

Supplementary Information II

CO₂ Reduction on Single-Atom Ir Catalysts with Chemical Functionalization

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1. INCAR files

Geometry relaxation (at the level of PBE-D3-sol)

The 4×4 rectangular MoS₂ supercell (see **Sec. 2**) is relaxed by ISIF=3, and then MoS₂-IrX₃ and the derivatives are relaxed by ISIF=2 as the INCAR in the following.

```
SYSTEM = MoS2
PREC   = Accurate
ISTART = 0
ICHARG = 2
ENCUT  = 400 ; LMAXMIX = 4
ISMEAR = 0 ; SIGMA = 0.20
LREAL  = Auto ; ISPIN = 2
NSW    = 1000 ; NELM = 100
ALGO   = Normal ; EDIFF = 1.0E-5
```

```
IBRION = 2
ISIF   = 2
EDIFFG = -0.005
```

```
LSOL = T ; IVDW = 12
```

Single-point energy calculation (at the level of r²SCAN, VASP version >= 6.2.0, or in version 5.4.4 by the patch in https://gitlab.com/dhamil/r2scan-subroutines/-/tree/master/vasp_patch_files)

```
SYSTEM = MoS2
PREC   = Accurate
ISTART = 0
ICHARG = 2
ENCUT  = 400 ; LMAXMIX = 4
ISMEAR = 0 ; SIGMA = 0.20
LREAL  = Auto ; ISPIN = 2
NSW    = 0 ; NELM = 100
ALGO   = Normal ; EDIFF = 1.0E-5
```

```
NELECT = 318 ; LVHAR = T
LCHARG = .FALSE. ; LWAVE = .FALSE.
METAGGA = R2SCAN ; LASPH = .TRUE.
```

MD simulation (Langevin dynamics)

```
SYSTEM = MoS2
PREC   = Accurate
ISTART = 0
ICHARG = 2
ENCUT  = 400 ; LMAXMIX = 4
ISMEAR = 0 ; SIGMA = 0.20
LREAL  = Auto ; ISPIN = 2
NSW    = 7000 ; NELM = 100
ALGO   = Normal ; EDIFF = 1.0E-5

IBRION = 0 ; ISIF   = 2
ISYM   = 0 ; NELMIN = 4

MDALGO = 3 ; POTIM = 1.0

LANGEVIN_GAMMA = 10 10 0 0
TEBEG = 300 ; TEEND = 300

IVDW = 12
```

Vibrational modes calculation

```
SYSTEM = MoS2
PREC   = Accurate
ISTART = 1
ICHARG = 1
ENCUT  = 400 ; LMAXMIX = 4
ISMEAR = 0 ; SIGMA = 0.20
LREAL  = Auto ; ISPIN = 2
NSW    = 1000 ; NELM = 100
ALGO   = Normal ; EDIFF = 1.0E-5

IBRION = 5 ; NFREE = 2 ; POTIM = 0.01

LSOL = T ; IVDW = 12
```

2. The Python code to calculate $E_{\text{ZPE}} + \int_0^T C_p dT - TS$ of solid phases

The following Python code processes the OUTCAR of vibrational modes calculation

```
# -*- coding: UTF-8 -*-

import os
import sys
import math

path="/OUTCAR" ; zpe=0.0 ; hv=[]
h=6.62607015e-34 ; thz=1.0e12 ; k=1.380649e-23 ; eV=1.6021766208e-19

if len(sys.argv)>1:
    path=sys.argv[1]+"/OUTCAR"

if not os.path.exists(path):
    print path+"does not exist!" ; exit()
if os.path.isdir(path):
    print path+"does not exist!" ; exit()

print "vibration modes:"
file = open(path,'r+')
line = file.readline()
while line:
    if line.find("f  = ")>0 and line.find("THz")>0:
        print "{:12.6f} THz".format(float(line.split()[3]))
        zpe=zpe+float(line.split()[3])*thz*h*0.5/eV
        hv.append(float(line.split()[3])*thz*h)
    line = file.readline()

print
print "ZPE: {:10.6f} eV".format(zpe)
print

print "Helmholtz free energy:"
for i in range(1,11):
    G=0.0 ; T=100.0*i
    for j in range(0,len(hv)):
        G=G-k*T*math.log(1.0/(1.0-math.exp(-hv[j]/k/T)))/eV
    print "{:6.1f} K   {:12.6f} eV".format(T,G)

file.close()
```

3. POSCAR for MoS₂-IrF₃ and the intermediates

MoS₂-IrF₃

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F
16	32	1	3

Cartesian

0.004552352	0.231383244	1.986045390
0.003282425	5.741579452	1.994830668
3.183601818	0.224536229	1.990910918
3.165097236	5.749958633	2.015470415
6.373533302	0.224537215	1.991066784
6.392061782	5.749769407	2.015296668
9.552549279	0.231398212	1.985667199
9.553498388	5.741444103	1.995100677
1.596979089	2.987014153	1.996594518
1.592131693	8.499751880	1.985540986
4.778590131	2.960438357	2.024796903
4.778387563	8.493107931	1.998265088
7.960442053	2.986906070	1.996050924
7.965315813	8.500104051	1.984305680
11.142557996	2.987525655	1.991999745
11.142778772	8.498111261	1.986180842
0.003253793	2.065109086	3.548062444
0.001471079	7.583668809	3.545989394
3.170244689	2.045099216	3.554143906
3.169440299	7.598876566	3.550667167
6.387544602	2.044883380	3.553793430
6.388483848	7.599091417	3.549863398
9.554085606	2.065044367	3.547877073
9.555750908	7.583671437	3.545579910
1.581468827	4.820879389	3.563383222
1.589353692	10.332814218	3.544619679
4.778397805	4.824279551	3.567488194
4.778766524	10.331048105	3.551324010
7.976155073	4.820418807	3.563019335
7.967989401	10.332774796	3.544173241
11.142622484	4.822415211	3.550734520
11.142885746	10.336064575	3.541121781
0.008574710	2.072423704	0.435387716
0.003921768	7.574090537	0.431003422
3.194917528	2.067223099	0.445430540
3.187993057	7.572248208	0.441084132
6.362619312	2.067422510	0.445021167
6.369352976	7.571991964	0.440652259
9.549516835	2.072458691	0.435154215
9.554151611	7.574089880	0.430723093
1.599484250	4.826120237	0.443936326
1.595630156	10.336207809	0.429494493
4.778205859	4.818020297	0.490616821
4.778570405	10.327578297	0.437848978
7.957978619	4.825885676	0.443550684
7.961548208	10.336579692	0.428802073
11.142844777	4.824340655	0.437149107
11.143091348	10.336517273	0.429386497
4.785786209	4.792983280	5.862736106
4.787054722	6.654999555	5.888934731
4.795056519	4.793650171	7.766236067
4.777898973	2.933370770	5.903369784

