

Atomic Coordinates for the structures for “the Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO₂ (110) Surface”

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We list all the atomic coordinates of the optimized structures used to compute the free energy in Table S1. The structure names follow Table S1.

CELL_PARAMETERS(bohr)

12.054346	0.000000	0.000000
0.000000	11.983792	0.000000
0	0	60

1

ATOMIC_POSITIONS(angstrom)

Ir	3.161645188	1.582314932	-6.437086798
Ir	-0.028942049	-0.004755284	-6.530800689
Ir	-0.011555946	1.583147185	-3.220033474
Ir	3.177503370	-0.001897245	-3.226546871
Ir	3.189366668	1.585414724	0.000147373
Ir	0.000000000	0.000000000	0.000000000
Ir	0.011559903	1.586493964	3.219458657
Ir	3.201376630	0.001897245	3.226546871
Ir	3.217765318	1.587752569	6.444805090
Ir	0.028942049	0.004755284	6.530800689
O	3.169062771	0.001510583	-7.614076994
O	-1.248766196	1.580475925	-6.354709232
O	1.192629324	1.579147840	-6.385638603
O	3.161182576	-0.004022581	-5.195282199
O	-0.008223144	-0.002740535	-4.458730858
O	1.952172343	1.583367247	-3.211903806
O	-1.975382346	1.583491266	-3.221198631
O	-0.011272036	-0.000651366	-1.983881839
O	3.189722756	-0.000152930	-1.235573952
O	-1.224343674	1.585542266	0.004718807
O	1.224220996	1.585510663	-0.003122349
O	3.189157244	0.000152930	1.235573952
O	0.011272036	0.000651366	1.983881839
O	1.975262943	1.586964900	3.224337554
O	-1.952117083	1.586938270	3.215119602
O	0.008223144	0.002740535	4.458730858

O	3.217707424	0.004022581	5.195282199
O	-1.189249255	1.588369069	6.430846308
O	1.246101482	1.589394529	6.402754553
O	3.209827229	-0.001510583	7.614076994
O	-0.070035646	0.076074999	-8.307191579
O	0.070035646	-0.076074999	8.307191579
Ir	3.161114682	4.753797431	-6.444805090
Ir	-0.029321666	3.161686751	-6.521443467
Ir	-0.011559903	4.755056036	-3.219458657
Ir	3.177420770	3.169255021	-3.226651274
Ir	3.189513332	4.756145276	-0.000147373
Ir	0.000000000	3.170780000	0.000000000
Ir	0.011555946	4.758412815	3.220033474
Ir	3.201459230	3.172294979	3.226651274
Ir	3.217234812	4.759235068	6.437086798
Ir	0.029321666	3.179863249	6.521443467
O	3.166056357	3.163530238	-7.614299041
O	-1.246101482	4.752155471	-6.402754553
O	1.189249255	4.753190931	-6.430846308
O	3.160875659	3.170051980	-5.195255723
O	-0.009670156	3.171448750	-4.458889689
O	1.952117083	4.754611730	-3.215119602
O	-1.975262943	4.754585100	-3.224337554
O	-0.011008762	3.167819603	-1.983653725
O	3.189737644	3.170709336	-1.235518213
O	-1.224220996	4.756049337	0.003122349
O	1.224343674	4.756007734	-0.004718807
O	3.189142356	3.170840664	1.235518213
O	0.011008762	3.173730397	1.983653725
O	1.975382346	4.758058734	3.221198631
O	-1.952172343	4.758192753	3.211903806
O	0.009670156	3.170101250	4.458889689
O	3.218014341	3.171498020	5.195255723
O	-1.192629324	4.762402160	6.385638603
O	1.248766196	4.761074075	6.354709232
O	3.212833643	3.178019762	7.614299041
O	-0.058564078	3.113283710	-8.305599999
O	0.058564078	3.228266290	8.305599999
O	-0.024568434	1.454928893	10.685813465
H	0.881234065	1.092967037	10.746675867
H	0.084252042	2.279642651	10.169244932
O	0.024568434	-1.454928893	-10.685813465
H	-0.881234065	-1.092967037	-10.746675867
H	-0.084252042	-2.279642651	-10.169244932

TS1

ATOMIC_POSITIONS(angstrom)

Ir	3.1371409500	1.5800531779	-6.3844413848
Ir	-0.0466403330	-0.0167157740	-6.4291070600
Ir	-0.0430006021	1.5885662028	-3.1856229642
Ir	3.1506437643	-0.0000623329	-3.1936570822
Ir	3.1892707233	1.5854496642	-0.0000935771
Ir	0.0000000000	0.0000000000	0.0000000000
Ir	0.0363570248	1.5852753446	3.1880255923
Ir	3.2282362357	0.0000623329	3.1936570822
Ir	3.2350394749	1.5879677830	6.3905590338

