

Supplementary Information

High-Efficiency CO₂ Electroreduction on Molybdenene: A Comparative Study Using Fixed-Charge and Fixed-Potential Methods

Song Yu^{a,b}, Huajian Pan^{b,c}, Xinzhuo Zhou^{a,b}, Dongxiao Yang^a and Gang Bi^{*,b}

^a College of Information Science and Electronic Engineering, Zhejiang University, Hangzhou 310027, People's Republic of China.

^b School of Information and Electrical Engineering, Hangzhou City University, Hangzhou 310015, People's Republic of China

^c College of Information Engineering, Zhejiang University of Technology, Hangzhou 310023, People's Republic of China.

*Correspondence and requests for materials should be addressed to

Gang Bi: big@hzcu.edu.cn

Coordinates of various transition states

TS1

76

Lattice vector (Angstrom)

0.9146520090E+01 -0.1319613892E+02 0.0000000000E+00

0.9146520090E+01 0.1319613892E+02 0.0000000000E+00

0.0000000000E+00 0.0000000000E+00 0.2000000000E+02

Position (normalized), move_x, move_y, move_z

1	0.550729840847859	0.443291934982605	0.639383415396080	1	1	1
6	0.491442603346316	0.506628062070496	0.638941900340317	1	1	1
8	0.411432410499355	0.462072009796832	0.660574486398389	1	1	1
8	0.537616678581077	0.586458240281275	0.660372529535684	1	1	1
42	0.124276038705336	0.042631095649219	0.446180387528760	1	1	1
42	0.124427004672464	0.209859717177547	0.444836710715108	1	1	1
42	0.124275249856734	0.376540618904533	0.445203020422315	1	1	1
42	0.124548553226860	0.542277236600667	0.445896341681665	1	1	1
42	0.124719480798230	0.708365850674131	0.444638066372044	1	1	1
42	0.124545546066102	0.874710150955230	0.446143556305819	1	1	1
42	0.291109217516652	0.042295322780973	0.446539058628038	1	1	1
42	0.290346602631204	0.209522520247661	0.443924024483924	1	1	1
42	0.289603226002900	0.376217530937708	0.444887569366246	1	1	1
42	0.291555849052196	0.541158004538918	0.446221447527232	1	1	1
42	0.291375269912075	0.707926848881924	0.446191187959696	1	1	1
42	0.290956250214423	0.874574668935549	0.444724707446064	1	1	1
42	0.457028511864898	0.042516352798552	0.446970239163548	1	1	1
42	0.458451299197148	0.210073208963329	0.445294226824011	1	1	1
42	0.456236579897653	0.375992361754590	0.443783367289918	1	1	1
42	0.458018928375140	0.541347118809924	0.450631036013649	1	1	1
42	0.458150918884200	0.707739470471919	0.446324568554722	1	1	1
42	0.457079442483678	0.874703988692535	0.446151477704077	1	1	1
42	0.623484006941053	0.042271933971964	0.445077090368482	1	1	1
42	0.624049071747939	0.209673162938436	0.445353429703772	1	1	1
42	0.622840850406482	0.376444258342579	0.444878337211283	1	1	1
42	0.623480145506028	0.543154736355614	0.443575250232888	1	1	1
42	0.623086380904921	0.709659163376356	0.444989954242197	1	1	1
42	0.622740971343482	0.874961866193440	0.445272069615800	1	1	1
42	0.789437331897265	0.042586053712040	0.446568102619202	1	1	1
42	0.789640160806995	0.209533968440356	0.443922360691897	1	1	1
42	0.789525983863667	0.375143002693759	0.445176351550749	1	1	1
42	0.789179296652231	0.540842846067685	0.444975139844362	1	1	1
42	0.789729346652734	0.708932991156118	0.443782072622602	1	1	1
42	0.789385252224764	0.874793764871838	0.444740462587070	1	1	1