MoS₂-IrF₃-HCOO

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F	C	O	H
16	32	1	3	1	2	1

Cartesian

12.676810569	0.234430330	1.949364394
12.668419569	5.749178731	1.949318945
3.130360128	0.230219386	1.954859644
3.117127992	5.756894306	2.004181743
6.315468874	0.226428596	1.934464872
6.330163745	5.758663704	2.002973855
9.496225642	0.237355003	1.941081136
9.493808487	5.746418523	1.954431832
1.541706318	2.985443508	1.967181116
1.537969630	8.502207880	1.953425705
4.725688519	2.970422678	2.006631345
4.721098885	8.502986468	1.948883384
7.901681536	2.991540803	1.963381469
7.907884503	8.507440516	1.936374754
11.086387612	2.991731672	1.952722520
11.085565962	8.503504213	1.942951828
12.670994529	2.065877653	3.516326547
12.668829256	7.587477647	3.508736789
3.119512712	2.043928542	3.533340394
3.127739078	7.615606019	3.524863422
6.335184688	2.025556170	3.513309360
6.326421177	7.628719145	3.508682549
9.498201244	2.066990016	3.511852920
9.494890365	7.591444174	3.504253328
1.501303863	4.824822263	3.512763977
1.534190076	10.337691397	3.510848880
4.720880385	4.836444902	3.577934206
4.728718307	10.337325428	3.507381380
7.928154154	4.824088025	3.533320129
7.908746363	10.339772230	3.496865928
11.082368885	4.828333792	3.511572480
11.082150385	10.339102710	3.502322435
12.684453510	2.076605410	0.397989303
12.679788387	7.583127411	0.388083979
3.145054430	2.079883035	0.416825451
3.128172854	7.564980732	0.407462306
6.300777796	2.084532058	0.406265035
6.311122017	7.566191649	0.400437526
9.490019640	2.082534011	0.394078083
9.497306002	7.577311985	0.384498388
1.552798503	4.829198780	0.415272117
1.541238307	10.338287985	0.393104106
4.722878748	4.826528914	0.475696027
4.714156205	10.334513313	0.384645537
7.888766528	4.833546716	0.413294025
7.908919342	10.341134923	0.374527685
11.081758906	4.826999023	0.391707756
11.089479233	10.342410230	0.384750664
4.830694370	4.836644641	5.897785425
6.241034788	6.151274301	5.863595605
4.957977338	4.840553020	7.833456993
6.181453000	3.459634005	5.845695734
2.430485504	4.880797795	6.427346468
3.096193168	5.958476918	6.219443083
3.057965374	3.777972914	6.236331463
1.381820029	4.902644573	6.751574278

MoS₂-IrF₃-COOH

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F	C	O	H
16	32	1	3	1	2	1

Cartesian

12.693324754	0.247419195	1.945279390
12.684996725	5.760421933	1.942175478
3.146659607	0.242072522	1.952359974
3.122509119	5.769935158	1.980843991
6.333887346	0.237465693	1.940024346
6.345242887	5.768773519	1.980976462
9.513215519	0.246806570	1.938488334
9.509878086	5.757619017	1.952023804
1.559032481	2.998943628	1.957518309
1.554401688	8.515121268	1.946341693
4.739010938	2.973859633	1.987159848
4.738397166	8.509179033	1.955415905
7.918317110	2.999395998	1.952106059
7.927071518	8.515252675	1.932670027
11.103127126	3.002378285	1.947369576
11.103366868	8.514052270	1.940270811
12.691390120	2.080822268	3.508138955
12.688051170	7.598109148	3.500976563
3.137271133	2.059639753	3.523085117
3.133888748	7.619351125	3.516938686
6.350872292	2.048313765	3.503999114
6.354084163	7.625882063	3.502351344
9.514481756	2.078223854	3.502438068
9.513936265	7.601887106	3.498846889
1.521146851	4.841091462	3.504422009
1.550726738	10.349072576	3.504798412
4.729212966	4.841557629	3.535954058
4.743521290	10.347111323	3.508461714
7.931942243	4.832371279	3.524949849
7.928602534	10.346774921	3.493982553
11.100657623	4.838781980	3.503299952
11.101228150	10.350497687	3.496724367
12.699715874	2.087943061	0.394661054
12.694830734	7.596151838	0.385009162
3.156568156	2.084354494	0.406949297
3.146691851	7.586264759	0.402056277
6.320093786	2.086125699	0.399569385
6.326125671	7.584384978	0.396885537
9.509167203	2.090062987	0.390277542
9.515887590	7.587287764	0.383579694
1.560920171	4.840536923	0.402389765
1.558324063	10.351868264	0.391492769
4.734538141	4.834973470	0.456179418
4.734386025	10.341726255	0.393297821
7.909693954	4.842828993	0.406214707
7.923740154	10.351846582	0.377364084
11.095909045	4.838325340	0.390465483
11.106457730	10.352423460	0.384553373
4.993592049	4.884789946	5.857717991
4.927472337	6.807141517	5.811489224
5.533076810	4.989598699	7.671792507
5.275137782	2.985671171	5.920376182
3.062784888	4.656978453	6.291685104
2.517867979	5.833651232	6.645685434
2.483814253	3.603187847	6.286039352
1.590366909	5.649764573	6.914356947