Ir	0.0466403330	0.0167157740	6.4291070600
O	3.1656945989	0.0037169819	-7.5575259943
O	-1.2812395185	1.5907930294	-6.2778953210
O	1.1722435753	1.5647139367	-6.3350350704
O	3.1338196016	-0.0054099800	-5.1485677457
O	-0.0316283255	0.0077789040	-4.4167908698
O	1.9222983665	1.5857026452	-3.1764076940
O	-2.0039233751	1.5867476802	-3.1912589004
O	-0.0383258941	0.0002950998	-1.9641617717
O	3.1812617162	0.0001183924	-1.2236098594
O	-1.2254774903	1.5855333748	0.0099290656
O	1.2255241478	1.5848192429	-0.0108870693
O	3.1976182838	-0.0001183924	1.2236098594
O	0.0383258941	-0.0002950998	1.9641617717
O	2.0012167420	1.5847150501	3.1952595801
O	-1.9251082775	1.5845045782	3.1795758867
O	0.0316283255	-0.0077789040	4.4167908698
O	3.2450703984	0.0054099800	5.1485677457
O	-1.1682679820	1.5935877047	6.3640416167
O	1.2615027761	1.5987616558	6.3277824958
O	3.2131954011	-0.0037169819	7.5575259943
O	-0.1705195300	0.0673489144	-8.2281491623
O	0.1705195300	-0.0673489144	8.2281491623
Ir	3.1438405251	4.7535822170	-6.3905590338
Ir	-0.0543394512	3.1547130094	-6.4104452704
Ir	-0.0363570248	4.7562746554	-3.1880255923
Ir	3.1498883082	3.1712962629	-3.1942873719
Ir	3.1896092767	4.7561103358	0.0000935771
Ir	0.0000000000	3.1707800000	0.0000000000
Ir	0.0430006021	4.7529937972	3.1856229642
Ir	3.2289916918	3.1702537371	3.1942873719
Ir	3.2417390500	4.7614968221	6.3844413848
Ir	0.0543394512	3.1868369906	6.4104452704
O	3.1399722580	3.1636468432	-7.5601382125
O	-1.2615027761	4.7427883442	-6.3277824958
O	1.1682679820	4.7479722953	-6.3640416167
O	3.1250573699	3.1708281284	-5.1477673017
O	-0.0391943559	3.1711724092	-4.4096568378
O	1.9251082775	4.7570454218	-3.1795758867
O	-2.0012167420	4.7568349499	-3.1952595801
O	-0.0342660002	3.1729612121	-1.9627945195
O	3.1824755101	3.1711038617	-1.2238486267
O	-1.2255241478	4.7567407571	0.0108870693
O	1.2254774903	4.7560166252	-0.0099290656
O	3.1964044899	3.1704461383	1.2238486267
O	0.0342660002	3.1685887879	1.9627945195
O	2.0039233751	4.7548023198	3.1912589004
O	-1.9222983665	4.7558573548	3.1764076940
O	0.0391943559	3.1703775908	4.4096568378
O	3.2538326301	3.1707218716	5.1477673017
O	-1.1722435753	4.7768360633	6.3350350704
O	1.2812395185	4.7507569706	6.2778953210
O	3.2389177420	3.1779031568	7.5601382125
O	-0.0327195210	3.0933343197	-8.2568420174
O	0.0327195210	3.2482156803	8.2568420174
O	-0.8553040248	1.1946370447	9.1770745741

H	-0.3617637990	0.9579947145	9.9926917250
H	-0.3862217523	2.2026732343	8.7698589605
O	0.8553040248	-1.1946370447	-9.1770745741
H	0.3617637990	-0.9579947145	-9.9926917250
H	0.3862217523	-2.2026732343	-8.7698589605

2

ATOMIC_POSITIONS(angstrom)

Ir	3.150238926	1.572612986	-6.448582522
Ir	-0.038951697	-0.015391839	-6.443279379
Ir	-0.014099180	1.576404667	-3.212262541
Ir	3.169993484	-0.006608885	-3.224218995
Ir	3.191006656	1.585884051	-0.000186370
Ir	0.000649593	0.000501410	0.000554584
Ir	0.026689175	1.592804785	3.213490925
Ir	3.210282180	0.007248472	3.223914792
Ir	3.230467575	1.598400283	6.443865331
Ir	0.041344410	0.014798149	6.443571335
O	3.144455608	-0.015668827	-7.623449884
O	-1.252836271	1.576569412	-6.414668167
O	1.187562308	1.564237368	-6.442869214
O	3.153417833	-0.009743477	-5.195960660
O	-0.024440165	-0.007488949	-4.443492486
O	1.949460167	1.577444275	-3.210036966
O	-1.982524459	1.578473411	-3.222256206
O	-0.016699837	-0.007097876	-1.980155937
O	3.188684419	-0.000831467	-1.236292696
O	-1.223054960	1.586437727	0.005460683
O	1.224973523	1.586376629	-0.006380304
O	3.191378085	0.002043698	1.236138009
O	0.017857595	0.007413631	1.981039083
O	1.990008809	1.592478971	3.220246933
O	-1.941824152	1.593257595	3.209567925
O	0.026162668	0.008130470	4.443880487
O	3.229425051	0.009773669	5.195732921
O	-1.179639484	1.608438525	6.394333118
O	1.274123110	1.586061693	6.397856201
O	3.236506517	0.015137033	7.623555276
O	-0.042747925	-0.123685465	-8.359308675
O	0.041749256	0.119061094	8.359976905
H	-0.157938107	-0.775642885	8.748068907
O	-0.667761977	-2.413125955	9.137293171
H	-0.533052014	-2.804374543	10.030253486
Ir	3.150780504	4.742879121	-6.443732464
Ir	-0.040735269	3.161226429	-6.453967373
Ir	-0.025493688	4.749159887	-3.213029426
Ir	3.169487109	3.163995569	-3.225835684
Ir	3.189173927	4.756969885	0.000321242
Ir	0.000659098	3.171328554	0.000345230
Ir	0.015236519	4.765377283	3.213040934
Ir	3.210679059	3.178168346	3.225709343
Ir	3.231096979	4.768653428	6.448296761
Ir	0.043440955	3.180185937	6.455797534
O	3.157793543	3.161675735	-7.625827098
O	-1.271712378	4.755259354	-6.397298736
O	1.182512934	4.733331739	-6.391371070

O	3.154582212	3.157732183	-5.199985580
O	-0.018929834	3.160369176	-4.444962505
O	1.943127300	4.749001369	-3.210589859
O	-1.988701875	4.749841033	-3.220271261
O	-0.016962612	3.163614532	-1.982514177
O	3.189409123	3.170256029	-1.235964136
O	-1.223668993	4.756349235	0.007168983
O	1.224391339	4.756315240	-0.004765159
O	3.190667083	3.172570654	1.236119165
O	0.018012049	3.178513698	1.983268660
O	1.983667677	4.763557971	3.223051981
O	-1.948305938	4.764448880	3.209657959
O	0.020295707	3.180975524	4.445454684
O	3.227316878	3.183500594	5.199871559
O	-1.185135936	4.776406481	6.443555446
O	1.255133846	4.764910526	6.413034160
O	3.220074595	3.179673993	7.625702618
O	-0.185197741	3.322101151	-8.370032176
O	0.188692043	3.026429834	8.372341996
H	0.145980424	0.771481577	-8.751153681
O	0.650077103	2.408482446	-9.142761750
H	0.509409539	2.801396779	-10.034075187

l'