42	0.956245090943250	0.042920186770894	0.447046829718553	1	1	1
42	0.956599171760963	0.209733489209491	0.446648216542278	1	1	1
42	0.956945378044968	0.375742627535085	0.444916217714699	1	1	1
42	0.956703816105702	0.542264510116971	0.446750857609925	1	1	1
42	0.956906066515915	0.708175251003218	0.446330270788588	1	1	1
42	0.956530284257801	0.874932134706373	0.446075584307143	1	1	1
42	0.039500855571403	0.125431873413952	0.550593543354244	1	1	1
42	0.039871570791816	0.291811212540117	0.550092699593824	1	1	1
42	0.040225497426314	0.458634053008319	0.550929051838091	1	1	1
42	0.040378225751740	0.625048664510135	0.550539743509541	1	1	1
42	0.040598603631543	0.792037109022342	0.550504682694764	1	1	1
42	0.040461919468642	0.958781312617658	0.550813706568795	1	1	1
42	0.206440250224386	0.124655940380471	0.549238887046145	1	1	1
42	0.206255269686531	0.291637243377245	0.548535757981888	1	1	1
42	0.206319923108474	0.458452275515045	0.551224085105757	1	1	1
42	0.206632818439306	0.625246875524207	0.551004837865625	1	1	1
42	0.207337486852109	0.791886024624191	0.548956774507580	1	1	1
42	0.207191381958914	0.958628793720185	0.550596323214337	1	1	1
42	0.373243923070961	0.125425175775285	0.550613167096618	1	1	1
42	0.372014340540856	0.291397898196815	0.547067121517776	1	1	1
42	0.370496804331787	0.458278662761638	0.558675160714303	1	1	1
42	0.373203242172560	0.625995463917324	0.551852046488301	1	1	1
42	0.373978467376872	0.792552246325772	0.551158948154493	1	1	1
42	0.374217384268041	0.958802547653522	0.550691765384983	1	1	1
42	0.539961042225882	0.125701618297045	0.550873641011570	1	1	1
42	0.539694316850587	0.291307879608835	0.550686380458383	1	1	1
42	0.540662554716777	0.458201242671676	0.550558943429900	1	1	1
42	0.540934266362556	0.628506178569814	0.558831796632233	1	1	1
42	0.540797937988786	0.792757274642328	0.551401820445647	1	1	1
42	0.540661649026433	0.958971564602524	0.551188797104193	1	1	1
42	0.706348551745550	0.125470397754361	0.549071651947175	1	1	1
42	0.707025645032285	0.292323773404058	0.550018220324720	1	1	1
42	0.707948516523546	0.459555078631965	0.550392204123177	1	1	1
42	0.707736236495315	0.627020587325125	0.546994496356298	1	1	1
42	0.707545998582398	0.792834328593500	0.548565123319976	1	1	1
42	0.707450472698190	0.959317495574222	0.550056860057629	1	1	1
42	0.873052453022697	0.126225481500522	0.552166295659204	1	1	1
42	0.873820935321553	0.293002658907495	0.548996813698402	1	1	1
42	0.873602455038939	0.459330354448792	0.550672375125242	1	1	1
42	0.873790122407373	0.625960453043500	0.550351869815507	1	1	1
42	0.874585289130613	0.792752777311355	0.549150082493714	1	1	1
42	0.873796010695234	0.959694087083105	0.550515564583532	1	1	1

TS1'

Lattice vector (Angstrom)

```
0.9146520090E+01 -0.1319613892E+02 0.0000000000E+00
0.9146520090E+01 0.1319613892E+02 0.0000000000E+00
0.0000000000E+00 0.0000000000E+00 0.2000000000E+02
```

Position (normalized), move_x, move_y, move_z

1	0.435815502688645	0.446284305700770	0.638937272875948	1	1	1
6	0.426006511911311	0.574868342971249	0.640206380096625	1	1	1
8	0.389498785507863	0.490342031405154	0.663962163106410	1	1	1
8	0.508653606450523	0.617877624575624	0.658663338210530	1	1	1
42	0.125396987154089	0.041909907245938	0.447005147551081	1	1	1
42	0.125715407693883	0.210040030164913	0.445195438730346	1	1	1
42	0.125383308165744	0.376238721452164	0.444110380944778	1	1	1
42	0.125466297349812	0.543004001542912	0.444955311100247	1	1	1
42	0.125304127054416	0.708919798949512	0.444684289564000	1	1	1
42	0.125338542821801	0.874830120154937	0.443837847810876	1	1	1
42	0.291739523749388	0.042284215653658	0.445640793862333	1	1	1
42	0.292225948236900	0.209083874596591	0.446327231799506	1	1	1
42	0.292155545001601	0.375685133245430	0.444367451336876	1	1	1
42	0.292259884409406	0.542812019799527	0.446074063901106	1	1	1
42	0.292074073153724	0.708475729487976	0.445956648078400	1	1	1
42	0.291666909167451	0.875173123800583	0.445356230566019	1	1	1
42	0.458187107804536	0.042009715891583	0.446633819378151	1	1	1
42	0.458212197344265	0.209380355946883	0.446579448390520	1	1	1
42	0.457194253920796	0.376581606914135	0.447440781810907	1	1	1
42	0.457739022618918	0.543863069479833	0.450514985124246	1	1	1
42	0.458560715054807	0.707962995523455	0.447791805925339	1	1	1
42	0.457433925989393	0.874526712830465	0.445831347500344	1	1	1
42	0.624397768138371	0.042244824190368	0.446140396741140	1	1	1
42	0.624566897039301	0.209483383665461	0.446155801608565	1	1	1
42	0.623931908449623	0.376260983579195	0.447413982132479	1	1	1
42	0.624001912689153	0.543773410160543	0.446680808434524	1	1	1
42	0.625929630875706	0.709113618438221	0.444649326273017	1	1	1
42	0.624308455003866	0.875190254917457	0.444130459926446	1	1	1
42	0.790689897117342	0.041505608483677	0.446199858710152	1	1	1
42	0.790858353640703	0.209219542328689	0.446090209610256	1	1	1
42	0.790904165762009	0.375884296014330	0.444959965780535	1	1	1
42	0.790454431644824	0.542320582491382	0.446089722900514	1	1	1
42	0.791550214259248	0.707988061217655	0.444476750886446	1	1	1
42	0.791145694460294	0.875368039624294	0.443544408930559	1	1	1
42	0.958415194621875	0.042035946635253	0.446375308655776	1	1	1
42	0.958470139543557	0.209755349779316	0.446672316260775	1	1	1
42	0.958330871391995	0.376197266531578	0.445744547611023	1	1	1
42	0.958124519072334	0.542089499919789	0.445105704320961	1	1	1