MoS₂-IrF₃-CO

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F	C	O
16	32	1	3	1	1

Cartesian

12.667821729	0.264471540	1.956444979
12.664388703	5.774327445	1.964089125
3.119450121	0.254901008	1.963772327
3.103087482	5.792025368	1.998394281
6.306826371	0.247472866	1.944842637
6.328040958	5.783763140	1.993405223
9.487626764	0.261084272	1.952919364
9.490471813	5.772547534	1.962088794
1.534975310	3.018998669	1.980558336
1.522418209	8.533536018	1.942531914
4.722462991	2.987141618	2.000437528
4.706690795	8.522411083	1.966127604
7.892603931	3.010690448	1.972513199
7.899321283	8.528157521	1.953365207
11.078098276	3.018843937	1.965875179
11.075304058	8.529733093	1.950699538
12.664602650	2.094163221	3.527679443
12.663512427	7.619464792	3.512447178
3.117523074	2.073335506	3.538232744
3.089953026	7.648792912	3.520688713
6.324022231	2.045932173	3.523406684
6.317123175	7.638447878	3.527953029
9.488919554	2.090710825	3.523753285
9.490332216	7.614721648	3.516312838
1.509813406	4.861974039	3.537382782
1.522362731	10.360804612	3.514230549
4.720898214	4.856787068	3.532374203
4.716673505	10.359791462	3.519062102
7.925132332	4.847900655	3.534472883
7.899985886	10.363116722	3.510325849
11.076904872	4.855881672	3.523995578
11.076153779	10.365237634	3.511523008
12.676624692	2.109677814	0.410041176
12.661847125	7.603180810	0.391031243
3.129595948	2.103090699	0.423057675
3.120717117	7.598772755	0.403909422
6.299309750	2.099669676	0.408519916
6.301535338	7.598774726	0.410286896
9.484384924	2.105320515	0.405305550
9.485633712	7.603893037	0.394261144
1.539475040	4.855858348	0.421922691
1.530196765	10.375254150	0.392835140
4.714546925	4.851042273	0.468057543
4.704206497	10.354121241	0.398403890
7.890629846	4.852228223	0.415908061
7.901231639	10.360838121	0.388553627
11.078850886	4.852190444	0.403625481
11.079274229	10.370151607	0.393445343
5.122166291	5.087357127	5.794267058
4.388115034	6.917200974	5.831674933
6.041181811	5.608845680	7.398209572
6.310614460	3.515145012	5.838798881
3.604092567	4.230717425	6.202913523
2.640469514	3.687575919	6.569050550

MoS₂-IrF₃-CHO

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F	C	O	H
16	32	1	3	1	1	1

Cartesian

12.708120530	0.273010442	1.935670078
12.704675364	5.784860390	1.938680112
3.160944601	0.270014358	1.945917606
3.144933231	5.796057599	1.978880465
6.348545041	0.271410723	1.940479577
6.364338860	5.799876950	1.977190375
9.528022675	0.275750837	1.930324137
9.528405808	5.786018088	1.941125989
1.573312543	3.026849265	1.939559430
1.570647111	8.540664859	1.944108009
4.757548523	3.007166763	1.983261108
4.756253836	8.539395466	1.951352209
7.934822950	3.030168611	1.945406795
7.943036419	8.547722741	1.922251284
11.117626257	3.031178804	1.934962124
11.119233141	8.541451989	1.930634081
12.705503843	2.108767983	3.492626250
3.146061008	2.093287063	3.508873880
3.155070522	7.643689712	3.516812623
6.368291582	2.088783574	3.508669734
6.374024926	7.658532814	3.494627774
9.531788003	2.107999251	3.492827415
9.529924686	7.630007593	3.487246633
1.546057821	4.857415523	3.499247432
1.563498071	10.377023548	3.497526348
4.755454946	4.866220792	3.538059890
4.756415055	10.377486758	3.504504263
7.954267157	4.861669832	3.516678810
7.944799591	10.376417760	3.487532437
11.116486720	4.864913619	3.493522704
11.115794804	10.377044573	3.487401009
12.712479146	2.112124452	0.380350128
12.713508674	7.620693449	0.380135328
3.177577520	2.112356879	0.397734046
3.164525381	7.613611257	0.400731899
6.335644448	2.116017555	0.396952182
6.341325064	7.614734132	0.389192738
9.522756678	2.117296312	0.381002091
9.531844904	7.617609979	0.372717343
1.583129292	4.873153508	0.394521803
1.574458814	10.375397383	0.385378674
4.754857864	4.866107125	0.452588014
4.752164930	10.372018247	0.390220247
7.925537467	4.872886752	0.398060195
7.934016473	10.386388940	0.371135250
11.116126347	4.867478031	0.379775316
11.120069965	10.379720024	0.375469029
12.702215724	7.623122512	3.495159745
4.993832550	4.822774281	5.864560604
5.176199094	6.734596192	5.863811374
5.561176417	4.784143188	7.676749825
4.869549402	2.888156504	5.882791281
3.064469727	4.808051745	6.336894035
2.444003473	5.760446900	6.691320539
2.685814104	3.769246818	6.282773018

