.647902	-0.047404
H	4.570889	1.701712	-0.506329
H	4.733410	1.077165	1.184498
H	5.490559	-2.180693	0.747891
H	4.330738	-1.521131	1.927646
H	3.829275	-2.857726	0.826591
H	-0.387685	4.840741	3.288840
H	-0.379595	3.067961	3.528258
H	0.918981	3.827979	2.594730
H	-2.981272	4.825256	2.449174
H	-3.605851	3.892813	1.045126
H	-3.180020	3.049236	2.548876
H	-0.475759	4.281287	-4.208341
H	0.021445	2.561391	-4.141919
H	-1.656292	3.013991	-3.734654
H	1.647988	5.078402	-2.583827
H	1.972565	4.438186	-0.940704
H	2.304465	3.423263	-2.356600
Cl	-1.690620	-3.229699	-1.611314
Cl	2.347299	0.946302	-2.805712
Cl	-3.021118	2.266892	-1.150668
C	2.157098	0.232250	5.819659
H	1.852490	1.115786	6.392648
H	2.020167	-0.669403	6.427368
H	3.219521	0.320461	5.509610
C	1.421822	0.140350	4.565572
N	0.917211	0.081330	3.508697

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C	-2.520466	-2.128201	4.011355
C	-3.569076	-2.311531	2.895630
P	-3.336194	-1.085122	1.445539
Mo	-0.805285	-0.354749	1.288209

P	-0.763171	-2.083965	3.282498
Mo	1.548905	-0.965453	-0.050766
P	2.318226	-2.828583	-1.731756
C	4.163204	-3.167186	-1.422873
C	4.974914	-1.867920	-1.294864
P	4.175131	-0.504788	-0.198071
S	1.481214	0.559941	-2.042576
Fe	-0.533162	-0.357264	-1.444339
Cl	-1.562800	-0.786769	-3.476713
Mo	0.628696	1.679745	-0.035125
P	0.219433	3.540795	-1.838597
C	-0.377928	5.160824	-1.023134
C	0.132204	5.302116	0.425094
P	-0.258059	3.735728	1.440972
S	1.413428	0.456243	1.949823
S	-0.647040	-2.263632	-0.168771
S	-1.758439	1.239211	-0.349247
C	-4.110183	-2.002153	-0.000971
C	-4.608075	0.265079	1.767103
C	-0.473666	-3.914994	2.947070
C	0.357819	-1.717477	4.741991
C	-2.094593	4.021211	1.772015
C	0.554975	4.067265	3.101375
C	1.716710	4.074051	-2.846474
C	-1.075141	3.228870	-3.170291
C	5.139105	-0.561174	1.418231
C	4.939145	0.993662	-1.050808
C	2.208240	-2.509953	-3.587280
C	1.566678	-4.545019	-1.568644
H	-2.578606	-2.954538	4.732276
H	-2.673739	-1.185884	4.543869
H	-4.582810	-2.181083	3.294550
H	-3.511138	-3.321598	2.470003
H	-0.344449	6.160511	0.916825
H	-0.042195	6.005662	-1.637533
H	1.216103	5.443956	0.448462
H	-1.474947	5.149997	-1.050259
H	4.206857	-3.747544	-0.496637
H	4.553991	-3.785582	-2.242326
H	5.111945	-1.406383	-2.281636
H	5.974308	-2.078297	-0.892727
H	0.278874	5.062109	3.471520
H	0.218915	3.302298	3.805674
H	1.638522	3.999715	2.977699
H	-2.232764	5.017378	2.209864
H	-2.659326	3.947021	0.838319
H	-2.456256	3.256685	2.460244
H	-1.095600	4.061444	-3.883537
H	-0.839407	2.297089	-3.692317
H	-2.057996	3.115326	-2.704426
H	1.459548	4.931790	-3.479306
H	2.531538	4.329509	-2.165798
H	2.032859	3.236287	-3.474707
H	6.215877	-0.490248	1.223544
H	4.820969	0.284343	2.035889
H	4.902196	-1.488921	1.942520
H	6.010889	0.812305	-1.199900
H	4.452567	1.150334	-2.017763
H	4.785120	1.884786	-0.442085
H	2.149020	-5.267824	-2.152756
H	1.570161	-4.826319	-0.512999