42	0.958364922985019	0.708457711123323	0.444551729210548	1	1	1
42	0.958184488249984	0.875037403149001	0.445774546273445	1	1	1
42	0.041455589266457	0.125142151346194	0.550521654717978	1	1	1
42	0.040778671620996	0.291806174278504	0.550103331706574	1	1	1
42	0.040876950388238	0.458917819526669	0.550022333198492	1	1	1
42	0.041009176500935	0.625159505239691	0.549326767805772	1	1	1
42	0.041276330706713	0.791840084244591	0.549047284254486	1	1	1
42	0.042070994459096	0.958992059709589	0.551603191927553	1	1	1
42	0.208196360545516	0.125772150926544	0.550820506403602	1	1	1
42	0.207819488709625	0.292209525876099	0.548360119332804	1	1	1
42	0.207035773722881	0.458090848330763	0.548159308466115	1	1	1
42	0.207025323548591	0.625310191524834	0.551191664847967	1	1	1
42	0.207837697942662	0.792096011025319	0.549863858529838	1	1	1
42	0.208538809298534	0.959101590367865	0.549330350809683	1	1	1
42	0.374885408542996	0.125322797828660	0.551153287948790	1	1	1
42	0.375432916764275	0.291842949194649	0.551852205849777	1	1	1
42	0.375121254015147	0.458351476212518	0.554595481929912	1	1	1
42	0.372466579962514	0.626309463251655	0.556070644848898	1	1	1
42	0.374702314687224	0.792353115025781	0.551895870535571	1	1	1
42	0.375001941773552	0.958800325303924	0.550947979116170	1	1	1
42	0.541220642988411	0.124973916667504	0.551366338590743	1	1	1
42	0.541457568080414	0.291475369110797	0.552199060962230	1	1	1
42	0.542738319678056	0.458261578834462	0.553998806122976	1	1	1
42	0.544815556882438	0.626228725538607	0.558214433270242	1	1	1
42	0.542803081442452	0.793197381284556	0.549458297215579	1	1	1
42	0.541527404991816	0.959059399977407	0.550448131290580	1	1	1
42	0.708204498014818	0.125524901637867	0.550858256543648	1	1	1
42	0.707980193054259	0.292106335766607	0.549977023564642	1	1	1
42	0.708508371875213	0.458931733327065	0.552055308762172	1	1	1
42	0.708664459592715	0.625676071510677	0.551022374645379	1	1	1
42	0.708592228822691	0.792670205736210	0.547466608510040	1	1	1
42	0.708682595612635	0.959391993141934	0.549557599181672	1	1	1
42	0.874955906254623	0.125948922649296	0.551276191116614	1	1	1

TS2

77

Lattice vector (Angstrom)

0.9146520090E+01	-0.1319613892E+02	0.0000000000E+00
0.9146520090E+01	0.1319613892E+02	0.0000000000E+00
0.0000000000E+00	0.0000000000E+00	0.2000000000E+02

Position (normalized), move_x, move_y, move_z

1	0.503128160849659	0.496650002629298	0.728964337012367	1	1	1
1	0.534326419455109	0.447928833546761	0.657389358067672	1	1	1
6	0.499034372182385	0.497103232267091	0.673809402387760	1	1	1