MoS₂-IrF₃-CH₃O

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F	C	O	H
16	32	1	3	1	1	3

Cartesian

12.663818934	0.259733776	1.913145185
12.657556031	5.771760405	1.913388520
3.115553921	0.257916927	1.921230406
3.098043778	5.780237484	1.956811696
6.305117066	0.255847818	1.909968704
6.314851687	5.789188287	1.944537908
9.483902404	0.262235995	1.905925125
9.481103634	5.772524538	1.921371073
1.525381044	3.013652695	1.918553561
1.527420565	8.527991947	1.923818588
4.708952420	2.991793433	1.947203130
4.711459477	8.526512959	1.923569441
7.889899237	3.015577482	1.919159591
7.898721926	8.533756125	1.896432936
11.072176020	3.017049243	1.913734376
11.075016518	8.528322437	1.909955740
3.101161952	2.082314725	3.487076461
3.115034983	7.627269724	3.496315777
6.321641493	2.072620651	3.476324081
6.327767454	7.645880928	3.468481302
9.484463827	2.093658617	3.472389579
9.482960882	7.617489084	3.468790054
1.491163158	4.844019543	3.480115533
1.521412389	10.366466949	3.478649259
4.716118910	4.847982456	3.495934606
4.713797349	10.365579293	3.478675485
7.898599778	4.849025501	3.493356705
7.899187755	10.362970203	3.464819789
11.071516727	4.851741688	3.475502431
11.071018275	10.365397294	3.467861712
12.666279333	2.098957121	0.356041789
12.670713817	7.610007415	0.356482677
3.123904331	2.097299090	0.367466584
3.117114904	7.598423868	0.375608690
6.293901501	2.100783352	0.363169685
6.296215474	7.604689364	0.357446149
9.479580963	2.104300467	0.353675559
9.489433180	7.601678825	0.348924994
1.533539508	4.857999628	0.368460603
1.529452025	10.361286876	0.359954797
4.703944374	4.854130671	0.417707898
4.705302411	10.359771751	0.360082239
7.882377684	4.859438209	0.369944721
7.893181286	10.371387492	0.341651775
11.067971416	4.854778180	0.356284678
11.076822935	10.365293482	0.349981710
12.658052208	7.609148668	3.476220369
12.660166649	2.094693613	3.474627137
4.874425059	4.810251173	5.788325071
5.374719450	6.682198221	5.914432406
5.233624714	4.702833001	7.703587413
4.835996404	2.884084523	5.849683285
2.660608672	5.944685074	7.142667770
3.049517663	5.306527281	5.922465324
1.585385512	6.145532463	7.010021210
3.213240027	6.889208608	7.266868353
2.833898559	5.293517638	8.011093140

MoS₂-IrF₃-CH₂OH

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	F	C	O	H
16	32	1	3	1	1	3

Cartesian

12.690645855	0.253244702	1.963477284
12.685365443	5.764770855	1.970437765
3.143406956	0.250058406	1.971922219
3.122067757	5.773315609	2.005933225
6.331760386	0.248840631	1.961213350
6.338526294	5.775879364	2.002699375
9.510727808	0.254764427	1.957968920
9.507190084	5.765555356	1.975947917
1.552841748	3.006171025	1.967612058
1.552353442	8.521921591	1.970243603
4.736476188	2.988440250	2.005511224
4.739418349	8.519619337	1.972180754
7.916474277	3.009327755	1.971560866
7.924504903	8.524198221	1.953422576
11.098792029	3.010614889	1.966374815
11.101432993	8.520720529	1.962585002
3.128431943	2.073972338	3.538322151
3.140796339	7.626341989	3.536787629
6.349722512	2.064313743	3.526890278
6.350140166	7.634465583	3.525072336
9.511131426	2.086226061	3.524564207
9.510594280	7.610152620	3.524130881
1.524997531	4.833712946	3.530722260
1.547781542	10.358296705	3.527638912
4.725188928	4.848127332	3.570238948
4.741032820	10.357002344	3.529081047
7.926645139	4.840281665	3.548272550
7.925871286	10.356464889	3.517268002
11.097705599	4.844447273	3.529798687
11.098439243	10.358764515	3.519385159
12.691765667	2.092653024	0.406646840
12.694418012	7.599776049	0.407967009
3.155808528	2.091126893	0.421066433
3.144612689	7.592416588	0.422594659
6.317971759	2.096277892	0.416882038
6.325027861	7.591404095	0.413726754
9.505790319	2.097721400	0.406077430
9.514128211	7.594059178	0.403524898
1.557857286	4.850936162	0.419259705
1.556303794	10.356577899	0.408896282
4.730192422	4.845622382	0.473437458
4.733371291	10.353231614	0.409448817
7.906752552	4.853499588	0.424938239
7.920027933	10.360998438	0.395447649
11.094770266	4.849319196	0.411402285
11.102998150	10.357535200	0.401670150
12.686365383	7.604512622	3.528483212
12.688172559	2.088013528	3.525393307
5.038807474	4.783391210	5.834594965
5.152840478	6.725314243	5.950289369
5.631997289	4.730292839	7.675064802
4.940279233	2.854105609	5.871688128
3.090819818	4.896593928	6.570048332
2.428574769	6.044492140	6.200730801
2.561195809	4.022925164	6.170285940
2.914761318	6.813337367	6.562371850
3.311102148	4.826309135	7.646782398