H	0.535386	-4.528425	-1.931891
H	2.558216	-3.385431	-4.146834
H	1.168296	-2.294261	-3.851999
H	2.810354	-1.635574	-3.850670
H	-5.138954	-2.291696	0.243166
H	-4.123416	-1.341306	-0.869807
H	-3.524588	-2.889409	-0.249975
H	-5.575356	-0.194816	2.004170
H	-4.272114	0.890306	2.596121
H	-4.716495	0.868996	0.861415
H	0.137688	-2.392968	5.577250
H	1.393854	-1.853731	4.419140
H	0.206939	-0.679201	5.046933
H	-0.613182	-4.482808	3.875050
H	-1.176359	-4.267281	2.186723
H	0.541937	-4.049144	2.571023
Cl	2.706481	3.133216	0.352189
Cl	2.492168	-2.807465	1.522874
Cl	-1.590446	1.026159	3.337877
Cl	-3.720465	-3.434658	-3.522574
H	-2.816970	-2.412281	-3.456339
C	-5.121986	0.165768	-4.081391
H	-5.699812	0.758044	-4.799602
H	-4.064868	0.165172	-4.370234
H	-5.476567	-0.870905	-4.102025
C	-5.260585	0.720202	-2.729773
N	-5.348416	1.146058	-1.632763

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C	-1.37483600	-4.18279000	-2.77502600
C	-2.12270800	-4.44834600	-1.45229700
P	-1.21611300	-3.67335200	0.03450500
Mo	0.01532700	-1.46961700	-0.72432100
P	-1.04708700	-2.32006000	-2.99304600
Mo	-0.36855800	1.27527900	-0.88907400
P	-2.41541200	2.93331300	-0.65150600
C	-2.15532900	4.31438700	-1.93162500
C	-0.73193100	4.89014000	-1.87900800
P	0.66776200	3.57923700	-1.75810600
S	0.38668800	2.09887600	1.37257400
Fe	-0.74478100	0.12296800	1.39082300
Cl	-5.08535400	1.54847300	2.46146600
Mo	1.84678200	0.31978100	0.47716300
P	2.97893900	0.76941600	2.80275500
C	4.54892000	-0.29668100	3.00678500
C	5.21744500	-0.59881300	1.64998400
P	3.95954700	-1.32911400	0.41617400
S	1.49422300	0.05843000	-1.93605300
S	-2.13268700	-0.48387700	-0.30838800
S	0.79108800	-1.57552700	1.63648600
C	-2.51965700	-3.59262600	1.38311300
C	-0.11179000	-5.07340600	0.64258000
C	-2.75549200	-1.73064400	-3.52676900
C	-0.01996100	-2.18701300	-4.55763700
C	3.87933000	-3.10222200	1.05811600
C	4.93281500	-1.47238400	-1.18350100
C	3.58504600	2.52184400	3.12565800
C	1.99756600	0.39665700	4.36655000