8	0.410360521385848	0.463251509593486	0.653983116240562	1	1	1
8	0.545800892689261	0.582499413030356	0.650254000596334	1	1	1
42	0.124600937936686	0.041808116294360	0.442366917320325	1	1	1
42	0.124523516429921	0.208139772275747	0.442150961208883	1	1	1
42	0.124355359751534	0.375167411506656	0.441103043171855	1	1	1
42	0.124642441326044	0.541472177870534	0.443013077014485	1	1	1
42	0.124718154979809	0.707776040314765	0.442374416407390	1	1	1
42	0.124563528146213	0.873959206586334	0.443534432261888	1	1	1
42	0.291090908855625	0.041202385367324	0.443525381005745	1	1	1
42	0.291549370229151	0.209137656165919	0.441197508072234	1	1	1
42	0.289284010084554	0.374679774511737	0.441848880441420	1	1	1
42	0.291690094683629	0.540255470551357	0.444251165291869	1	1	1
42	0.290826869323050	0.707274923512049	0.443977919343704	1	1	1
42	0.290692138047490	0.873856392205419	0.442107015686072	1	1	1
42	0.457134347052188	0.041050327111732	0.444076547429237	1	1	1
42	0.458501755356927	0.209086691295178	0.443223998023345	1	1	1
42	0.457379574997324	0.376843727960043	0.446211329087318	1	1	1
42	0.457677107354658	0.540761812198781	0.451755764317302	1	1	1
42	0.457447702896890	0.706507485863054	0.443717182150873	1	1	1
42	0.456878402299653	0.873815515878055	0.442882226553787	1	1	1
42	0.623839830335225	0.040727781449674	0.443045654908380	1	1	1
42	0.624226976124203	0.208123991695835	0.443747279805890	1	1	1
42	0.623703273977904	0.374825717140914	0.444252260360481	1	1	1
42	0.621949317963156	0.541002656150578	0.445333021527289	1	1	1
42	0.623490169423231	0.708171763241110	0.442546631312570	1	1	1
42	0.622835210441677	0.873777796361267	0.442474665298522	1	1	1
42	0.790258437190431	0.041274957732341	0.443867181624618	1	1	1
42	0.790195650149467	0.208365908627111	0.442622628049672	1	1	1
42	0.790089399564369	0.374105002230680	0.443302969691163	1	1	1
42	0.789577240671195	0.539566145267490	0.443040197557756	1	1	1
42	0.789169292975248	0.706463926554210	0.442275896232787	1	1	1
42	0.789875414597619	0.873613324218686	0.444105945397699	1	1	1
42	0.957084879593759	0.041515398577848	0.445699065654798	1	1	1
42	0.957339797113107	0.208527160353707	0.442545856616514	1	1	1
42	0.957503014764330	0.374395493101491	0.442432733746195	1	1	1
42	0.957591171148764	0.541241601675505	0.443891656654249	1	1	1
42	0.957212968538208	0.707388543083771	0.444313488965600	1	1	1
42	0.956660033485364	0.873481325352325	0.443539429495231	1	1	1
42	0.039928971230492	0.124242814255134	0.548937016962720	1	1	1
42	0.040300599469390	0.290837315048230	0.546055027105714	1	1	1
42	0.040253939144492	0.457820457178580	0.547929988775804	1	1	1
42	0.040537381248890	0.623628773720462	0.548097137384543	1	1	1
42	0.040384644044750	0.790935677509756	0.548661716580698	1	1	1
42	0.040924884820666	0.957229259331537	0.547975748733543	1	1	1

42	0.206489971199643	0.123522040775093	0.545861953809431	1	1	1
42	0.206909388307516	0.290934962785735	0.545738996087479	1	1	1
42	0.206998282148772	0.456718607246730	0.547418547272619	1	1	1
42	0.206428776983895	0.624303755436533	0.548901290567775	1	1	1
42	0.207147525013625	0.791367257636235	0.546961376683404	1	1	1
42	0.207270691223692	0.957799833084307	0.548198355901316	1	1	1
42	0.373763248518985	0.124595558877029	0.547938594397196	1	1	1
42	0.371219190331705	0.289765123597475	0.546537943157712	1	1	1
42	0.369358915706621	0.457270930253805	0.560627973542491	1	1	1
42	0.372549755258568	0.626117663775793	0.550014330687432	1	1	1
42	0.374467083084965	0.792080966852098	0.548280179795994	1	1	1
42	0.374530873041186	0.957987145082698	0.547767761645269	1	1	1
42	0.540380207306490	0.123956068344320	0.548816457895390	1	1	1
42	0.540339563030536	0.289907166381343	0.549204675487232	1	1	1
42	0.543973232975572	0.453893518736781	0.550812797410829	1	1	1
42	0.539128850809939	0.626875427777983	0.557326368517788	1	1	1
42	0.541606213028754	0.791497838745517	0.547633966203065	1	1	1
42	0.540718200747860	0.958688641673231	0.548481271107190	1	1	1
42	0.707195362144502	0.124054185942782	0.547705107449850	1	1	1
42	0.707997649763374	0.290632992389819	0.548732190190635	1	1	1
42	0.708924599703348	0.457817156082226	0.548561620320668	1	1	1
42	0.708852224777802	0.626440641557293	0.546601455058223	1	1	1
42	0.707453510167205	0.791583496372491	0.546814874654776	1	1	1
42	0.707558829955202	0.958564589719648	0.547761516283420	1	1	1
42	0.873828824470998	0.124235733892726	0.548941797239793	1	1	1
42	0.874389598637241	0.291503638567637	0.547389446701587	1	1	1
42	0.874771443584665	0.457893389657845	0.548518182649763	1	1	1
42	0.874063462497609	0.624268589707007	0.548413673961891	1	1	1
42	0.874994145723628	0.791772385286932	0.547402932558884	1	1	1
42	0.874178535208068	0.958146026864001	0.549845296814136	1	1	1