ATOMIC_POSITIONS(angstrom)

Ir	2.9924184900	1.5757658060	-6.3774423200
Ir	-0.1996547640	-0.0158409430	-6.4471403560
Ir	-0.1071527540	1.5806977880	-3.1881109760
Ir	3.0824649840	-0.0028212000	-3.1923163340
Ir	3.1894464790	1.5854259390	0.0005683240
Ir	0.0000000000	0.0000000000	0.0000000000
Ir	0.1051328550	1.5863607490	3.1831478340
Ir	3.2964150160	0.0028212000	3.1923163340
Ir	3.3858861680	1.5900736430	6.4008087840
Ir	0.1996547640	0.0158409430	6.4471403560
O	3.0284516430	0.0098563090	-7.5519781840
O	-1.4251614270	1.5722196470	-6.2370951930
O	1.0273916270	1.5715732720	-6.3421709150
O	2.9900641160	-0.0146973720	-5.1467754670
O	-0.1093744100	-0.0103273220	-4.4179820700
O	1.8574164500	1.5828366490	-3.1575213170
O	-2.0713413430	1.5829700910	-3.2116919030
O	-0.0984544310	0.0000203400	-1.9654552940
O	3.1771303840	0.0013109190	-1.2245303270
O	-1.2249229610	1.5851713820	0.0314180580
O	1.2250229120	1.5851369220	-0.0274213610
O	3.2017496160	-0.0013109190	1.2245303270
O	0.0984544310	-0.0000203400	1.9654552940
O	2.0698752800	1.5867412010	3.2107985230
O	-1.8587778120	1.5866162860	3.1544957370
O	0.1093744100	0.0103273220	4.4179820700
O	3.3888258840	0.0146973720	5.1467754670
O	-1.0176645150	1.5902710380	6.4277253040
O	1.4141215140	1.5975923450	6.3257983040
O	3.3504383570	-0.0098563090	7.5519781840
O	-0.3105565820	0.1243517220	-8.2285845600

O	0.3105565820	-0.1243517220	8.2285845600
Ir	2.9929938320	4.7514763570	-6.4008087840
Ir	-0.1988782510	3.1498478450	-6.3636075290
Ir	-0.1051328550	4.7551892510	-3.1831478340
Ir	3.0824713690	3.1700180180	-3.1935736360
Ir	3.1894335210	4.7561340610	-0.0005683240
Ir	0.0000000000	3.1707800000	0.0000000000
Ir	0.1071527540	4.7608622120	3.1881109760
Ir	3.2964086310	3.1715319820	3.1935736360
Ir	3.3864615100	4.7657841940	6.3774423200
Ir	0.1988782510	3.1917021550	6.3636075290
O	2.9962981610	3.1485026980	-7.5528136520
O	-1.4141215140	4.7439576550	-6.3257983040
O	1.0176645150	4.7512889620	-6.4277253040
O	2.9913038350	3.1716684560	-5.1463940170
O	-0.1107079560	3.1773036030	-4.3983175880
O	1.8587778120	4.7549337140	-3.1544957370
O	-2.0698752800	4.7548087990	-3.2107985230
O	-0.0970198890	3.1655853630	-1.9612053680
O	3.1778282860	3.1701014450	-1.2236765890
O	-1.2250229120	4.7564230780	0.0274213610
O	1.2249229610	4.7563786180	-0.0314180580
O	3.2010517140	3.1714485550	1.2236765890
O	0.0970198890	3.1759646370	1.9612053680
O	2.0713413430	4.7585799090	3.2116919030
O	-1.8574164500	4.7587233510	3.1575213170
O	0.1107079560	3.1642463970	4.3983175880
O	3.3875861650	3.1698815440	5.1463940170
O	-1.0273916270	4.7699767280	6.3421709150
O	1.4251614270	4.7693303530	6.2370951930
O	3.3825918390	3.1930473020	7.5528136520
O	-0.3084758220	3.0837117580	-8.2991882550
O	0.3084758220	3.2578382420	8.2991882550
O	-1.4343733150	1.4754380790	9.4519704860
H	-0.8888637640	0.8075985260	9.9102718770
H	-0.7798942410	2.1620699480	9.1581099320
O	1.4343733150	-1.4754380790	-9.4519704860
H	0.8888637640	-0.8075985260	-9.9102718770
H	0.7798942410	-2.1620699480	-9.1581099320
H	0.3410765440	4.2032934720	8.5910226830
H	-0.3410765440	-4.2032934720	-8.5910226830

TS1'

ATOMIC_POSITIONS(angstrom)

Ir	3.1219447183	1.5832270326	-6.3893085832
Ir	-0.0681316313	-0.0177671716	-6.4276530486
Ir	-0.0389419559	1.5884799515	-3.1835025535
Ir	3.1511950344	0.0031257663	-3.1957390598
Ir	3.1891618464	1.5850767218	0.0000992192
Ir	0.0000000000	0.0000000000	0.0000000000
Ir	0.0380569197	1.5759523614	3.1828624222
Ir	3.2276849656	-0.0031257663	3.1957390598
Ir	3.2547963613	1.5840790132	6.4015258362
Ir	0.0681316313	0.0177671716	6.4276530486
O	3.1266495706	0.0071603990	-7.5758040354