C	1.45253500	3.54545900	-3.46802600
C	1.90587900	4.60357600	-0.77019100
C	-2.69331100	3.86933500	0.95929700
C	-4.12716500	2.28846700	-1.07722400
H	-1.96878800	-4.53291500	-3.62932100
H	-0.40601900	-4.69059200	-2.79263900
H	-2.22731000	-5.52603200	-1.27421700
H	-3.13176400	-4.01927000	-1.47690200
H	6.03424300	-1.32104500	1.77951300
H	5.24450500	0.22632500	3.67513200
H	5.62510600	0.31080800	1.20030500
H	4.24725200	-1.22583400	3.50727100
H	-2.36342900	3.86868500	-2.90770900
H	-2.89474700	5.10393900	-1.74165200
H	-0.61384600	5.52737300	-0.99300900
H	-0.53364700	5.51450000	-2.75967200
H	5.90471000	-1.94538900	-0.99831000
H	4.35227800	-2.07600000	-1.88542300
H	5.07457900	-0.46981500	-1.59379000
H	4.88866700	-3.53175700	1.05979800
H	3.47469300	-3.11128000	2.07440600
H	3.22669200	-3.68761100	0.40959500
H	2.60037600	0.60950000	5.25712500
H	1.09732400	1.01788000	4.37538600
H	1.69120400	-0.65278000	4.36750200
H	4.08214800	2.57452800	4.10141700
H	4.27218700	2.81590600	2.32981000
H	2.72594600	3.19844000	3.11273800
H	1.72223200	4.56003400	-3.78428200
H	2.35170500	2.92396900	-3.42235300
H	0.74807000	3.09881100	-4.17280400
H	1.99593400	5.59503900	-1.23105100
H	1.55058700	4.70892300	0.25910800
H	2.87516200	4.10476200	-0.75526700
H	-4.80471800	3.13306800	-1.25126800
H	-4.05951000	1.67203600	-1.97646400
H	-4.50567600	1.70219000	-0.23508200
H	-3.41435900	4.67904500	0.79516500
H	-3.11502900	3.17822700	1.69624200
H	-1.74919800	4.27735700	1.33039700
H	-2.99805700	-4.57215800	1.50030100
H	-2.03561200	-3.31647800	2.32487700
H	-3.28489200	-2.84307500	1.16780600
H	-0.73211600	-5.92339800	0.95066800
H	0.57715300	-5.36909100	-0.15029200
H	0.47194100	-4.71668900	1.49609400
H	-0.48540100	-2.75711600	-5.37043300
H	0.04261400	-1.13136700	-4.83640800
H	0.98302900	-2.56965200	-4.35480500
H	-3.07138200	-2.29546400	-4.41233200
H	-3.47331900	-1.88138600	-2.71558900
H	-2.70950600	-0.66509800	-3.75651700
Cl	3.80159600	1.80315900	-0.24143000
Cl	-1.30501300	1.38257400	-3.29764100
Cl	1.69550500	-3.26072700	-1.56877700
Cl	-5.47626600	-1.64552200	2.29915700
H	-5.31739400	-0.11563200	2.32871000
C	-3.48054600	-0.28449500	4.93885300
H	-2.99769600	-0.40919800	5.91464700
H	-4.09483500	0.62348700	4.92591400
H	-4.14565800	-1.13010900	4.72624700

C	-2.48927800	-0.18087800	3.87190900
N	-1.71112300	-0.10215200	2.99854100

mofe-cl-sph (los dos coordinados)

E(CH_3CN)= -1422.4735185 a. u

C	4.766169	0.206422	-3.183945
C	4.244346	-1.190292	-3.564012
P	2.386672	-1.368010	-3.195860
Mo	1.911909	-0.422749	-0.817953
P	4.068184	0.912306	-1.526835
Mo	0.295452	1.573453	0.573060
P	-1.038329	3.781720	0.021869
C	-0.509834	5.136848	1.265943
C	-0.225900	4.639429	2.704608
P	-0.079219	2.732566	2.905510
S	-1.933816	0.569798	0.848820
Fe	-1.496093	0.037802	-1.318500
Mo	-0.069749	-1.031419	1.248664
P	-2.002645	-2.760356	1.748740
C	-1.515686	-3.779738	3.289635
C	-0.013106	-4.152430	3.373054
P	1.150703	-3.224714	2.149611
S	2.055284	0.168270	1.561391
S	0.558574	1.289404	-1.813741
S	0.013542	-1.945114	-0.950046
C	1.534722	-0.579926	-4.683310
C	2.103050	-3.203656	-3.502937
C	4.067173	2.734006	-2.029630
C	5.538981	0.840735	-0.348098
C	1.611518	-4.636040	0.978652
C	2.716414	-3.020729	3.172779
C	-3.705660	-2.123386	2.231115
C	-2.428607	-4.125602	0.516234
C	1.271208	2.562225	4.204049
C	-1.648076	2.380355	3.898795
C	-2.919927	3.865063	0.142800
C	-0.684588	4.636873	-1.615572
H	4.486143	0.937415	-3.954140
H	5.862314	0.204493	-3.117799
H	4.730386	-1.960831	-2.957768
H	4.431580	-1.402084	-4.626345
H	0.133168	-5.225436	3.193439
H	-1.783783	-3.152535	4.143310
H	0.361514	-3.923962	4.376152
H	-2.142863	-4.681552	3.306808
H	0.402879	5.563795	0.843646
H	-1.290223	5.910096	1.266379
H	-1.012925	4.967246	3.396172
H	0.724599	5.056219	3.053401
H	3.016071	-3.980033	3.614339
H	3.504997	-2.648489	2.513456
H	2.518916	-2.286423	3.958390
H	2.020893	-5.479406	1.550516
H	0.723057	-4.961005	0.428245
H	2.356784	-4.263784	0.272558
H	-3.166365	-4.807799	0.958352
H	-2.833389	-3.659993	-0.387262
H	-1.524477	-4.680816	0.248187

