

Electronic Supplementary Information

**Ab Initio Molecular Dynamics Simulations on the Adsorption of
1-Hydroxyethane-1,1-Diphosphonic Acid on Iron (100) Surface**

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1. The Cartesian coordinates of CH₃C(OH)(PO₃H)₂- 2-, in angstroms

Charge: -2 Spin: Singlet

C	-0.00110900	0.61301400	0.00602100
O	0.07148100	1.15173600	1.37656100
H	0.54498400	0.43301700	1.84191200
C	0.02812400	1.79423600	-0.96165900
H	-0.85275400	2.41720100	-0.79470100
H	0.93926000	2.38184600	-0.83124500
H	0.00011700	1.42048200	-1.98772000
O	-2.70735000	0.91847000	0.00333700
O	-1.80326900	-1.13343300	-1.32666600
O	2.72991200	0.81605700	-0.13572800
H	2.69395300	1.23474700	0.73204100
O	1.78819500	-1.18936700	-1.34098000
P	-1.71688900	-0.20084300	-0.16870900
O	-1.76436100	-1.12062600	1.21442800
P	1.58200200	-0.41905600	-0.08947700
O	1.71219600	-1.01012900	1.29697700
H	-1.67877000	-0.49397400	1.94289500

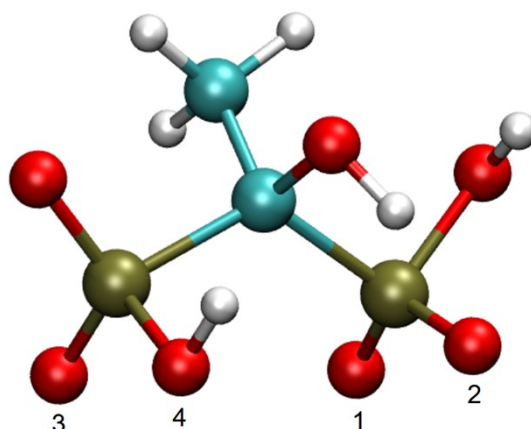


Figure S1. The optimized structure of the deprotonated HEDP

2. The Cartesian coordinates of Snapshots of Fe–HEDP–water model along the simulation trajectory, in angstroms. The parameters of supercells: 11.466 nm × 11.466 nm × 24.300 angstroms, $\alpha = \beta = \gamma = 90^\circ$.

(a) 0 fs

H	10.6124370000	1.5359540000	8.2568930000
H	1.4414420000	4.5029000000	8.2881410000
H	6.9142400000	9.6374510000	8.4265400000
H	9.6988060000	3.9861780000	8.5213210000
H	1.8560440000	3.0550030000	8.7160080000
H	3.7431500000	9.8213800000	8.8272550000
H	9.3515560000	10.6855970000	8.8551630000
H	7.8448180000	1.5083900000	9.0493560000
H	1.5195720000	11.7099550000	9.1300650000
H	9.6796030000	7.1561630000	9.3131530000
H	11.0693710000	6.4343480000	9.3184460000
H	10.6340790000	10.0111450000	9.4482180000
H	6.2305770000	8.7003810000	9.4771130000
H	2.5217720000	6.2698230000	10.1428200000
H	3.3391850000	9.1986590000	10.2060850000
H	1.3379380000	11.1534620000	10.5822400000
H	3.4467250000	2.9402280000	10.7910010000
H	10.3821900000	0.9265670000	10.8121840000
H	12.1763790000	8.4384500000	10.9508100000
H	6.3622180000	6.0219440000	10.9634550000
H	8.5403740000	8.8230870000	11.0265350000
H	1.4910710000	5.6096410000	11.1188010000
H	10.0514610000	4.6361020000	11.1834690000
H	9.0152560000	1.1030170000	11.5517100000
H	0.7664240000	3.0663600000	11.5659010000
H	11.0107220000	7.7388050000	11.7283420000
H	9.1480760000	9.9524980000	11.9216910000
H	6.7403850000	2.1621710000	11.9962540000
H	5.5418480000	8.8919040000	12.0135570000
H	4.2932010000	3.8508000000	12.0976390000
H	4.3056400000	2.0497100000	12.1021710000
H	8.9108700000	4.8530090000	12.2345270000
H	3.5001310000	10.9141370000	12.2426830000
H	4.3514070000	7.9234200000	12.3222940000
H	1.6207470000	3.2732120000	12.8608120000
H	11.4466370000	-0.2097470000	12.9229200000
H	7.9185640000	7.1933060000	13.0204430000
H	5.9247560000	0.0306730000	13.2178800000
H	2.6893250000	11.7793730000	13.2648720000