O	-1.3077946331	1.5975853828	-6.2785830270
O	1.1581695465	1.5696900663	-6.3551634606
O	3.1229975926	-0.0028935469	-5.1537380163
O	-0.0299745996	0.0103215956	-4.4183602140
O	1.9259041062	1.5886836835	-3.1769601012
O	-2.0023945914	1.5898124190	-3.1941044582
O	-0.0346751685	0.0052544768	-1.9631898269
O	3.1844034045	0.0010845215	-1.2266187908
O	-1.2258022034	1.5863923857	0.0102625357
O	1.2258937136	1.5857837742	-0.0101423207
O	3.1944765955	-0.0010845215	1.2266187908
O	0.0346751685	-0.0052544768	1.9631898269
O	2.0021381575	1.5805529765	3.1963171434
O	-1.9262142380	1.5808316839	3.1788578930
O	0.0299745996	-0.0103215956	4.4183602140
O	3.2558924074	0.0028935469	5.1537380163
O	-1.1556377933	1.5967252989	6.3934644753
O	1.2900282540	1.5924084895	6.3640659273
O	3.2522404294	-0.0071603990	7.5758040354
O	-0.2484142360	0.1846171793	-8.2427509727
O	0.2484142360	-0.1846171793	8.2427509727
Ir	3.1240836387	4.7574709868	-6.4015258362
Ir	-0.0701231675	3.1549574918	-6.3451404618
Ir	-0.0380569197	4.7655976386	-3.1828624222
Ir	3.1506775414	3.1749333087	-3.1980189102
Ir	3.1897181536	4.7564832782	-0.0000992192
Ir	0.0000000000	3.1707800000	0.0000000000
Ir	0.0389419559	4.7530800485	3.1835025535
Ir	3.2282024586	3.1666166913	3.1980189102
Ir	3.2569352817	4.7583229674	6.3893085832
Ir	0.0701231675	3.1865925082	6.3451404618
O	3.1052414164	3.1629379519	-7.5811467783
O	-1.2900282540	4.7491415105	-6.3640659273
O	1.1556377933	4.7448347011	-6.3934644753
O	3.1169510741	3.1765727295	-5.1565214587
O	-0.0395425350	3.1799893761	-4.3889412961
O	1.9262142380	4.7607183161	-3.1788578930
O	-2.0021381575	4.7609970235	-3.1963171434
O	-0.0329482451	3.1759019915	-1.9616331685
O	3.1850099692	3.1715327397	-1.2264580747
O	-1.2258937136	4.7557762258	0.0101423207
O	1.2258022034	4.7551576143	-0.0102625357
O	3.1938700308	3.1700172603	1.2264580747
O	-1.2258937136	4.7557762258	0.0101423207
O	1.2258022034	4.7551576143	-0.0102625357
O	3.1938700308	3.1700172603	1.2264580747
O	0.0329482451	3.1656480085	1.9616331685
O	2.0023945914	4.7517375810	3.1941044582
O	-1.9259041062	4.7528763165	3.1769601012
O	0.0395425350	3.1615606239	4.3889412961
O	3.2619389259	3.1649772705	5.1565214587
O	-1.1581695465	4.7718599337	6.3551634606
O	1.3077946331	4.7439646172	6.2785830270
O	3.2736485836	3.1786120481	7.5811467783
O	-0.0924826936	3.0985613564	-8.3786907635
O	0.0924826936	3.2429886436	8.3786907635

O	-0.3059128935	1.0763182288	9.3999588564
H	0.5143857355	0.9183021074	9.9207518199
H	-0.1261328942	2.2081621715	8.8588210116
O	0.3059128935	-1.0763182288	-9.3999588564
H	-0.5143857355	-0.9183021074	-9.9207518199
H	0.1261328942	-2.2081621715	-8.8588210116
H	-0.5403716234	3.9266184115	8.6885164982
H	0.5403716234	-3.9266184115	-8.6885164982

2'

ATOMIC_POSITIONS(angstrom)

Ir	3.2256718790	1.5893245770	-6.4056700970
Ir	0.0243052750	0.0088524750	-6.4083750240
Ir	0.0167361840	1.5774483400	-3.1769720390
Ir	3.2020043030	-0.0020381930	-3.1988809930
Ir	3.1900403430	1.5851573320	-0.0000575290
Ir	0.0000000000	0.0000000000	0.0000000000
Ir	-0.0085844170	1.5848813980	3.1817502330
Ir	3.1768756970	0.0020381930	3.1988809930
Ir	3.1634655290	1.5918852870	6.3860616990
Ir	-0.0243052750	-0.0088524750	6.4083750240
O	3.2822953570	-0.0150127810	-7.6104087370
O	-1.1921309330	1.5872937140	-6.3761221900
O	1.2644829810	1.5936946300	-6.3904316730
O	3.2193199630	0.0043444900	-5.1617511110
O	0.0189145990	0.0011922100	-4.3974957730
O	1.9769223280	1.5808686690	-3.1899538790
O	-1.9497998370	1.5813835890	-3.1843692230
O	0.0111954100	-0.0054115640	-1.9587956590
O	3.1888382870	-0.0013997800	-1.2272671260
O	-1.2250785820	1.5860969390	-0.0045153920
O	1.2261282810	1.5859065950	0.0045975910
O	3.1900417130	0.0013997800	1.2272671260
O	-0.0111954100	0.0054115640	1.9587956590
O	1.9537500580	1.5885278860	3.1893709810
O	-1.9734341080	1.5868072990	3.1932572640
O	-0.0189145990	-0.0011922100	4.3974957730
O	3.1595700370	-0.0043444900	5.1617511110
O	-1.2497603190	1.5651471690	6.3453300160
O	1.2042815940	1.5924790100	6.3514311310
O	3.0965946430	0.0150127810	7.6104087370
O	0.0720066780	0.0628357480	-8.3508360950
O	-0.0720066780	-0.0628357480	8.3508360950
Ir	3.2154144710	4.7496647130	-6.3860616990
Ir	0.0336427410	3.1795171840	-6.3482368720
Ir	0.0085844170	4.7566686020	-3.1817502330
Ir	3.1997991360	3.1669372640	-3.1973225060
Ir	3.1888396570	4.7564026680	0.0000575290
Ir	0.0000000000	3.1707800000	0.0000000000
Ir	-0.0167361840	4.7641116600	3.1769720390
Ir	3.1790808640	3.1746127360	3.1973225060
Ir	3.1532081210	4.7522254230	6.4056700970
Ir	-0.0336427410	3.1620328160	6.3482368720