TS2'

77

Lattice vector (Angstrom)

0.9146520090E+01	-0.1319613892E+02	0.0000000000E+00
0.9146520090E+01	0.1319613892E+02	0.0000000000E+00
0.0000000000E+00	0.0000000000E+00	0.2000000000E+02

Position (normalized), move_x, move_y, move_z

1	0.369489630852367	0.385236990600001	0.631720374159160	1	1	1
1	0.529584412764476	0.469967454145194	0.658142430692629	1	1	1
6	0.483002639329690	0.507291637127333	0.644132206686221	1	1	1
8	0.396277812476501	0.462150251307913	0.663833840747211	1	1	1
8	0.515285117641122	0.594448519154431	0.658601033613351	1	1	1
42	0.125268370207994	0.042199922806704	0.447142660826340	1	1	1

42	0.126888643747866	0.209861201085253	0.447464350272688	1	1	1
42	0.126516514432031	0.376566720557117	0.447691523562219	1	1	1
42	0.126052404698932	0.542713089945604	0.446811600765832	1	1	1
42	0.125699260948023	0.709442601985000	0.444630429788619	1	1	1
42	0.125467589761786	0.875284263688401	0.445005107238336	1	1	1
42	0.292218917740070	0.042649235141131	0.446558920879425	1	1	1
42	0.292442033535370	0.209596386273468	0.446948071437146	1	1	1
42	0.291862614246103	0.376003440243255	0.446703223361848	1	1	1
42	0.293815742996983	0.542650780301034	0.445645278984155	1	1	1
42	0.292748717125145	0.708924340984632	0.446917227912138	1	1	1
42	0.291922120314608	0.875561108267365	0.445560611103661	1	1	1
42	0.458649659836347	0.042484178757559	0.446680986160535	1	1	1
42	0.459282711048434	0.209973308474764	0.445203821959026	1	1	1
42	0.459828888967379	0.376882794034564	0.444825452367249	1	1	1
42	0.459921603851603	0.543616442133754	0.447955007586493	1	1	1
42	0.460046694052931	0.707677445770216	0.447158940980851	1	1	1
42	0.458845377031547	0.874712361271846	0.445586187430128	1	1	1
42	0.625117718136004	0.042108774244432	0.443426763997272	1	1	1
42	0.625883828938457	0.209120539900972	0.444988789033655	1	1	1
42	0.625369194023211	0.376987026541080	0.444122461156854	1	1	1
42	0.626040360205385	0.543887823588402	0.444817884465702	1	1	1
42	0.625576208434237	0.709978220994474	0.443600289147800	1	1	1
42	0.624595844032073	0.875460538305962	0.444650738894135	1	1	1
42	0.791657482874776	0.041806109565813	0.445428651789457	1	1	1
42	0.791391858808778	0.209317228576268	0.443402192026972	1	1	1
42	0.791514952914925	0.375426713869216	0.444994805016612	1	1	1
42	0.791682455939938	0.542010702596385	0.444482798484340	1	1	1
42	0.791924174250152	0.709720125148055	0.443297005121693	1	1	1
42	0.791767311173209	0.875477584946818	0.442442858228230	1	1	1
42	0.958153839800322	0.042533924994734	0.445951870771092	1	1	1
42	0.958473116403212	0.209349812903885	0.447922857850362	1	1	1
42	0.958929914547723	0.375662203869667	0.445896548161911	1	1	1
42	0.958303852543542	0.542777786285095	0.445634275821113	1	1	1
42	0.958774428808451	0.709338401142028	0.444280056896114	1	1	1
42	0.958122240042814	0.875455778498323	0.444534067176194	1	1	1
42	0.042255690206421	0.126000098805313	0.551975328747941	1	1	1
42	0.042440283696300	0.292224479574121	0.552552835538795	1	1	1
42	0.041432476966147	0.459156458255202	0.551742673312606	1	1	1
42	0.041460393051472	0.626065172748810	0.549754751018467	1	1	1
42	0.041755343294990	0.792897950459842	0.549661965771417	1	1	1
42	0.042520534491495	0.959574589337029	0.550855158138993	1	1	1
42	0.208887406963295	0.125621302595837	0.551963715587581	1	1	1
42	0.208691103657345	0.292484229029639	0.552915419836646	1	1	1
42	0.207545303001129	0.459329251900241	0.551141777408085	1	1	1