H	11.4900490000	5.3510180000	13.3025250000
H	6.2181810000	5.1174790000	13.4245210000
H	7.4515750000	-0.0199870000	13.5580300000
H	9.9672580000	2.8955470000	13.7258950000
H	10.2087820000	0.0665210000	13.8407890000
H	8.4879100000	2.4143370000	13.8967440000
H	5.9880130000	3.7739230000	14.1958670000
H	3.8210400000	6.0861540000	14.3032660000
H	8.3190950000	6.9264670000	14.5098350000
H	3.3874490000	4.6047830000	14.5631860000
H	10.6027240000	5.4065660000	14.5908490000
H	0.8520310000	1.8274850000	15.2383600000
H	1.6733440000	2.7954780000	16.1551230000
C	5.6224220000	2.9605600000	10.6182340000
C	4.3383990000	2.9490020000	11.4522500000
O	7.0653910000	1.3258440000	8.4667760000
O	4.4775120000	4.5144220000	8.5263800000
O	4.3969710000	1.3140220000	8.5572130000
O	10.1372630000	10.1393140000	8.6016030000
O	6.8937620000	4.5471500000	8.6282290000
O	10.4330710000	6.9036610000	8.7225760000
O	6.8827890000	8.6961770000	8.7326850000
O	1.1545320000	3.7402170000	8.8505830000
O	3.3117460000	9.0268990000	9.2313400000
O	1.7257480000	11.9115400000	10.0773060000
O	5.5892800000	6.0302320000	10.3446260000
O	5.6724940000	0.0639720000	10.3645550000
O	2.4263110000	5.9301450000	11.0679030000
O	9.7306320000	1.6146170000	11.0979360000
O	9.1559090000	5.0438110000	11.2944690000
O	8.3460470000	9.7235770000	11.3890090000
O	6.7474610000	2.9941010000	11.4557190000
O	11.7402110000	8.3991060000	11.8388630000
O	1.0455360000	2.6123500000	12.3999580000
O	5.1807590000	8.2946290000	12.7155560000
O	2.9776860000	10.8501820000	13.0811780000
O	8.4470720000	7.5695560000	13.7681490000
O	11.0735280000	-0.4148550000	13.8167110000
O	6.5583570000	-0.2138860000	13.9382830000
O	11.3213360000	5.8925250000	14.1139130000
O	3.0656610000	5.4583860000	14.1788310000
O	6.4921590000	4.6250010000	14.2385260000
O	9.2526350000	2.7873890000	14.4024210000
O	0.8232820000	2.7270290000	15.6517900000

P	5.6910180000	1.4443920000	9.5203150000
P	5.6451680000	4.4891860000	9.5481660000
Fe	1.4332000000	1.4332000000	2.0000000000
Fe	4.2996000000	1.4332000000	2.0000000000
Fe	7.1660000000	1.4332000000	2.0000000000
Fe	10.0324000000	1.4332000000	2.0000000000
Fe	1.4332000000	4.2996000000	2.0000000000
Fe	4.2996000000	4.2996000000	2.0000000000
Fe	7.1660000000	4.2996000000	2.0000000000
Fe	10.0324000000	4.2996000000	2.0000000000
Fe	1.4332000000	7.1660000000	2.0000000000
Fe	4.2996000000	7.1660000000	2.0000000000
Fe	7.1660000000	7.1660000000	2.0000000000
Fe	10.0324000000	7.1660000000	2.0000000000
Fe	1.4332000000	10.0324000000	2.0000000000
Fe	4.2996000000	10.0324000000	2.0000000000
Fe	7.1660000000	10.0324000000	2.0000000000
Fe	10.0324000000	10.0324000000	2.0000000000
Fe	0.0000000000	0.0000000000	3.4332000000
Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
Fe	2.8664000000	2.8664000000	3.4332000000
Fe	5.7328000000	2.8664000000	3.4332000000
Fe	8.5992000000	2.8664000000	3.4332000000
Fe	0.0000000000	5.7328000000	3.4332000000
Fe	2.8664000000	5.7328000000	3.4332000000
Fe	5.7328000000	5.7328000000	3.4332000000
Fe	8.5992000000	5.7328000000	3.4332000000
Fe	0.0000000000	8.5992000000	3.4332000000
Fe	2.8664000000	8.5992000000	3.4332000000
Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
Fe	1.4332000000	1.4332000000	4.8664000000
Fe	4.2996000000	1.4332000000	4.8664000000
Fe	7.1660000000	1.4332000000	4.8664000000
Fe	10.0324000000	1.4332000000	4.8664000000
Fe	1.4332000000	4.2996000000	4.8664000000
Fe	4.2996000000	4.2996000000	4.8664000000
Fe	7.1660000000	4.2996000000	4.8664000000
Fe	10.0324000000	4.2996000000	4.8664000000
Fe	1.4332000000	7.1660000000	4.8664000000
Fe	4.2996000000	7.1660000000	4.8664000000