O	3.1693241370	3.1804902670	-7.5978402020
O	-1.2042815940	4.7490709900	-6.3514311310
O	1.2497603190	4.7764128310	-6.3453300160
O	3.2017051000	3.1633904990	-5.1575180900
O	0.0083238870	3.1598528640	-4.3916127660
O	3.1595700370	-0.0043444900	5.1617511110
O	-1.2497603190	1.5651471690	6.3453300160
O	1.2042815940	1.5924790100	6.3514311310
O	3.0965946430	0.0150127810	7.6104087370
O	0.0720066780	0.0628357480	-8.3508360950
O	-0.0720066780	-0.0628357480	8.3508360950
Ir	3.2154144710	4.7496647130	-6.3860616990
Ir	0.0336427410	3.1795171840	-6.3482368720
Ir	0.0085844170	4.7566686020	-3.1817502330
Ir	3.1997991360	3.1669372640	-3.1973225060
Ir	3.1888396570	4.7564026680	0.0000575290
Ir	0.0000000000	3.1707800000	0.0000000000
Ir	-0.0167361840	4.7641116600	3.1769720390
Ir	3.1790808640	3.1746127360	3.1973225060
Ir	3.1532081210	4.7522254230	6.4056700970
Ir	-0.0336427410	3.1620328160	6.3482368720
O	3.1693241370	3.1804902670	-7.5978402020
O	-1.2042815940	4.7490709900	-6.3514311310
O	1.2497603190	4.7764128310	-6.3453300160
O	3.2017051000	3.1633904990	-5.1575180900
O	0.0083238870	3.1598528640	-4.3916127660
O	1.9734341080	4.7547427010	-3.1932572640
O	-1.9537500580	4.7530221140	-3.1893709810
O	0.0094886210	3.1706032130	-1.9601987230
O	3.1913464490	3.1704597030	-1.2276734770
O	-1.2261282810	4.7556534050	-0.0045975910
O	1.2250785820	4.7554530610	0.0045153920
O	3.1875335510	3.1710902970	1.2276734770
O	-0.0094886210	3.1709467870	1.9601987230
O	1.9497998370	4.7601664110	3.1843692230
O	-1.9769223280	4.7606913310	3.1899538790
O	-0.0083238870	3.1816971360	4.3916127660
O	3.1771849000	3.1781595010	5.1575180900
O	-1.2644829810	4.7478553700	6.3904316730
O	1.1921309330	4.7542562860	6.3761221900
O	3.2095658630	3.1610597330	7.5978402020
O	0.0824726180	3.2738549010	-8.4327377060
O	-0.0824726180	3.0676950990	8.4327377060
O	0.9604057580	0.7364708400	9.0049790460
H	1.8328881020	0.4028478480	8.5665838720
H	0.3752109120	2.1882710970	8.7259187900
O	-0.9604057580	-0.7364708400	-9.0049790460
H	-1.8328881020	-0.4028478480	-8.5665838720
H	-0.3752109120	-2.1882710970	-8.7259187900
H	-1.0347538560	3.0170931670	8.6904250470
H	1.0347538560	-3.0170931670	-8.6904250470

3

ATOMIC_POSITIONS(angstrom)

Ir	3.201658871	1.586938240	-6.461705251
Ir	0.012926874	-0.001940565	-6.450297473

Ir	-0.001377896	1.582477840	-3.210819804
Ir	3.188081204	-0.000415462	-3.227665100
Ir	3.190572024	1.585515770	0.000059066
Ir	0.000823543	-0.000059497	0.000050102
Ir	0.003143521	1.586088346	3.213420473
Ir	3.191980077	0.000427448	3.227787711
Ir	3.176575965	1.580622903	6.448821772
Ir	-0.012744396	0.002152697	6.450479967
O	3.204447326	-0.002088350	-7.629504675
O	-1.207595000	1.585585258	-6.453198904
O	1.233181408	1.583700819	-6.453079774
O	3.197916086	0.006040408	-5.200685590
O	0.000742780	0.003374023	-4.442925672
O	1.964154212	1.584179120	-3.219608329
O	-1.967200148	1.584527036	-3.214850250
O	-0.003045023	-0.002409784	-1.975690543
O	3.185561432	-0.000597951	-1.237032379
O	-1.222719126	1.585648384	0.000560478
O	1.224963545	1.585512286	-0.000921939
O	3.195051267	0.000465195	1.237146249
O	0.004414543	0.002410445	1.975789511
O	1.968505657	1.586745379	3.217010717
O	-1.962245029	1.586870320	3.221419283
O	0.000216730	-0.003313495	4.443081061
O	3.181465972	-0.005808655	5.200811380
O	-1.242380810	1.579823497	6.392641718
O	1.216819666	1.576804688	6.399582356
O	3.174574904	0.002381875	7.629635564
O	0.023988031	-0.106155181	-8.343723722
O	-0.024643140	0.106414861	8.343931391
H	-0.040017949	-0.826012013	8.734875656
O	-0.045564146	-2.362289186	9.241689593
Ir	3.202507078	4.761195420	-6.448707341
Ir	0.012120145	3.174764346	-6.470041860
Ir	-0.001965370	4.755501850	-3.213288497
Ir	3.187949138	3.169596274	-3.230095395
Ir	3.190001621	4.755886491	0.000075831
Ir	0.000825934	3.170713101	0.000031015
Ir	0.002561996	4.759098094	3.210946406
Ir	3.192113126	3.171962955	3.230240053
Ir	3.177429673	4.754881662	6.461823572
Ir	-0.011924897	3.166991568	6.470102858
O	3.204384004	3.180490665	-7.634711427
O	-1.216629212	4.764961027	-6.399445442
O	1.242558663	4.761937969	-6.392726970
O	3.198136712	3.169187677	-5.204811213
O	0.001296667	3.164211805	-4.448475418
O	1.963432570	4.754706359	-3.221084197
O	-1.967324527	4.754844923	-3.217047945
O	-0.004289780	3.168749323	-1.984275215
O	3.185418854	3.170859982	-1.238442040
O	-1.223286213	4.755892255	0.001048654
O	1.224393890	4.755762646	-0.000407066
O	3.195208785	3.170558115	1.238597682
O	0.005675784	3.172792835	1.984349894
O	1.968385066	4.757018516	3.214777190