4. POSCAR for MoS₂-IrCl₃ and the intermediates

MoS₂-IrCl₃

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl
16	32	1	3

Cartesian

12.723480763	0.233308174	1.952912211
12.724150677	5.743076837	1.969861388
3.175830470	0.223938265	1.961609870
3.164050447	5.743480258	2.019312680
6.366076996	0.223365247	1.960589141
6.374314742	5.744129409	2.020037621
9.545771233	0.232813365	1.952846497
9.545436655	5.743735188	1.970062703
1.580346360	2.987490175	1.968493909
1.577147291	8.501548873	1.946767122
4.769698023	2.970623402	2.021043450
4.769581565	8.494190726	1.972357929
7.959223613	2.987565078	1.969504952
7.962890313	8.501155309	1.947396696
11.133322586	2.988057526	1.959851235
11.133686752	8.498748586	1.949898303
12.715019206	2.063430687	3.519655466
12.718440852	7.590586742	3.514359295
3.145820507	2.042120543	3.521780372
3.148262318	7.612707833	3.515194654
6.394234642	2.040552690	3.520249128
6.391160471	7.613081686	3.516027033
9.551914264	2.062256892	3.520192206
9.549915901	7.591392925	3.515290916
1.561842252	4.816248927	3.546992242
1.576518535	10.333650625	3.509936035
4.770607680	4.812530103	3.631660938
4.771098925	10.335414110	3.524928093
7.978375729	4.817452946	3.547144234
7.964503267	10.332957452	3.510568738
11.135244322	4.824284807	3.521788716
11.134561510	10.335644072	3.507358730
12.726573901	2.075073530	0.402490683
12.721390600	7.570503777	0.396468937
3.191919226	2.076300217	0.425250120
3.181762778	7.558144271	0.421750210
6.348603839	2.076452649	0.425212495
6.357465600	7.558434024	0.422452837
9.540924027	2.074853259	0.402396023
9.546130088	7.570112841	0.396146886
1.601714958	4.830589068	0.427895933
1.588402687	10.339648707	0.393817797
4.769874795	4.820757180	0.493119247
4.769591808	10.325210339	0.408383310
7.937705175	4.831811812	0.429280214
7.952821113	10.338594164	0.393510163
11.133661716	4.827000994	0.409322903
11.134580477	10.337730162	0.394018739
4.877543233	4.781529827	6.038610339
4.757020482	6.994479587	6.116882563
5.150780662	4.792020065	8.286503553
4.777696785	2.571122796	6.157296896

MoS₂-IrCl₃-HCOO

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	O	H
16	32	1	3	1	2	1

Cartesian

12.696186495	0.232412100	1.924539357
12.686151436	5.749283857	1.923252344
3.151085745	0.230525729	1.933549941
3.146780427	5.751536177	2.003442943
6.333514834	0.218797060	1.898935884
6.341548495	5.752829881	2.002846897
9.515758614	0.235129006	1.9111111027
9.511970526	5.744417848	1.933644265
1.560688110	2.981370213	1.947304010
1.557624181	8.498851740	1.932584196
4.743903665	2.976843891	2.003622502
4.735755063	8.503025233	1.921568513
7.922736421	2.988462917	1.938703805
7.929845251	8.504485168	1.905126572
11.106691404	2.989146235	1.927227825
11.105917550	8.501075807	1.916732639
12.687815979	2.061790889	3.493827581
12.686711341	7.585665542	3.485626876
3.134813200	2.040115433	3.520677090
3.148414434	7.620431949	3.509339094
6.361081089	2.011977534	3.473921418
6.343238834	7.641468930	3.472560644
9.520151371	2.061440853	3.485914767
9.514477204	7.591584123	3.479092419
1.511690286	4.821038063	3.483237922
1.552971102	10.336577063	3.487497270
4.746324612	4.830386701	3.616567850
4.750082354	10.336849733	3.481232524
7.951142155	4.816643806	3.518521786
7.928808895	10.336939090	3.464698792
11.102704541	4.825387642	3.487220407
11.100120477	10.336956173	3.475019038
12.706886916	2.075244688	0.373468809
12.702126200	7.582163539	0.362541117
3.171274976	2.085577238	0.403309837
3.146284819	7.550331455	0.392151028
6.311722512	2.090817922	0.385495946
6.326157915	7.551668524	0.381191336
9.509261280	2.082733750	0.366658308
9.518815336	7.570773819	0.357755125
1.583474302	4.829981638	0.401709862
1.563235757	10.335933168	0.371483788
4.743167745	4.825134683	0.471929424
4.727012415	10.331840490	0.354383849
7.897335817	4.836396939	0.400341898
7.929799730	10.336832651	0.340938233
11.098950593	4.825539417	0.367432013
11.111267761	10.339655935	0.357426926
4.745444923	4.841597708	6.092324257
6.383135155	6.401649070	6.218357086
4.613519592	4.872346997	8.380872011
6.241589763	3.150899320	6.232385635
2.257752868	4.914661106	6.298119426
2.945297615	5.989859590	6.178770065
2.882476833	3.800277318	6.201905012
1.176269271	4.948465941	6.490369439