Fe	7.1660000000	7.1660000000	4.8664000000
Fe	10.0324000000	7.1660000000	4.8664000000
Fe	1.4332000000	10.0324000000	4.8664000000
Fe	4.2996000000	10.0324000000	4.8664000000
Fe	7.1660000000	10.0324000000	4.8664000000
Fe	10.0324000000	10.0324000000	4.8664000000
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Fe	8.5992000000	0.0000000000	6.2996000000
Fe	0.0000000000	2.8664000000	6.2996000000
Fe	2.8664000000	2.8664000000	6.2996000000
Fe	5.7328000000	2.8664000000	6.2996000000
Fe	8.5992000000	2.8664000000	6.2996000000
Fe	0.0000000000	5.7328000000	6.2996000000
Fe	2.8664000000	5.7328000000	6.2996000000
Fe	5.7328000000	5.7328000000	6.2996000000
Fe	8.5992000000	5.7328000000	6.2996000000
Fe	0.0000000000	8.5992000000	6.2996000000
Fe	2.8664000000	8.5992000000	6.2996000000
Fe	5.7328000000	8.5992000000	6.2996000000
Fe	8.5992000000	8.5992000000	6.2996000000

(b) 75 fs

H	11.4073176871	1.1331082719	6.4943041314
H	1.8447051352	4.2565627874	8.9156741366
H	5.9606283510	8.9184609534	9.3714715955
H	10.0415731474	3.0159940883	5.5682368124
H	1.1572300452	2.9148611568	9.3396449358
H	4.0371267062	9.9430641791	9.2246854352
H	9.5185056598	9.9022700745	9.6770108964
H	7.4662289774	2.3764033837	8.7594381387
H	1.7302721876	12.0299638253	8.8830394064
H	10.0392099914	7.7046358302	8.8240824234
H	9.9463868868	6.4725200597	9.8134882300
H	10.9605912068	9.6190099864	9.3301244072
H	6.4652915831	7.6078094998	8.8283992232
H	3.4790407785	6.0803782467	10.6122670720
H	3.7136776936	9.2127751712	10.5095068934
H	1.9727143404	11.5619636747	10.3076739606
H	3.2049126861	2.8466479544	10.4109623514
H	10.5861108480	2.0335736513	11.5131648102
H	11.8728785093	7.4707010341	12.4976104255
H	6.7449887755	5.8976650256	10.7247419414

H	8.0580929779	9.2515943740	12.3859962980
H	2.2036477697	5.4862547132	11.2593899757
H	9.0283511956	4.4013480508	10.7406726500
H	10.1173241780	0.8744067159	10.6954065234
H	1.5110776407	2.2656140484	12.6728132927
H	11.2148725668	8.8505223552	12.5184612512
H	9.4465414120	9.2181193040	11.8282116004
H	7.0850117471	2.1907498623	11.1324863625
H	4.5376872173	8.4310476083	13.1036200046
H	3.8904620000	4.0279937518	11.5376069160
H	3.9813396552	2.3279197788	11.9395336186
H	10.0229960665	5.2921769879	11.5546384525
H	2.1737805095	11.0206761591	13.3090939794
H	4.8815958537	7.2055921288	12.2226555823
H	0.3985751233	3.0990339963	13.3117518291
H	10.0422161035	-0.8395164129	13.0138096995
H	7.9245565379	7.0680355927	15.0628477186
H	5.7776531714	-0.5030843192	13.6967896691
H	2.2982645181	9.7502138357	12.5145717302
H	11.4449624751	6.1673437909	14.8102521249
H	5.9960662529	4.3866993762	13.1191608426
H	6.5803155579	0.1833316025	12.6939027267
H	9.8799173736	2.8362388848	14.8597684610
H	10.4614086569	-0.0534744133	14.2319164601
H	9.7781920741	1.7057904165	13.7911213809
H	6.1918323666	4.2310240613	14.6561654858
H	2.7389417637	5.3922386906	13.8564294944
H	7.0726267063	7.0363282966	13.8372228072
H	3.8822075376	5.1303265388	14.8300018682
H	10.6449210041	6.7284339490	13.6449358676
H	0.9403090754	2.9133285763	16.6544965194
H	1.4262773372	3.7381221837	15.4437426770
C	5.3914931939	2.9377679018	10.3578064190
C	4.0201025188	3.0217095718	11.0975177169
O	7.1880436712	1.4354797779	8.9647868589
O	4.6694376309	4.8472705744	8.3106480879
O	4.5323722150	1.0885323338	8.2633402746
O	10.1938672455	10.1043532455	9.0068465130
O	7.1028917123	4.3520740891	8.5424477293
O	10.4477302727	6.8270155581	9.0040143379
O	6.5983324575	8.5731789418	8.7169459347
O	1.0361731232	3.7158471049	8.7697737109
O	3.7068453796	9.0906881274	9.5516463511
O	1.2780957613	12.0109887079	9.7803034129