42	0.207674866320607	0.625799137920561	0.551823607671969	1	1	1
42	0.208296967227248	0.792694291714202	0.549445510692441	1	1	1
42	0.208755489723313	0.959324654294138	0.550978971499365	1	1	1
42	0.374947139598321	0.125104449563497	0.552141281686820	1	1	1
42	0.374954027688186	0.291188551244908	0.550613233729753	1	1	1
42	0.374252750894213	0.460479443564172	0.554134987520425	1	1	1
42	0.373186371074617	0.627670601733908	0.551513865015610	1	1	1
42	0.375287763358054	0.793265688738753	0.552179961359432	1	1	1
42	0.375696409528347	0.958953938241924	0.550850307761390	1	1	1
42	0.541696922634057	0.125392182059271	0.550297340432925	1	1	1
42	0.541211365081347	0.291490321776511	0.549677088019608	1	1	1
42	0.542978233379025	0.456734725064948	0.549927477355291	1	1	1
42	0.542386133508554	0.626259273381449	0.559903837652670	1	1	1
42	0.543035868130037	0.792750024468399	0.551077671864298	1	1	1
42	0.542029694640552	0.959113971288819	0.549804508124928	1	1	1
42	0.708874049423570	0.125584876928275	0.548088050438531	1	1	1
42	0.708602470239253	0.292303296837551	0.549500828747075	1	1	1
42	0.709442098855205	0.459298028850506	0.550144094353938	1	1	1
42	0.708296155665827	0.626269257284495	0.547929532892619	1	1	1
42	0.708170912362278	0.792466300822374	0.547722326732875	1	1	1
42	0.709153134094469	0.959071215706494	0.549328680240459	1	1	1
42	0.875738262981018	0.126709783303419	0.551742583305455	1	1	1
42	0.875452806818717	0.293008581223979	0.549713959020756	1	1	1
42	0.875526846618674	0.459467282132907	0.550243819539655	1	1	1
42	0.875566160479984	0.625935644000862	0.549670727774654	1	1	1
42	0.875234872927604	0.792533543835851	0.548275466455823	1	1	1
42	0.875541991961772	0.959506623724016	0.549600035910593	1	1	1

TS3

77

Lattice vector (Angstrom)

0.9146520090E+01	-0.1319613892E+02	0.0000000000E+00
0.9146520090E+01	0.1319613892E+02	0.0000000000E+00
0.0000000000E+00	0.0000000000E+00	0.2000000000E+02

Position (normalized), move_x, move_y, move_z

1	0.467965147001359	0.495497326687310	0.699408364422887	1	1	1
1	0.351676211623773	0.488279895126662	0.694025320624796	1	1	1
1	0.422470768265277	0.418880519518978	0.627990862845453	1	1	1
6	0.414306620329502	0.499980310774774	0.667383364171704	1	1	1
8	0.442007483182995	0.579070835835082	0.630443248843052	1	1	1
42	0.127598058356430	0.043410040417759	0.444123777423365	1	1	1
42	0.127678539677306	0.210703696392467	0.442674532080570	1	1	1
42	0.127504278213169	0.376854412746926	0.443995951968322	1	1	1
42	0.127824685451079	0.543566765091219	0.444872439872723	1	1	1

42	0.127393737234614	0.709997301917506	0.444262052813952	1	1	1
42	0.127635499318451	0.875807379962219	0.442956311394614	1	1	1
42	0.293908291828996	0.043072978836690	0.444769561829630	1	1	1
42	0.294876220161238	0.210109613261930	0.444625867308859	1	1	1
42	0.293941782776523	0.376503161667036	0.444690256852568	1	1	1
42	0.294872556279756	0.543273533596716	0.447656192712375	1	1	1
42	0.294151078326112	0.709244544769703	0.445565349586453	1	1	1
42	0.293754558107725	0.876163538778271	0.444397493908510	1	1	1
42	0.460483615788209	0.042982949312554	0.444653348849891	1	1	1
42	0.460870672464486	0.210284254574410	0.444841226886984	1	1	1
42	0.460735314496806	0.376933726630893	0.445230513908945	1	1	1
42	0.460616328879345	0.544614124829949	0.448159031828684	1	1	1
42	0.460333040280673	0.708743758941077	0.446890398323287	1	1	1
42	0.459860563558031	0.875882633625092	0.444563587982165	1	1	1
42	0.627361108411099	0.042858040335486	0.443526018243359	1	1	1
42	0.627633549728200	0.209754942674283	0.443940160137612	1	1	1
42	0.627214148125243	0.375904551926956	0.444993792331040	1	1	1
42	0.626892371944491	0.542651262351107	0.444632448076923	1	1	1
42	0.628149526968461	0.709707060075284	0.443118657562293	1	1	1
42	0.626525932160378	0.875814533931656	0.443839431683620	1	1	1
42	0.793856443349173	0.042705695172050	0.444523353701530	1	1	1
42	0.793458012311441	0.210148239106777	0.443035075343357	1	1	1
42	0.793997187223516	0.376022229124733	0.444009185063305	1	1	1
42	0.793754443672570	0.542844470242729	0.445202534885902	1	1	1
42	0.793755158079386	0.709324592900939	0.444421346977724	1	1	1
42	0.793443890034351	0.876201291309878	0.443025197549969	1	1	1
42	0.960848638168418	0.043123770919741	0.443856448610208	1	1	1
42	0.961232487066993	0.210116662491880	0.443434611039564	1	1	1
42	0.961309112344885	0.376097422311730	0.443132285024327	1	1	1
42	0.960914746907490	0.542793492510252	0.444746391126717	1	1	1
42	0.960895344837824	0.709697414271877	0.443542590915633	1	1	1
42	0.961071089986422	0.876313567599151	0.444348292271305	1	1	1
42	0.044119631311034	0.126409310698018	0.548277425649584	1	1	1
42	0.044201677963829	0.293122985581383	0.548419993471973	1	1	1
42	0.043710884953416	0.459847977973274	0.549586587276258	1	1	1
42	0.043317309683349	0.626287875325660	0.549667082660645	1	1	1
42	0.043586257508330	0.792771674736275	0.548341385514399	1	1	1
42	0.043953339514909	0.959727397851009	0.548932087994847	1	1	1
42	0.211123617413953	0.127298164821270	0.548600799155146	1	1	1
42	0.211485050316371	0.294356548427289	0.548288931739562	1	1	1
42	0.209763428990662	0.459641532618991	0.550602348039285	1	1	1
42	0.209753021747298	0.626482034312628	0.551845915895494	1	1	1
42	0.210075377111579	0.793418293991451	0.549297679712112	1	1	1
42	0.210919189014452	0.960248598251667	0.548954137124415	1	1	1