O	-1.962965863	4.757353056	3.219967837
O	-0.000265726	3.177415630	4.448649279
O	3.181194553	3.172578670	5.204930659
O	-1.232983258	4.758056626	6.453133208
O	1.207795667	4.756211924	6.453352559
O	3.174333301	3.161354937	7.634818264
O	0.009059816	3.346794825	-8.409615967
O	-0.009714933	2.994947808	8.409589153
H	0.039446767	0.826187307	-8.734820249
O	0.044249470	2.362364426	-9.241700805

4

ATOMIC_POSITIONS(angstrom)

Ir	3.192655594	1.587058441	-6.443261255
Ir	0.004105881	0.004585790	-6.530929063
Ir	-0.001198234	1.580935756	-3.215485902
Ir	3.188337132	0.002264774	-3.222555576
Ir	3.190383541	1.585539212	0.000508537
Ir	0.000914773	-0.000042719	0.000132884
Ir	0.002538235	1.581339649	3.216366145
Ir	3.191907917	-0.002278274	3.222889827
Ir	3.186290012	1.573719464	6.435029149
Ir	-0.003479871	-0.004211291	6.530905116
O	3.193299168	0.005334332	-7.612042192
O	-1.210861326	1.583536208	-6.417356367
O	1.217524922	1.584267666	-6.417053626
O	3.191501340	0.008092514	-5.191841672
O	-0.000270752	-0.000347155	-4.460695453
O	1.963278427	1.585999531	-3.215991333
O	-1.965787569	1.585793784	-3.215009356
O	-0.001411800	0.000532726	-1.977973009
O	3.188651844	0.000008527	-1.233976935
O	-1.222740061	1.585906603	0.000780855
O	1.224641858	1.586004157	-0.001041727
O	3.192088471	-0.000079087	1.234315492
O	0.002961445	-0.000574456	1.978233681
O	1.967006518	1.583591465	3.214508997
O	-1.961928409	1.583652859	3.215233477
O	0.001476111	0.000438863	4.460891333
O	3.188152557	-0.007940638	5.192168134
O	-1.229434957	1.570722926	6.390611373
O	1.222803432	1.569889686	6.393891959
O	3.186163895	-0.005187875	7.612350252
O	0.008934484	-0.016637328	-8.301815732
O	-0.008627626	0.017100251	8.301831593
O	-0.023426594	-2.176646362	9.110133492
Ir	3.193186169	4.768028103	-6.434690389
Ir	0.003163821	3.178194184	-6.448457700
Ir	-0.001185143	4.760200860	-3.216147138
Ir	3.188382497	3.171909482	-3.225370030
Ir	3.190355041	4.755936143	-0.000161617
Ir	0.000914191	3.170736223	0.000149560
Ir	0.002580559	4.760627320	3.215725142
Ir	3.191857155	3.169624782	3.225705322
Ir	3.186837951	4.754679643	6.443534780
Ir	-0.002604854	3.163761270	6.448526502

O	3.193846600	3.183408744	-7.615457878
O	-1.222191494	4.772043800	-6.393467275
O	1.230015090	4.771164089	-6.390568559
O	3.191462409	3.172452648	-5.195180737
O	-0.000703203	3.168173277	-4.443989207
O	1.963279929	4.757884032	-3.214810033
O	-1.965645820	4.757924267	-3.214297353
O	-0.001880999	3.171380103	-1.983891831
O	3.188686086	3.171076215	-1.234551517
O	-1.222790778	4.755460434	0.001361488
O	1.224592949	4.755553644	-0.000453992
O	3.192057203	3.170404227	1.234904608
O	0.003427267	3.170154961	1.984171307
O	1.967167922	4.755752145	3.215241671
O	-1.961909662	4.755538287	3.216453677
O	0.002002686	3.173381799	4.444144824
O	3.188238725	3.169219459	5.195503586
O	-1.216910302	4.757602350	6.416839062
O	1.211453946	4.758360223	6.417543844
O	3.185418920	3.158353511	7.615778066
O	0.004293636	3.234261963	-8.392338665
O	-0.004970742	3.108940027	8.392313080
O	0.024442041	2.179050864	-9.110909220

5

ATOMIC_POSITIONS(angstrom)

Ir	3.167741727	1.597274457	-6.454330222
Ir	-0.020137254	0.019976789	-6.531585521
Ir	0.024349542	1.585871427	-3.212655762
Ir	3.208635034	0.007860426	-3.222055242
Ir	3.189197183	1.585422851	-0.000671063
Ir	0.000000000	0.000000000	0.000000000
Ir	-0.024791011	1.573513352	3.220874671
Ir	3.170244966	-0.007860426	3.222055242
Ir	3.205856152	1.555608495	6.431255015
Ir	0.020137254	-0.019976789	6.531585521
O	3.186703724	0.011159052	-7.620870735
O	-1.239666978	1.594472569	-6.402332867
O	1.193560137	1.611592526	-6.535352074
O	3.144712803	0.024332235	-5.188917382
O	0.046785889	0.018187589	-4.461241340
O	1.986888836	1.591260635	-3.197893323
O	-1.942059142	1.592285209	-3.233992454
O	0.007125527	0.002000361	-1.980417928
O	3.210443950	-0.000159149	-1.237816678
O	-1.224320677	1.586229056	-0.002810536
O	1.223912377	1.586327443	-0.000672183
O	3.168436050	0.000159149	1.237816678
O	-0.007125527	-0.002000361	1.980417928
O	1.942547740	1.578710958	3.236468658
O	-1.987422301	1.577531781	3.203769332
O	-0.046785889	-0.018187589	4.461241340
O	3.234177197	-0.024332235	5.188917382
O	-1.206732464	1.568398484	6.449580562
O	1.246350173	1.546730963	6.281560103