O	5.8509603218	5.4556198785	10.5775948029
O	5.4381851672	0.2374999628	10.4825451032
O	2.7859670372	6.2713668404	11.2438681303
O	9.7604419589	1.6346480907	11.1824848080
O	9.3637332287	5.2936167238	10.8826608105
O	8.6607850554	9.8069596098	11.8549021497
O	6.5186181937	2.9943454610	11.2377677253
O	11.5810098259	8.2034852645	11.9153324780
O	0.9370445663	3.0246589414	12.5434876683
O	5.1203654002	8.1093367319	12.4452543693
O	2.8243531182	10.5617849899	12.7370768127
O	7.9580606122	7.2739143383	14.1298416292
O	10.8391784040	-0.4488101385	13.4491735178
O	6.6589134667	-0.1368225330	13.6050145199
O	11.3934661743	6.1155166199	13.8471382159
O	3.0561600252	5.6762706317	14.7411692292
O	5.9368431113	4.8414278519	13.9634799169
O	9.2763522398	2.4118001059	14.2315704389
O	0.9234275151	2.9340235554	15.6885113316
P	5.6056757340	1.2615336144	9.4399287752
P	5.7569193138	4.4127585329	9.2863881076
Fe	1.4332000000	1.4332000000	2.0000000000
Fe	4.2996000000	1.4332000000	2.0000000000
Fe	7.1660000000	1.4332000000	2.0000000000
Fe	10.0324000000	1.4332000000	2.0000000000
Fe	1.4332000000	4.2996000000	2.0000000000
Fe	4.2996000000	4.2996000000	2.0000000000
Fe	7.1660000000	4.2996000000	2.0000000000
Fe	10.0324000000	4.2996000000	2.0000000000
Fe	1.4332000000	7.1660000000	2.0000000000
Fe	4.2996000000	7.1660000000	2.0000000000
Fe	7.1660000000	7.1660000000	2.0000000000
Fe	10.0324000000	7.1660000000	2.0000000000
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Fe	4.2996000000	10.0324000000	2.0000000000
Fe	7.1660000000	10.0324000000	2.0000000000
Fe	10.0324000000	10.0324000000	2.0000000000
Fe	0.0000000000	0.0000000000	3.4332000000
Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
Fe	2.8664000000	2.8664000000	3.4332000000
Fe	5.7328000000	2.8664000000	3.4332000000

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Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
Fe	1.5754629089	1.5015336408	5.0739506068
Fe	4.4120874980	1.4642436372	5.1774306505
Fe	7.4054213777	1.7236917899	5.0591138623
Fe	9.7202284989	1.3095307901	5.0895066993
Fe	1.5612362923	4.4060101068	5.0299547642
Fe	4.3548027489	4.2928388278	5.0589493014
Fe	7.0889212049	4.3256954886	4.8694121456
Fe	9.8476805694	4.6214248959	4.9187190477
Fe	1.3480361290	7.1177319295	5.2078600222
Fe	4.4855784222	7.1277163773	5.0403762332
Fe	7.2635837267	7.0604695556	4.9876392964
Fe	9.8795164821	7.0987846564	5.0775680967
Fe	1.4883388449	10.0202432759	5.0603609830
Fe	4.5037783249	10.0654916176	5.1427932156
Fe	6.9465749795	9.9284384564	5.0549016985
Fe	9.8870143683	10.2356021997	5.0294230232
Fe	0.0134594923	-0.1325786208	5.8898895462
Fe	2.9019229432	0.0105372376	5.7777677960
Fe	5.9574039174	0.1555694140	5.8940094572
Fe	8.3883192673	-0.0647829892	5.9390119967
Fe	0.0850731481	2.8212517974	6.4053911420
Fe	2.9104731888	2.9801527170	5.8290024998
Fe	5.6914526870	2.8583875435	6.0993090447
Fe	8.6837067503	3.0188794743	6.0463058109
Fe	-0.0225843793	5.5842870420	5.8580228741
Fe	2.9790463961	5.7996017497	5.9191811093
Fe	5.5867191454	5.6428617395	6.1618074050
Fe	8.4663787198	5.6904403752	6.0649083187
Fe	-0.1309738193	8.6400522887	5.7020399097
Fe	2.8823267624	8.5672520363	5.6734423783
Fe	5.8125653646	8.4325499449	5.9964256943
Fe	8.5571019443	8.6777713440	5.7913904888