MoS₂-IrCl₃-COOH

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	O	H
16	32	1	3	1	2	1

Cartesian

12.727284025	0.254614315	1.915794760
12.718033441	5.769029763	1.915103197
3.179998278	0.248301779	1.933367848
3.166007462	5.769627008	1.983464360
6.367278745	0.241742054	1.918803900
6.366469233	5.764799107	1.995749921
9.546744619	0.254442849	1.908288747
9.542264614	5.765801087	1.929672211
1.587888491	3.005756764	1.930648237
1.585074927	8.521190310	1.920444369
4.770141850	2.988057198	1.985210180
4.770661926	8.514306543	1.942261606
7.959483082	3.009669742	1.926527321
7.964946336	8.521813837	1.905763298
11.137916393	3.008987082	1.917592287
11.136849689	8.520972174	1.910539418
12.721860981	2.085978687	3.483304381
12.718756463	7.605041536	3.477115929
3.154569983	2.066441555	3.502745032
3.159544078	7.630166596	3.500297964
6.400694042	2.057498637	3.473212123
6.395020634	7.639119369	3.481857181
9.554329901	2.082895381	3.477558792
9.551364980	7.610136851	3.476594090
1.544842132	4.843504427	3.481427431
1.578784996	10.355953058	3.482583165
4.748233072	4.826777273	3.590973318
4.776367198	10.356021389	3.494499624
7.978508498	4.834885756	3.514814675
7.967598681	10.353535822	3.470979631
11.135877820	4.844952863	3.478436172
11.134401429	10.358151500	3.468331099
0.005855046	2.094906493	0.360774398
0.001633517	7.602496178	0.353073701
3.197470866	2.094409938	0.388884507
3.185232221	7.581149076	0.388403162
6.347635763	2.098013453	0.382347740
6.353941152	7.572669368	0.388592109
9.542456560	2.098528569	0.356807038
9.547960783	7.591409351	0.352968127
1.607092292	4.852503850	0.382790193
1.596535830	10.359098289	0.363345668
4.769857725	4.841472542	0.457091182
4.767247107	10.344273584	0.372645371
7.926625414	4.858509160	0.393173173
7.952538885	10.358053602	0.347928964
11.127004300	4.847444672	0.360755399
11.139752398	10.359849282	0.351664126
4.823520292	4.780271603	6.007448435
4.999859504	7.051449214	6.072155833
5.206611157	4.801561871	8.260955215
5.093401701	2.512417772	6.107614040
2.830464015	4.678860383	6.305022836
2.295089402	5.902357496	6.541047096
2.197071563	3.647947773	6.326239109
1.340887067	5.746247694	6.724790335

MoS₂-IrCl₃-CO

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	O
16	32	1	3	1	1

Cartesian

0.003233484	0.263162108	1.903675646
12.724158264	5.777148100	1.911980063
3.183632544	0.256510357	1.926335245
3.170824510	5.782589673	1.974511594
6.373097820	0.254699853	1.915730536
6.372342933	5.781544329	1.998176724
9.552251118	0.264870833	1.900075227
9.548766501	5.776142178	1.926130801
1.592243978	3.014230887	1.916278452
1.590304602	8.529966998	1.911616474
4.774639684	2.996376588	1.985151172
4.778200169	8.524883510	1.938202381
7.962144531	3.017790380	1.924725175
7.970855693	8.533307369	1.898414642
11.141393423	3.019536453	1.908896416
11.142706697	8.530375674	1.902748197
12.725906263	2.093809736	3.470058441
12.724404076	7.615414164	3.470015228
3.150790050	2.075647780	3.494445384
3.163022056	7.640821093	3.495024741
6.407604099	2.067295045	3.479350805
6.406247579	7.657554488	3.479962051
9.560504796	2.091669276	3.471683562
9.557612709	7.622110019	3.470912874
1.557664581	4.847247561	3.474987745
1.581301158	10.364543804	3.472800255
4.745427094	4.839039538	3.577275574
4.781236027	10.367065509	3.490505517
7.986894187	4.843892406	3.512789309
7.974228784	10.365299396	3.465161920
11.141849389	4.852645113	3.473142385
11.140723508	10.368307307	3.458748460
0.007679725	2.104571165	0.348405242
0.006707526	7.608917392	0.346112363
3.206148267	2.103599081	0.381626599
3.193487417	7.593084793	0.380831882
6.351536137	2.109739411	0.380563587
6.359949138	7.581810711	0.384154767
9.543644653	2.110312511	0.350139029
9.553065181	7.600122964	0.346496589
1.612029591	4.864999362	0.373979919
1.603156640	10.367550401	0.353092961
4.779067340	4.851767969	0.455727577
4.774627545	10.354607448	0.368418470
7.929764073	4.870334495	0.394157134
7.955675267	10.370576053	0.341656134
11.132135252	4.859575858	0.355251804
11.143171768	10.368112824	0.341328569
4.770297759	4.813812309	6.026969552
5.030075448	7.125392055	6.117509604
5.421080482	4.817724959	8.215097785
4.970152633	2.497153838	6.156036854
3.001786455	4.848100722	6.324813366
1.891139582	4.880708438	6.664102077

MoS₂-IrCl₃-CHO

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	O	H
16	32	1	3	1	1	1

Cartesian

12.725970750	0.266517837	1.893605888
12.719191945	5.782426728	1.908079088
3.178099302	0.263409174	1.917877495
3.168280277	5.784577864	1.976205558
6.367538972	0.260814970	1.909830570
6.368950117	5.782443811	1.984574646
9.546972982	0.268968685	1.889852583
9.543525540	5.781928695	1.918450594
1.584768041	3.021229964	1.908294111
1.585436628	8.535181236	1.906427294
4.771045438	3.008706856	1.983783543
4.771275698	8.532347440	1.929058135
7.957930823	3.024530256	1.916329265
7.964777150	8.539870503	1.891099960
11.135436268	3.025882436	1.897835433
11.137433113	8.535635248	1.894352138
12.717302833	2.099086228	3.456113935
3.143421371	2.084006593	3.482365310
3.159874104	7.647087903	3.487332165
6.400285873	2.075987960	3.472207785
6.397352816	7.658584720	3.463461697
9.556973900	2.097823241	3.457707763
9.553221469	7.628752654	3.459776342
1.550194429	4.848824448	3.473427296
1.575382317	10.370950563	3.461726606
4.758226783	4.853297221	3.595696986
4.774515261	10.374519583	3.477845788
7.981034143	4.850705214	3.500205874
7.971011981	10.371300763	3.454045951
11.134802012	4.858501604	3.463016450
11.134786838	10.373639812	3.446798623
0.002733303	2.109135759	0.341919698
0.002664775	7.612541603	0.343988948
3.203029713	2.113397295	0.380024463
3.187573886	7.595352882	0.379555114
6.343760806	2.116928207	0.379971676
6.353372521	7.590254282	0.376610830
9.537857443	2.114373651	0.343210772
9.546650543	7.606437738	0.342125483
1.609438510	4.872549364	0.373651497
1.598456808	10.370114813	0.347623378
4.771194898	4.855821553	0.455009155
4.769852793	10.362236951	0.362091102
7.927417476	4.873400554	0.385339335
7.948105159	10.375908557	0.335865244
11.128562628	4.866488863	0.349542722
11.137779072	10.370952534	0.334275551
12.717379459	7.622569287	3.461587131
4.884831112	4.836447531	6.066806316
5.106106175	7.095969979	6.117377281
5.431931502	4.828545029	8.269984126
4.934430190	2.553468565	6.164857149
2.900074793	4.876469898	6.339355707
2.264066412	5.830929132	6.662639976
2.481828218	3.861154339	6.215186715