O	3.192186276	-0.011159052	7.620870735
O	-0.138023448	-0.154717716	-8.326937498
O	0.138023448	0.154717716	8.326937498
Ir	3.173023848	4.785941505	-6.431255015
Ir	-0.035943179	3.203328030	-6.402152113
Ir	0.024791011	4.768036648	-3.220874671
Ir	3.208137490	3.177429630	-3.228487622
Ir	3.189682817	4.756137149	0.000671063
Ir	0.000000000	3.170780000	0.000000000
Ir	-0.024349542	4.755688573	3.212655762
Ir	3.170742510	3.164120370	3.228487622
Ir	3.211138273	4.744275543	6.454330222
Ir	0.035943179	3.138221970	6.402152113
O	3.293112591	3.204815227	-7.648157515
O	-1.246350173	4.794819037	-6.281560103
O	1.206732464	4.773161516	-6.449580562
O	3.161910242	3.181484813	-5.204918871
O	0.075118843	3.164770317	-4.439167732
O	1.987422301	4.764018219	-3.203769332
O	-1.942547740	4.762839042	-3.236468658
O	0.011499751	3.180241226	-1.983133864
O	3.209041508	3.172336821	-1.236497717
O	-1.223912377	4.755232557	0.000672183
O	1.224320677	4.755320944	0.002810536
O	3.169838492	3.169213179	1.236497717
O	-0.011499751	3.161308774	1.983133864
O	1.942059142	4.749264791	3.233992454
O	-1.986888836	4.750299365	3.197893323
O	-0.075118843	3.176779683	4.439167732
O	3.216979758	3.160065187	5.204918871
O	-1.193560137	4.729957474	6.535352074
O	1.239666978	4.747077431	6.402332867
O	3.085777409	3.136734773	7.648157515
O	0.408853981	2.926079637	8.483979538
H	0.283444094	1.941643056	8.670634171
H	1.405516300	3.064316107	8.515259785
O	-0.408853981	-2.926079637	-8.483979538
H	-0.283444094	-1.941643056	-8.670634171
H	-1.405516300	-3.064316107	-8.515259785

TS2 (computed by 1x3 large supercell)

CELL_PARAMETERS (angstrom)

6.3788851605459698	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.5123243877191008	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.1047464399999999

ATOMIC_POSITIONS (angstrom)

Ir	6.377590	0.004362	0.006514
Ir	6.375138	9.500626	6.360331
Ir	6.379205	0.028615	22.761261
Ir	3.190010	9.508490	3.227772
Ir	3.186451	0.012275	25.887529
Ir	0.001109	1.593527	3.205173
Ir	6.376004	1.609318	25.912598
Ir	3.184640	1.577769	6.445609
Ir	3.189117	1.610604	22.672791
Ir	3.188042	1.588912	0.005814

Ir	6.377434	3.174801	0.006128
Ir	-0.002992	3.168958	6.484695
Ir	6.376265	3.203271	22.626741
Ir	3.190443	3.167622	3.218636
Ir	3.186757	3.183661	25.897766
Ir	0.000701	4.752547	3.212126
Ir	6.375983	4.768240	25.904879
Ir	3.187661	4.746027	6.413778
Ir	3.188023	4.778908	22.702330
Ir	3.188199	4.760244	0.005649
Ir	6.377706	6.345938	0.006293
Ir	0.000811	6.322600	6.490369
Ir	6.379584	6.358184	22.629894
Ir	3.189741	6.336991	3.217537
Ir	3.186142	6.353003	25.897034
Ir	0.000302	7.911132	3.205652
Ir	6.375547	7.926412	25.913189
Ir	3.186641	7.913901	6.442169
Ir	3.192039	7.946858	22.670153
Ir	3.188208	7.931645	0.005214
O	0.001396	9.509888	1.983167
O	5.398904	8.605840	9.228541
O	6.375680	0.009988	24.702391
O	3.189120	9.504083	5.201680
O	3.205062	0.020574	21.492161
O	3.187222	0.004957	27.880270
O	-0.000519	9.509177	4.417843
O	1.010698	0.909073	19.877584
O	6.376426	0.010419	27.135630
O	3.170445	9.502743	7.622412
O	3.188995	0.018698	23.913845
O	3.189257	0.002493	1.235320
O	1.220566	1.591663	0.005039
O	1.209820	1.580976	6.442764
O	1.215999	1.618666	22.690439
O	4.412101	1.585611	3.220854
O	4.408474	1.601984	25.892841
O	5.155401	1.591573	0.004882
O	5.159851	1.578597	6.449108
O	5.160857	1.611574	22.672075
O	1.968847	1.585794	3.221005
O	1.964799	1.602232	25.893194
O	0.000563	3.165291	1.978677
O	0.001412	3.338238	8.275880
O	6.378092	3.175655	24.677277
O	3.191006	3.154998	5.185011
O	3.184543	3.210389	21.512466
O	3.187629	3.172529	27.884169
O	6.376863	3.156636	4.441676
O	6.345560	3.349083	20.843586
O	6.376843	3.180080	27.138697
O	3.185145	3.175151	7.604826
O	3.189097	3.187254	23.931938
O	3.188941	3.170654	1.232521
O	1.221429	4.760000	0.005423
O	1.220398	4.744949	6.279335