(c) 107 fs

H	11.0980519621	1.7779833238	7.4242471697
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H	1.7828175163	3.6141257899	8.3193140796
H	5.3744152601	8.7414113008	8.6442993936
H	10.1948065315	3.4523355154	5.7880661703
H	0.7292782580	2.6968291070	8.9206370425
H	4.4485832220	10.1030291719	10.0069294105
H	9.4669159231	10.1306555413	9.8225905670
H	7.2882364172	2.2963303384	8.6781234773
H	1.8055512945	11.5140003942	9.1118885250
H	10.2455824708	7.6375836929	9.1960876999
H	10.4206292714	6.1405503960	9.4760271566
H	11.0288819652	10.3062430679	9.5853653323
H	6.5621817836	7.7003720119	8.9333863025
H	2.7785387359	6.7061079240	10.3554116081
H	4.2804037230	8.6132119327	10.2948788731
H	1.5936492665	11.9740304741	10.6021964187
H	3.2431290143	2.9591698440	10.2481490832
H	10.5108560098	2.0828093017	11.7788418428
H	12.1694676253	7.7846042262	12.3349687412
H	6.4208788185	5.1736585498	11.0608782787
H	8.1041437176	10.2611450474	12.0705862111
H	2.2491891618	5.6318495772	11.3039698427
H	9.1419049572	4.4800783636	10.2584042976
H	10.2262292952	1.2002524416	10.4956182052
H	0.9616027684	2.2010725268	12.8916922884
H	11.6277590460	9.2390547079	12.4950502237
H	8.6439205244	8.7261691713	12.1710550405
H	7.2363688583	2.7807272002	10.9450696126
H	4.4016694773	8.3701760004	13.0076556048
H	4.0042006145	3.8245296857	11.5672680616
H	4.0060328735	2.0283198369	11.5011588576
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H	1.8677064828	9.9985482435	13.0909118517
H	4.6149077444	7.1669998509	12.1378863920
H	0.5640004069	3.5621407376	13.4342991638
H	10.1324678915	-0.9365058609	12.7768107349
H	7.3261238918	6.5872743360	14.7427176894
H	5.8070950690	-0.6985149668	13.3615217443
H	2.7683211840	9.9673598788	11.8068018376
H	11.5177269438	6.0648101664	14.7627383736
H	6.1137590277	4.2226175636	13.1545720686
H	6.5572454311	0.5398810953	12.8199451223
H	10.0236776001	2.5469365682	14.7701829817
H	10.5521922867	-1.1060314274	14.1721485380
H	9.5001855956	1.5052035422	13.7778422818

H	6.2766968942	4.3841489656	14.6165675894
H	2.4876269584	5.6211596382	14.0225982616
H	7.2685010231	7.4021200505	13.4555156523
H	3.9019504520	5.8914720432	14.5586598049
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H	1.0171281579	3.5235616487	16.4894971265
H	1.9156443129	3.0759073806	15.3135884333
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C	4.0908307052	2.9395584185	10.9122356662
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O	4.8470001098	5.0705044583	8.1453889161
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O	10.1920064052	10.0857801671	9.1396569488
O	7.1667015508	4.0223824825	8.5611621529
O	10.4636636341	6.7920079955	8.7807560739
O	6.3402761348	8.5482312430	8.4608787491
O	0.8618624097	3.6162678210	8.6130336166
O	3.9490019670	9.2996421499	9.6523255540
O	1.2743005141	12.0674202672	9.6763841050
O	6.0455867592	5.5936576209	10.2901333168
O	5.3822142915	0.0683016410	10.3462039328
O	2.9145416083	6.3299405746	11.2756660544
O	9.7924831650	1.7078066589	11.2113942469
O	9.2695587849	5.2178049467	10.8891342246
O	8.8606418150	9.6516587969	11.9455350671
O	6.3751298563	3.0497705515	11.3116030779
O	11.4880764644	8.3882104186	12.0007829137
O	0.9227131649	3.1334334055	12.6033871346
O	5.0744881715	8.0125055132	12.3594509591
O	2.6214612835	10.4321208113	12.6493830170
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O	9.2708022019	2.3867225375	14.1619794573
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Fe	7.1660000000	1.4332000000	2.0000000000
Fe	10.0324000000	1.4332000000	2.0000000000

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Fe	7.1660000000	4.2996000000	2.0000000000
Fe	10.0324000000	4.2996000000	2.0000000000
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Fe	8.5992000000	0.0000000000	3.4332000000
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Fe	8.5992000000	2.8664000000	3.4332000000
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Fe	2.8664000000	5.7328000000	3.4332000000
Fe	5.7328000000	5.7328000000	3.4332000000
Fe	8.5992000000	5.7328000000	3.4332000000
Fe	0.0000000000	8.5992000000	3.4332000000
Fe	2.8664000000	8.5992000000	3.4332000000
Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
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Fe	4.3970678481	1.4352369939	4.9169787113
Fe	7.2505007825	1.7897382005	4.9865386342
Fe	9.8312325955	1.3109969837	5.0368073736
Fe	1.5138465603	4.4053560744	5.0047928202
Fe	4.4221589628	4.2825165221	4.8372980991
Fe	7.0261263460	4.2978876395	4.9138278536
Fe	9.8406834143	4.5451112228	4.7903925623
Fe	1.3563498496	7.1463966064	4.9861572040
Fe	4.5178105131	7.1245011354	4.8947203531
Fe	7.1530014170	6.9134117652	4.9585263674
Fe	9.8181678773	6.9770863223	4.9604731087
Fe	1.4935936307	9.9752484300	4.8138806825
Fe	4.6035119250	10.1023842890	5.0283336116
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Fe	8.1953282834	-0.1109852030	5.9170346771
Fe	0.1251000271	2.9547792207	6.2805848883
Fe	3.0101599809	2.9722797391	5.8374037655
Fe	5.7826166072	2.9011489774	6.0679390155
Fe	8.6093394762	3.2625429882	5.9807968112
Fe	-0.0335242289	5.5409657776	5.8380302826
Fe	2.9976209695	5.7869805126	5.7810663134
Fe	5.7601216351	5.5752720969	6.2299275095
Fe	8.3062221728	5.6870393351	6.2092690164
Fe	-0.1921182563	8.6360278820	5.6724304555
Fe	2.9618331004	8.5896077641	5.6898525953
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(d) 265 fs