MoS₂-IrCl₃-HCOH

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	O	H
16	32	1	3	1	1	2

Cartesian

12.700622496	0.260490086	1.930474937
12.695483957	5.773816928	1.945409775
3.152177106	0.254042057	1.946015656
3.141446338	5.779073873	1.995705962
6.342534400	0.253265071	1.935817450
6.343854882	5.777748631	2.005131990
9.521108825	0.261640309	1.925109029
9.518052862	5.773621788	1.950159967
1.561820724	3.011429614	1.941213459
1.557855768	8.528331635	1.934452355
4.745891406	2.992100926	1.994275600
4.747742206	8.522742886	1.958130896
7.931662290	3.014640220	1.941550821
7.937667241	8.529471593	1.924900413
11.110276166	3.017071582	1.936095059
11.110852004	8.527320457	1.931053400
3.125357203	2.074262584	3.511072993
3.132450670	7.639706760	3.510977030
6.374354952	2.068914967	3.496690989
6.370060065	7.645379609	3.502676785
9.525176108	2.089937001	3.494991660
9.523532049	7.618456242	3.497261405
1.537204501	4.842340487	3.508937061
1.552848386	10.362820399	3.497288525
4.731423001	4.834695215	3.584352434
4.750836861	10.365294797	3.510334194
7.949724941	4.840731077	3.529423773
7.940230820	10.363254700	3.489022553
11.108395399	4.850035037	3.501595557
11.108333187	10.366501772	3.486188650
12.704286920	2.101956655	0.375837684
12.702125441	7.602950847	0.375341959
3.169391364	2.099291059	0.399236567
3.160314138	7.591323279	0.402522534
6.324374258	2.104040280	0.394583009
6.330353035	7.584934918	0.401841886
9.517346531	2.105902485	0.373378657
9.522746815	7.598963295	0.373217054
1.577580402	4.862818988	0.402297899
1.568939702	10.365003730	0.376459807
4.745413817	4.850042264	0.467977971
4.743666198	10.352656050	0.388967767
7.906899736	4.866489520	0.408638604
7.926525268	10.365882844	0.365842246
11.105726363	4.858133006	0.384941176
11.112904234	10.364079280	0.368654877
12.694692654	7.615374085	3.498845398
12.695816259	2.091632154	3.496906757
4.891360691	4.800303647	5.961276293
4.894509971	7.190671875	6.177614927
5.822924018	4.796732327	8.027014732
4.876462114	2.476388542	6.136913896
3.044155883	4.842890755	6.294029355
2.379595722	5.885026855	6.694939733
2.449255624	3.916914035	6.271830201
3.028696073	6.672691566	6.670562625

MoS₂-IrCl₃-CH₂OH

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	O	H
16	32	1	3	1	1	3

Cartesian

12.707776848	0.257238845	1.930759102
12.702421326	5.769598756	1.943103522
3.160830989	0.253148200	1.949518621
3.145892961	5.770996929	2.008503228
6.348218050	0.251607122	1.940107346
6.347408918	5.772266322	2.012438178
9.528093232	0.260508893	1.926889867
9.523463009	5.771175642	1.951428354
1.564382597	3.009316586	1.936657876
1.568239725	8.524287578	1.943791211
4.751106192	3.000446927	2.009095103
4.755882462	8.522330268	1.957979500
7.938545792	3.016222692	1.949715614
7.948115022	8.529244915	1.921771616
11.115868396	3.014170111	1.935544163
11.120069207	8.524087182	1.930727214
3.125977234	2.075378231	3.511803150
3.149903722	7.635012237	3.520655632
6.379201399	2.067076909	3.500725329
6.380046569	7.647733769	3.493905067
9.534546564	2.088293425	3.497715294
9.532595998	7.616918120	3.496061563
1.530044744	4.828571968	3.507297635
1.559738148	10.361917631	3.499915898
4.734520312	4.843836558	3.623734415
4.757295882	10.362906470	3.512209654
7.956248829	4.842492920	3.536304832
7.949352429	10.360271099	3.489296436
11.115534577	4.847399336	3.501074612
11.116558795	10.362848651	3.486001492
12.708137979	2.097141237	0.372888111
12.714890989	7.602383168	0.377917774
3.183289621	2.100962230	0.405258983
3.167278630	7.583609676	0.411722288
6.326684439	2.108529644	0.406145789
6.337453141	7.579902021	0.403430536
9.519442764	2.105550642	0.376509279
9.532070991	7.595158399	0.372123979
1.587416118	4.861098539	0.401598662
1.578712258	10.359154137	0.381486565
4.748212967	4.849310654	0.478756875
4.751110744	10.353004937	0.390209109
7.908913273	4.863496720	0.413796753
7.932853417	10.367738971	0.366806760
11.110218507	4.855229564	0.383815058
11.119566960	10.361550348	0.369573832
12.701173298	7.608651292	3.500619531
12.701538981	2.089287849	3.494711518
4.993397827	4.785373159	5.990918875
5.152405375	7.078097284	6.167275310
5.735424706	4.732100345	8.160165548
4.890920656	2.510829387	6.111730337
2.957412026	4.867035188	6.568192244
2.282945782	5.989143421	6.139120460
2.485458691	3.983046688	6.125360727
2.693784606	6.777179357	6.550613642
3.058580664	4.800586501	7.660504580