42	0.377797353305133	0.125979306187562	0.550693105841648	1	1	1
42	0.377974066816431	0.293534707317332	0.549824521023873	1	1	1
42	0.376122263661948	0.459918781760142	0.558028920090868	1	1	1
42	0.373298463890061	0.629523340292560	0.554978070693511	1	1	1
42	0.377298375307551	0.793418980837025	0.550782915492720	1	1	1
42	0.377503302682483	0.960061863252690	0.550003150747363	1	1	1
42	0.544043471138010	0.126000388471222	0.548959127437810	1	1	1
42	0.544558176215929	0.292092331196166	0.550969763822360	1	1	1
42	0.547499792707830	0.457122787921318	0.549145573758649	1	1	1
42	0.543749862756846	0.623266116616091	0.554056516148667	1	1	1
42	0.544427069260371	0.793417875099305	0.548620474833266	1	1	1
42	0.544141882902057	0.960471198451637	0.549509781483397	1	1	1
42	0.710643199150027	0.126127064764497	0.548927416634979	1	1	1
42	0.711333524679370	0.292907402042610	0.548919454414919	1	1	1
42	0.712227062202191	0.459586025430787	0.550951880754293	1	1	1
42	0.708920281304036	0.625454488340603	0.549566773914940	1	1	1
42	0.709337102308692	0.791594073348242	0.547999970105980	1	1	1
42	0.710322232129116	0.959416041746296	0.548743020698418	1	1	1
42	0.876745262766186	0.126485745166690	0.548649152567130	1	1	1
42	0.877429042480216	0.292824209596289	0.548332173703348	1	1	1
42	0.877916097806956	0.459525433279521	0.549591752961845	1	1	1
42	0.877682633666823	0.625821193439720	0.550092742002341	1	1	1
42	0.876454408692743	0.792382332152239	0.548682829121858	1	1	1
42	0.876955998605169	0.959225940710428	0.548849444193891	1	1	1

TS3'

77

Lattice vector (Angstrom)

0.9146520090E+01	-0.1319613892E+02	0.0000000000E+00
0.9146520090E+01	0.1319613892E+02	0.0000000000E+00
0.0000000000E+00	0.0000000000E+00	0.2000000000E+02

Position (normalized), move_x, move_y, move_z

1	0.513564861795714	0.578904774485112	0.664907430558824	1	1	1
1	0.374572558253096	0.387385803932895	0.634018452599704	1	1	1
1	0.532999727822116	0.474537334207507	0.660303040295846	1	1	1
6	0.488023366063383	0.510758389126159	0.642466348977121	1	1	1
8	0.399683504523744	0.466337689776532	0.663583216521076	1	1	1
42	0.126079031992673	0.043620472086288	0.446208555907094	1	1	1
42	0.126855138660219	0.210651079686277	0.445580794014419	1	1	1
42	0.126854214753156	0.377612283412562	0.447066765180804	1	1	1
42	0.126645581310734	0.543513583913964	0.446238981596879	1	1	1
42	0.125892210734058	0.710153412641729	0.444657359413914	1	1	1
42	0.126230934784003	0.876315871252520	0.445019523266710	1	1	1
42	0.292782527956931	0.043439964903207	0.445748972881961	1	1	1