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H	1.2878878393	2.7152687653	8.1655929635
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H	9.7270978997	10.7007119026	9.3975781553
H	7.9896557088	2.1545547519	8.9749108923
H	2.0601942263	11.6174769398	8.9798586929
H	10.0677269929	7.4976660358	7.8460165840
H	10.3566456570	7.2376909338	9.2977389021
H	11.3105518208	10.7347452519	9.3612628713
H	6.0996704989	7.4156315473	8.0915163795
H	1.4792741418	6.8636231487	11.4882135012
H	5.0281357720	8.9441107145	10.5330050947
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H	3.8278945398	3.8444396813	8.8429722772
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H	11.4456486529	7.5118106910	12.6717887091
H	7.7589069656	5.4149151790	10.6790403966
H	8.1048001555	10.2446642000	12.3309599412
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H	1.8758066494	9.6989822122	12.3500999111
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H	0.5949065606	4.2457864955	12.6533188448
H	10.1234042703	-0.8407393878	13.8504042132
H	6.5701533705	7.1392687431	13.3657985679
H	5.7908053450	0.4163434621	13.0054718073
H	2.8673862439	9.6500288940	11.1205734384
H	10.9533933802	5.4377651438	14.4904120147
H	5.7297729946	4.3560899288	12.9522573271
H	5.6938655922	0.1472675271	11.4896540725
H	10.2973957360	2.6791122287	14.7586519538
H	10.1941706857	0.6688456629	14.0486276824
H	9.6547943197	2.2680347171	13.4052995383
H	6.2856128244	4.7348076307	14.3075859224
H	2.8543838532	5.6249498777	13.9154236893
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H	4.1293534122	5.1622378709	14.5902331153
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H	1.9832584345	4.2394216482	15.1451460128
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C	4.1487656653	3.7163298946	9.8923043895
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O	10.5348274271	10.1466892607	9.4875460542
O	7.9318124659	4.2325718014	8.5308638394
O	10.4077581906	6.7966839141	8.4339306581
O	5.8515852557	8.3249776824	7.8922029171
O	0.3555870167	2.8653627870	7.9148284730
O	4.5866347775	9.3757888697	9.7925788735
O	1.2850407559	11.7186220194	9.5392099760
O	6.8551724816	5.6744583712	10.3079634975
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O	9.0810810599	4.8809082464	11.1002081004
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O	10.7686574792	-0.1070188723	13.8298674812
O	6.2714147185	0.0343489737	12.2597643217
O	10.9246567091	5.7031428657	13.5459562603
O	3.1904323462	5.3917099979	14.8145181439
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O	1.0962157718	3.8797206102	15.3939485803
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Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
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Fe	5.7328000000	2.8664000000	3.4332000000
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Fe	4.2811253608	1.4831259311	4.3082177775
Fe	7.2253450235	1.5841119096	4.6522981398
Fe	10.2784330884	1.0599453687	4.9727461086
Fe	1.4116569157	4.2550059027	4.4604611803
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Fe	4.5762898874	7.0422096341	5.0204880115
Fe	7.0684042304	6.8298638075	5.2516863512
Fe	9.6424334742	6.9962063628	4.9567735528
Fe	1.4883801036	9.9289245873	4.4308046331
Fe	4.4218204305	9.8423114952	4.8694068343
Fe	7.0244161022	10.0829963203	4.5936502765
Fe	9.9297917021	10.0805754061	4.8680394295
Fe	0.3572348212	-0.3243280200	5.7147415294
Fe	2.9390268219	0.0550944309	5.7425762397
Fe	5.6363481731	0.2165879585	5.7891145231
Fe	8.3511512353	-0.0187401669	5.8716029924
Fe	-0.0864620592	3.2375946832	5.8640610274
Fe	2.9252478828	2.7189999466	5.7372939201
Fe	5.5546767065	2.7897243317	5.8606136614
Fe	8.7625092601	2.7341129100	5.8101505731
Fe	0.1027042073	5.8439889768	5.7344710340
Fe	2.7469376802	5.8093854812	5.8149677514
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(e) 524 fs

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H	9.9699828863	3.7501656001	6.7742746547
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H	5.4079744466	10.8653058372	9.6634512140
H	9.5819207429	9.4542056095	10.7309242081