MoS₂-IrCl₃-CH₂

MoS2

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	H
16	32	1	3	1	2

Cartesian

0.017184272	0.248961361	1.965851486
0.015022363	5.762104602	1.992245615
3.195768388	0.241430434	1.975818425
3.189107558	5.772252525	2.022151351
6.387886008	0.242923117	1.978234947
6.392911504	5.770408224	2.046769410
9.566186550	0.250269664	1.967525929
9.565352002	5.762297771	1.994641274
1.611003097	2.999836540	1.976168305
1.603081720	8.516970167	1.962102354
4.790961544	2.974751560	2.024068832
4.793039948	8.510717155	1.991822869
7.976302256	3.003555693	1.984918267
7.981524250	8.517592380	1.969289184
11.156974432	3.005734096	1.978939027
11.155633844	8.515583164	1.971772462
3.170665756	2.057701332	3.539279699
3.174918726	7.629290767	3.538421988
6.413202398	2.059841299	3.541435599
6.407873430	7.636148252	3.549174070
9.570503439	2.078515578	3.537816703
9.569288792	7.607691362	3.541249931
1.608710177	4.835088123	3.546551764
1.599025818	10.349199384	3.528692126
4.777237025	4.815206540	3.602356017
4.791357196	10.352491134	3.545251191
7.996980836	4.830654115	3.571626842
7.984627251	10.352769061	3.532447815
11.155740060	4.836718558	3.545921445
11.156185405	10.355744120	3.524996638
0.019426632	2.092655488	0.414040312
0.013525825	7.585816003	0.413962044
3.212645981	2.086928925	0.427885465
3.207481647	7.583428991	0.428360850
6.375274472	2.089550499	0.432739370
6.379804550	7.573780416	0.441318490
9.562519850	2.095105739	0.416966900
9.565982465	7.586823239	0.417073406
1.619546402	4.853343213	0.438900106
1.610629258	10.354744768	0.406021625
4.798150795	4.839421604	0.501169749
4.793530055	10.342433226	0.424517430
7.956026536	4.855582392	0.451799929
7.972099928	10.353520053	0.410058163
11.153477676	4.847522202	0.430181809
11.154677149	10.351454331	0.408473611
0.016507957	7.608866800	3.536776006
0.017721411	2.078710389	3.534094393
4.752228659	4.767859205	5.964660048
4.800140813	7.106981904	6.124528646
5.699292196	4.771449251	8.012349606
4.795861858	2.425399913	6.156704426
2.907549497	4.752609398	6.115740538
2.375117045	3.801528315	6.247990727
2.368745461	5.699965415	6.248442531

MoS₂-IrCl₃-CH₃

MoS₂

1.0

12.7285366058	0.0000000000	0.0000000000
0.0000000000	11.0232362747	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Mo	S	Ir	Cl	C	H
16	32	1	3	1	3

Cartesian

12.713526124	0.244349214	1.931041628
12.703802124	5.759155824	1.934856474
3.165986977	0.239197743	1.954200417
3.153089419	5.757140695	2.011749744
6.353932427	0.235267579	1.937044561
6.353447251	5.758089455	2.008926272
9.533281844	0.246770187	1.922463030
9.528105371	5.757539516	1.944094598
1.570998854	2.997019827	1.946769953
1.571281747	8.511144885	1.941371113
4.757835304	2.983259520	2.007742822
4.758304927	8.506541033	1.963591278
7.944801108	3.001429524	1.942336559
7.952057123	8.514826915	1.918504983
11.121825551	3.000747521	1.932004392
11.123085718	8.511751330	1.925650686
3.137031011	2.061353139	3.520357311
3.146563824	7.620827485	3.525177240
6.389659043	2.049989864	3.494361043
6.387280582	7.631470812	3.495605290
9.539223066	2.074716596	3.492540717
9.536890884	7.602040852	3.490738273
1.525015550	4.827772026	3.507296741
1.563276252	10.347191481	3.501245379
4.750717369	4.820728928	3.618028164
4.764758637	10.349096229	3.514734507
7.963722585	4.827317686	3.530055583
7.955591812	10.345428654	3.486155570
11.118689168	4.835523409	3.494568765
11.119507783	10.348912259	3.482832611
12.719690398	2.085673001	0.375738628
12.719148701	7.592343656	0.371617861
3.184862364	2.086687957	0.410319008
3.172744160	7.568091141	0.414426252
6.330922804	2.091465759	0.401264690
6.337709196	7.567940022	0.403376594
9.526977214	2.090989737	0.370910540
9.534970666	7.583046596	0.366556346
1.595669418	4.845536968	0.405139923
1.585570440	10.348094906	0.382241830
4.752299217	4.833709990	0.478238016
4.752526062	10.335858266	0.393264256
7.912769643	4.850057047	0.407284014
7.937292453	10.352588376	0.362770930
11.114656025	4.840070427	0.376725160
11.126665170	10.350403731	0.366003476
12.702167927	7.596020430	3.495114446
12.703363607	2.075363448	3.497026861
4.989764509	4.782320570	6.000854969
5.049906203	7.057918391	6.108267903
5.619039795	4.781301507	8.193148971
5.008010760	2.507298640	6.128805876
2.970051444	4.803153213	6.445741057
2.527127099	3.888081321	6.040889621
2.540158185	5.700690783	5.989797711
2.897543078	4.834725767	7.539176941