42	0.292931784405098	0.209808178872789	0.446445141122607	1	1	1
42	0.292310382630005	0.376291882325685	0.446956592363903	1	1	1
42	0.293594779482126	0.543259101883769	0.445917346950150	1	1	1
42	0.292521849083307	0.709725611650527	0.446057481769587	1	1	1
42	0.292415914739075	0.876518689570158	0.445837978377165	1	1	1
42	0.459175209372063	0.043624317302815	0.446567371074891	1	1	1
42	0.459642430172869	0.210356918845355	0.445857315042907	1	1	1
42	0.459114296819188	0.377235815981966	0.446999890686967	1	1	1
42	0.460051406009448	0.543314189233851	0.447354130216312	1	1	1
42	0.459067356253851	0.709666959717196	0.446379416536390	1	1	1
42	0.459424584114467	0.876547358572811	0.446196316823795	1	1	1
42	0.625674333713268	0.043298758616116	0.444477400288265	1	1	1
42	0.626324513774844	0.209609323844692	0.445426330947274	1	1	1
42	0.625487851997908	0.376376968657523	0.445435343924053	1	1	1
42	0.625943250947873	0.542893709475395	0.445462314110943	1	1	1
42	0.625634055819151	0.710456343501414	0.444426008070449	1	1	1
42	0.625566573615121	0.876340023572018	0.446680044605889	1	1	1
42	0.792467309445552	0.043428224226219	0.446592930284508	1	1	1
42	0.792362408817159	0.210136878253986	0.444536722160209	1	1	1
42	0.792470628840207	0.375925701209059	0.445802357880740	1	1	1
42	0.792638655614606	0.542566519968479	0.445225788411813	1	1	1
42	0.792175844354346	0.710017092123288	0.445242576130781	1	1	1
42	0.792142495218034	0.876350508871193	0.444879421728847	1	1	1
42	0.959289274991139	0.043483391928147	0.446127533701169	1	1	1
42	0.959395986153194	0.210064016865485	0.447340359297200	1	1	1
42	0.959277740389795	0.376597815397340	0.446265278528378	1	1	1
42	0.959217134633270	0.543284935764593	0.445867087385514	1	1	1
42	0.959172119888505	0.709851600449620	0.444977701597634	1	1	1
42	0.959210223842820	0.876695392975110	0.446395099655344	1	1	1
42	0.042895461826443	0.126873077349730	0.550813998637994	1	1	1
42	0.042979021075300	0.293499005731593	0.551464863054330	1	1	1
42	0.041936548190734	0.460149388732194	0.552007804953002	1	1	1
42	0.042560145685140	0.626636308828747	0.549997643296224	1	1	1
42	0.042451954040088	0.793245491114103	0.550126461227018	1	1	1
42	0.042691079955683	0.959467207895634	0.550858020879208	1	1	1
42	0.209612696353591	0.127060232689301	0.550443946533027	1	1	1
42	0.209984354364322	0.294133139404601	0.551813428974917	1	1	1
42	0.208842814548715	0.460453064950633	0.551198768058318	1	1	1
42	0.208669789239533	0.626878282804462	0.551720526158927	1	1	1
42	0.209100770063652	0.793533498324891	0.549895502916474	1	1	1
42	0.209260624699653	0.959737130775581	0.550635855174237	1	1	1
42	0.375878097965935	0.126303905880469	0.551771163584395	1	1	1
42	0.376598230222226	0.292991035556763	0.551515178393677	1	1	1
42	0.375280230829310	0.461061324738749	0.557069322369327	1	1	1

42	0.373861029578372	0.628212083706920	0.550572400333812	1	1	1
42	0.375664273221447	0.794102077905454	0.551822421308777	1	1	1
42	0.375689994769011	0.959836270944837	0.551213256607739	1	1	1
42	0.542393734239036	0.126334517179117	0.550945505967300	1	1	1
42	0.542497790199832	0.292512489800104	0.551351426786555	1	1	1
42	0.545045108892152	0.458386790511690	0.551936563170047	1	1	1
42	0.540498058332924	0.625455608851050	0.553222748586263	1	1	1
42	0.541947282003755	0.792543508913689	0.551108095399191	1	1	1
42	0.541988169734908	0.960156477095026	0.551034103176717	1	1	1
42	0.709225584656740	0.126479240179564	0.549201103853652	1	1	1
42	0.709711161203479	0.293135623692040	0.550568648996972	1	1	1
42	0.710457015139283	0.460091619409577	0.550746974999619	1	1	1
42	0.709299666751374	0.626351233661411	0.548616125979592	1	1	1
42	0.708303364942625	0.792367231415823	0.549635384550554	1	1	1
42	0.709176701285274	0.959631165129993	0.550970963078264	1	1	1
42	0.876114309145017	0.126760188582171	0.551689744076611	1	1	1
42	0.876212535879173	0.293828064669667	0.550853825886669	1	1	1
42	0.876352996137254	0.460088612151389	0.550991790770637	1	1	1
42	0.876371488364020	0.626655358885529	0.550548771335056	1	1	1
42	0.875643814931407	0.792948905426315	0.550015385185192	1	1	1
42	0.875567542880225	0.959835060166257	0.550545641044351	1	1	1