H	8.4885811077	2.8094272053	8.4094648291
H	1.2710497978	11.3482481796	8.0267745633
H	10.2839581802	5.8673472664	9.2181248324
H	10.3828405729	7.2913072546	9.9633743957
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H	7.8527662573	10.3850368288	12.2289118576
H	2.9872798604	6.0568026117	11.5341876553
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H	10.3529649486	2.2548837189	10.7233059657
H	1.9929731213	3.9815766529	13.0832378686
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H	4.0200424476	2.3773137285	9.7177076326
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H	2.0984092456	10.8811222572	11.5503872069
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H	8.4217257128	1.2071888974	13.0216485782
H	5.8291675483	8.1150584492	13.3702513299
H	5.5690500663	0.4639572542	12.9063387042
H	3.2674794882	10.8836912891	10.4416340588
H	10.7619165805	5.1642581452	14.8339158952
H	6.3063714203	4.6647298065	13.0951963785
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H	10.7718530779	2.8204848801	15.9067437183
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H	6.2319104215	8.0280182875	14.9155521850
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O	5.9559197202	8.5265240514	7.8967998310
O	0.4930703794	3.2411272136	7.9590332935
O	4.6003231109	10.2519517682	9.5406464881
O	0.9301168162	11.8814144788	8.7971267542
O	7.0457100294	5.7295587501	10.3409216753
O	6.5960718796	0.5356849951	9.8431582326
O	3.1993111742	6.6707618724	12.2485065465
O	10.6989008666	3.1653498398	10.6533841660
O	9.3461025511	5.0144244468	11.8120749813
O	8.4790306817	9.6348394437	12.1843380009
O	6.0578386944	3.1597273701	11.1259982289
O	12.5858020317	8.0861392856	12.7390893234
O	1.2438704138	4.0345164073	12.4448333639
O	4.7646867789	8.8448213833	11.8994886913
O	2.5079543138	11.3988169675	10.8411739261
O	6.4141619113	7.6670257932	14.0337460317
O	9.3828300096	1.3494027998	12.9234571118
O	6.4671409061	0.2431243537	12.6198216001
O	10.7539262775	5.9955155672	14.2982623004
O	3.2165625948	4.5753074486	14.4084658841
O	6.1238195592	4.7527139679	14.0548244089
O	9.8585780619	2.4892141380	15.7602125739
O	0.9116648977	3.9045256954	15.8144638076
P	6.7177931805	1.7652586632	8.9436580357
P	6.7570262659	4.8432558751	9.0703180048
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Fe	7.1660000000	1.4332000000	2.0000000000
Fe	10.0324000000	1.4332000000	2.0000000000
Fe	1.4332000000	4.2996000000	2.0000000000
Fe	4.2996000000	4.2996000000	2.0000000000
Fe	7.1660000000	4.2996000000	2.0000000000
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Fe	1.4332000000	7.1660000000	2.0000000000
Fe	4.2996000000	7.1660000000	2.0000000000

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Fe	4.2996000000	10.0324000000	2.0000000000
Fe	7.1660000000	10.0324000000	2.0000000000
Fe	10.0324000000	10.0324000000	2.0000000000
Fe	0.0000000000	0.0000000000	3.4332000000
Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
Fe	2.8664000000	2.8664000000	3.4332000000
Fe	5.7328000000	2.8664000000	3.4332000000
Fe	8.5992000000	2.8664000000	3.4332000000
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Fe	2.8664000000	5.7328000000	3.4332000000
Fe	5.7328000000	5.7328000000	3.4332000000
Fe	8.5992000000	5.7328000000	3.4332000000
Fe	0.0000000000	8.5992000000	3.4332000000
Fe	2.8664000000	8.5992000000	3.4332000000
Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
Fe	1.4616339415	1.6136473478	4.8036102957
Fe	4.1701132516	1.4080923640	4.4956922797
Fe	7.0709452296	1.4645157126	4.5023142537
Fe	10.1896597119	1.3079481323	5.0058919318
Fe	1.4731486491	4.2019182708	4.4174491305
Fe	4.4738885845	4.5653079624	4.9188379059
Fe	7.0014053512	4.4723115829	4.8561693516
Fe	10.0026937242	4.4231304138	4.6749396735
Fe	1.5240927775	7.1109681388	4.4128639224
Fe	4.7487443973	7.0198019693	4.9855234549
Fe	7.1144378709	6.8292432827	5.0192457820
Fe	9.6888972605	6.7756446904	5.0096074372
Fe	1.3217052995	9.6555185253	5.0707298254
Fe	4.5932107048	9.8674964556	4.9586262435
Fe	7.0435975185	10.0655552027	4.8177487485
Fe	10.1890587695	10.1395173077	4.8574094449
Fe	0.4243031514	-0.0123003213	5.8994219215
Fe	2.9028432809	-0.0504427608	5.6987215606
Fe	5.8082559741	0.0465376700	5.9817847840
Fe	8.4073458885	0.1414936737	5.7617544577
Fe	0.0843297942	3.1171625184	5.9576543855
Fe	3.0677841071	3.0061531369	5.7684785257