O	1.219613	4.775142	22.829224
O	4.413107	4.752647	3.210006
O	4.409573	4.767418	25.903328
O	5.154813	4.759947	0.005222
O	5.155784	4.748858	6.301288
O	5.156039	4.781304	22.823280
O	1.967045	4.752448	3.210199
O	1.963198	4.767395	25.904058
O	0.000583	6.341363	1.978778
O	0.046717	6.169191	8.272156
O	6.372455	6.364761	24.675894
O	3.189122	6.336689	5.183403
O	3.183392	6.350149	21.510693
O	3.187743	6.349805	27.883448
O	6.374194	6.345089	4.440102
O	0.035355	6.196916	20.840052
O	6.377149	6.354886	27.139288
O	3.187765	6.316209	7.602444
O	3.186489	6.369054	23.931234
O	3.188846	6.348274	1.231804
O	1.220586	7.929627	0.004401
O	1.214443	7.913909	6.438066
O	1.216122	7.951445	22.669504
O	4.411417	7.918451	3.220001
O	4.407513	7.934897	25.893219
O	5.155731	7.929607	0.005011
O	5.160238	7.906520	6.430257
O	5.166591	7.946776	22.668394
O	1.967749	7.918525	3.221175
O	1.964499	7.935186	25.892614
O	5.743424	7.897615	10.183788
O	0.263336	1.430642	10.131993
O	0.642885	1.586828	18.909708
O	0.040926	8.056610	18.810711
H	5.761813	1.413807	10.544257
H	0.272044	2.274617	9.626446
H	6.017555	7.421046	18.194946
H	0.443885	7.476072	19.487770

1''

ATOMIC_POSITIONS (angstrom)

Ir	3.0954102170	1.5842503650	-6.4604047740
Ir	-0.0937676610	-0.0027512120	-6.4401377880
Ir	-0.0596342600	1.5831831780	-3.2150423340
Ir	3.1305999620	-0.0009855370	-3.2309359580
Ir	3.1894413270	1.5853870820	0.0000000000
Ir	0.0000000000	0.0000000000	0.0000000000
Ir	0.0596342600	1.5875903480	3.2150423340
Ir	3.2482826920	0.0009855370	3.2309359580
Ir	3.2834724360	1.5865231610	6.4604047740
Ir	0.0937676610	0.0027512120	6.4401377880
O	3.0974903710	-0.0011520260	-7.6364965910
O	-1.3178937410	1.5850209340	-6.4082963190
O	1.1296229330	1.5870545220	-6.4323670330
O	3.0944093710	-0.0021630790	-5.2073051710
O	-0.0635776850	-0.0022243160	-4.4437101790

O	1.9079761080	1.5842599340	-3.2023713220
O	-2.0265837770	1.5840959960	-3.2372606200
O	-0.0573901690	-0.0014288700	-1.9840053730
O	3.1822523260	0.0004433320	-1.2390552170
O	-1.2240048810	1.5853826170	0.0193752180
O	1.2240048810	1.5853909100	-0.0193752180
O	3.1966303270	-0.0004433320	1.2390552170
O	0.0573901690	0.0014288700	1.9840053730
O	2.0265837770	1.5866775300	3.2372606200
O	-1.9079761080	1.5865135930	3.2023713220
O	0.0635776850	0.0022243160	4.4437101790
O	3.2844732830	0.0021630790	5.2073051710
O	-1.1296229330	1.5837190040	6.4323670330
O	1.3178937410	1.5857525920	6.4082963190
O	3.2813922820	0.0011520260	7.6364965910
O	-0.1239002270	0.0878774010	-8.3755328850
O	0.1239002270	-0.0878774010	8.3755328850
H	-0.1603185440	-0.8198529100	-8.7605163140
H	0.1603185440	0.8198529100	8.7605163140
Ir	3.0954102170	4.7550270810	-6.4604047740
Ir	-0.0937676610	3.1680255040	-6.4401377880
Ir	-0.0596342600	4.7539598940	-3.2150423340
Ir	3.1305999620	3.1697911790	-3.2309359580
Ir	3.1894413270	4.7561637980	0.0000000000
Ir	0.0000000000	3.1707767160	0.0000000000
Ir	0.0596342600	4.7583670640	3.2150423340
Ir	3.2482826920	3.1717622530	3.2309359580
Ir	3.2834724360	4.7572998770	6.4604047740
Ir	0.0937676610	3.1735279280	6.4401377880
O	3.0974903710	3.1696246900	-7.6364965910
O	-1.3178937410	4.7557976500	-6.4082963190
O	1.1296229330	4.7578312380	-6.4323670330
O	3.0944093710	3.1686136370	-5.2073051710
O	-0.0635776850	3.1685524000	-4.4437101790
O	1.9079761080	4.7550366500	-3.2023713220
O	-2.0265837770	4.7548727120	-3.2372606200
O	-0.0573901690	3.1693478460	-1.9840053730
O	3.1822523260	3.1712200480	-1.2390552170
O	-1.2240048810	4.7561593330	0.0193752180
O	1.2240048810	4.7561676260	-0.0193752180
O	3.1966303270	3.1703333840	1.2390552170
O	0.0573901690	3.1722055860	1.9840053730
O	2.0265837770	4.7574542460	3.2372606200
O	-1.9079761080	4.7572903090	3.2023713220
O	0.0635776850	3.1730010320	4.4437101790
O	3.2844732830	3.1729397950	5.2073051710
O	-1.1296229330	4.7544957200	6.4323670330
O	1.3178937410	4.7565293080	6.4082963190
O	3.2813922820	3.1719287420	7.6364965910
O	-0.1239002270	3.2586541170	-8.3755328850
O	0.1239002270	3.0828993150	8.3755328850
H	-0.1603185440	2.3509238060	-8.7605163140
H	0.1603185440	3.9906296260	8.7605163140