H	-4.324844	-2.942160	2.619377
H	-3.587613	-1.346498	2.991150
H	-4.178715	-1.690218	1.345611
H	1.063835	3.211535	5.064727
H	1.303532	1.516640	4.521528
H	2.224316	2.834289	3.742874
H	-1.647518	2.981983	4.817275
H	-2.524296	2.629403	3.292247
H	-1.676731	1.317184	4.144590
H	-1.138812	5.636259	-1.630430
H	0.399666	4.713969	-1.735865
H	-1.103487	4.017481	-2.412965
H	-3.259675	4.889035	-0.061028
H	-3.338230	3.177457	-0.596779
H	-3.240349	3.561215	1.144482
H	1.867754	-1.046620	-5.618737
H	0.452863	-0.703010	-4.570916
H	1.743516	0.493561	-4.703582
H	2.462241	-3.488656	-4.499847
H	2.639779	-3.765379	-2.733775
H	1.033665	-3.416201	-3.417453
H	6.432409	1.284882	-0.805398
H	5.270370	1.396406	0.555888
H	5.716485	-0.204443	-0.082488
H	5.030267	2.989949	-2.491310
H	3.254123	2.903870	-2.743155
H	3.879803	3.350134	-1.149111
Cl	-0.305300	-0.827802	3.863922
Cl	2.198623	3.436013	0.695664
Cl	3.775786	-2.256995	-0.357796
S	-3.075082	-1.562490	-1.916270
H	-4.641278	0.513107	-0.441077
C	-5.298929	0.067650	-1.180851
C	-4.778418	-0.905514	-2.066211
C	-6.642034	0.473568	-1.272804
C	-5.636379	-1.448044	-3.052540
C	-7.495680	-0.077725	-2.251216
H	-7.019384	1.228983	-0.584483
C	-6.981364	-1.040285	-3.142626
H	-5.240550	-2.183619	-3.749233
H	-8.533949	0.242345	-2.322044
H	-7.621493	-1.469845	-3.912584
Cl	-2.580352	1.699941	-2.582161

mofe-sph

E(CH_3CN)= -1407.3697422 a. u

C	5.75908900	1.31234500	-2.93802600
C	4.35562600	1.40885500	-3.00447100
C	3.56772400	0.25030200	-3.17375000
C	4.20570900	-1.00491000	-3.28547400
C	5.60934800	-1.09893500	-3.22526200
C	6.39345100	0.05879000	-3.04892700
S	1.73509500	0.36275400	-3.37469600
Fe	0.73866600	0.11653500	-1.40382800
S	-1.42130400	0.40653500	-2.10090000
Mo	-0.93714700	1.50414100	0.06065500
S	-1.62220500	-0.05556100	1.82582800
Mo	0.76588100	-0.29833700	1.33478900
S	1.07161300	-1.93211500	-0.49117500

Mo	-1.29933800	-1.25970800	-0.29485700
P	-1.63185200	-3.61686700	0.90642000
C	-2.64488800	-3.68932900	2.48657000
P	-1.67166200	-2.87795100	-2.33152500
C	-3.14979900	-2.51716000	-3.44141800
C	-1.99611500	-4.66057400	-1.72045700
C	-2.63076000	-4.68949500	-0.31528200
C	-0.29226700	-3.11906700	-3.59175400
C	-0.18994700	-4.78854300	1.24619000
P	3.32627200	-0.80157500	1.71141300
C	3.81893200	-2.61326600	1.85968800
P	1.31544800	1.05514300	3.54783400
C	2.00027700	2.81005600	3.43801500
S	1.59316700	1.60817300	0.11082500
C	3.93036800	-0.03899800	3.36203600
C	2.79009500	0.17909900	4.37557100
C	4.60605000	-0.15131200	0.49568900
C	0.01735200	1.14968800	4.90006400
P	-0.67201600	3.72082700	-1.31618200
C	-0.66472700	3.66530600	-3.20037800
P	-3.45880600	2.35387700	-0.12555900
C	-4.40947000	2.53764000	1.48914300
C	-2.13542300	4.85934200	-0.89400300
C	-3.48089500	4.11227900	-0.91132400
C	0.80467100	4.82289400	-0.93618800
C	-4.74671000	1.54742800	-1.24330200
Cl	-3.86970300	-1.57197700	-0.18646300
Cl	0.66111800	-2.10613200	3.20437900
Cl	-1.04048100	3.34820100	1.90998100
H	-2.66212100	-5.71798900	0.06875800
H	-3.64864100	-4.29090600	-0.33573500
H	-2.64122200	-5.16742700	-2.44927900
H	-1.02918800	-5.18043600	-1.71849600
H	-3.82201500	3.96697900	-1.94445900
H	-1.92398500	5.25166200	0.10458100
H	-4.24884500	4.70122700	-0.39382400
H	-2.15199500	5.69688500	-1.60469600
H	4.70210900	-0.69630100	3.78214600
H	4.41274800	0.91451800	3.11087900
H	3.13737800	0.79606500	5.21522300
H	2.42405700	-0.77357200	4.76684400
H	-5.37825600	3.02049700	1.31294200
H	-4.56767700	1.53876400	1.90672700
H	-3.80854900	3.12251000	2.18864900
H	-5.63189900	2.19363600	-1.29822400
H	-4.32446500	1.41181100	-2.24339900
H	-5.01481300	0.56603400	-0.84914900
H	-0.52484000	4.67121400	-3.61374400
H	0.14654400	3.00971800	-3.53113400
H	-1.60754300	3.24465600	-3.56186400
H	0.67663300	5.80779200	-1.40103600
H	0.88571100	4.92599900	0.14868200
H	1.71366400	4.34933500	-1.31731000
H	0.45044000	1.55143000	5.82392900
H	-0.78986800	1.79989200	4.55257000
H	-0.37601500	0.14492700	5.07523000
H	2.32853500	3.14033100	4.43093700
H	2.84397600	2.82523000	2.74169100
H	1.22141000	3.47129100	3.05544500
H	4.89024500	-2.69633900	2.07731300
H	3.22979900	-3.07714000	2.65326400

H	3.59561400	-3.11576600	0.91422900
H	5.61699200	-0.35848100	0.86643800
H	4.47099400	-0.63348400	-0.47537100
H	4.47082700	0.92465600	0.35901400
H	-0.60722200	-3.82584100	-4.36871000
H	-0.04371500	-2.15525200	-4.04383600
H	0.60254100	-3.49559900	-3.08788700
H	-3.25300700	-3.30343800	-4.19874200
H	-4.04908500	-2.45508000	-2.82526900
H	-2.99314100	-1.55180200	-3.93158900
H	-2.90523800	-4.72623600	2.73099300
H	-2.05131300	-3.25331800	3.29411200
H	-3.55159600	-3.09727800	2.33920500
H	-0.57756900	-5.74707400	1.61336400
H	0.37965800	-4.95124600	0.32599400
H	0.46390200	-4.33852600	1.99425800
H	3.60372100	-1.89855900	-3.42792000
H	6.08676600	-2.07189600	-3.32258500
H	3.87300600	2.38029100	-2.93387800
H	7.47786400	-0.01314000	-3.00692100
H	6.35408500	2.21428700	-2.80960400