Fe	5.6791612141	2.8061868272	5.8099534105
Fe	8.5619701958	2.8274902808	5.7691617027
Fe	0.2056579643	5.6353494673	5.7320328219
Fe	2.8419501367	5.8793156012	5.8084709534
Fe	5.8450227310	5.5373003044	6.4714143705
Fe	8.5024897753	5.1976058414	6.3353099539
Fe	-0.1785211578	8.1402299853	5.7884780757
Fe	2.8749333600	8.5612970307	5.8212672958
Fe	6.1790798835	8.5518062917	6.0131298142
Fe	8.6655926823	8.5660253233	5.7279549318

(f) 671 fs

H	9.5661905275	-1.3421360865	6.3657993933
H	-0.3980929871	1.8787239323	8.1821913653
H	5.6344013432	9.2452276024	8.6286287758
H	10.3779055549	5.7501413029	7.1240949377
H	-0.6686849998	3.2186276140	8.8901523496
H	5.3734769992	10.9874260272	10.1049925883
H	10.6293703009	9.7677427433	11.1913664288
H	8.4005434007	3.0923173751	8.4717369785
H	2.1656781988	10.6007631803	7.8698878108
H	10.0207801548	6.0799805697	9.3730489665
H	10.8256973843	7.3017317131	9.9356478717
H	11.3680063132	9.5719774838	9.7781701971
H	5.7371870633	7.7110138256	8.3541031072
H	2.4519901569	7.6644918489	12.3886084189
H	4.7631312089	9.7809347017	10.9085632990
H	1.6960616332	11.9095499040	8.4762506097
H	4.2470842144	3.9381952730	9.5903892513
H	11.5934455925	3.3518300170	11.1830200681
H	11.9116219017	7.5311774467	13.1656210367
H	7.6991421453	5.9463892242	11.1022001268
H	9.4393226554	11.3940163911	12.5659026449
H	3.1069569716	6.6747797115	11.4040681539
H	9.7978537335	5.5590013049	11.6873020540
H	10.3546643717	2.3212568364	11.1555699575
H	2.0326259177	3.9223537630	12.4254457367
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H	8.1324130350	3.1216428915	10.8353043550
H	4.7472330180	9.3775817893	13.0943703208
H	4.6898376964	4.3090424409	11.2889033785
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H	9.1253820093	4.4353207749	12.4061285533

H	1.9589078862	12.0993154739	10.7134769463
H	4.4448254383	8.1271329642	12.3409393957
H	0.9783223862	5.0727876700	12.6125815753
H	8.2557290826	2.0211446591	13.2079137245
H	6.0633194598	7.7387543873	13.8870932898
H	5.9284867757	1.0244442251	13.2240274179
H	3.3514051196	11.4651242102	10.3752139936
H	11.7222480530	5.5430395318	14.8438184663
H	6.4252451539	4.3328318534	13.2052480993
H	6.6647300146	1.0314473608	11.8323369343
H	11.3513171155	3.0728975106	15.1779158813
H	9.7408293385	2.3999443734	13.4355509222
H	10.8484294543	1.6469048034	15.5311798815
H	6.3928473947	5.3667840329	14.3019709726
H	3.1388199169	5.6258483728	13.8027776146
H	6.2567920620	7.4336041492	15.4716383190
H	4.2580277249	4.5836776942	14.1884684271
H	10.4857327360	5.7596199067	13.7755114161
H	1.2555214923	5.1592500196	16.7075884783
H	2.1498940243	4.6063907348	15.4609422372
C	6.3510698313	3.5421405417	9.9277208682
C	4.8682229099	3.6295693536	10.4204657679
O	8.1112910015	2.1447708718	8.4948711203
O	5.6754311018	5.5773594153	8.3692150954
O	5.6465475582	1.9755838353	7.7055272270
O	11.3603880645	9.2907537627	10.7102843753
O	8.2030556918	5.0480797225	8.4860372892
O	10.6819614861	6.3459637411	10.0363962812
O	6.0941160466	8.5838091103	8.0684517705
O	-0.3303248828	2.8224388051	8.0370500218
O	4.6668839940	10.3017633695	10.1013699525
O	1.3274531452	11.0696375658	8.0513302273
O	6.9393355430	6.0684812312	10.4575775811
O	6.5505067173	0.7653389541	9.8797385901
O	3.2235707197	7.0085970492	12.3066168316
O	10.7978748037	3.0517058475	10.6925810064
O	9.1590651834	5.4109232365	12.4098637710
O	9.4630609907	10.4298888673	12.4167190343
O	7.2254927419	3.3393356266	11.1007061457
O	12.3458243289	8.3634283575	12.9006155500
O	1.2466886152	4.3241894107	12.0233501148
O	5.1867968481	8.7560905932	12.5008685291
O	2.8062609150	12.2873132737	10.2769445517
O	6.3856679663	7.1160591796	14.5667232299

O	9.0432011055	2.3943361557	12.7269001323
O	6.5566789544	0.5073706883	12.6893688765
O	11.4340891369	5.8496596108	13.9377185150
O	3.2664718543	4.7676833361	14.2594121368
O	6.0332702062	4.4736794456	14.0865846172
O	10.9543983300	2.2659864267	14.7836608962
O	1.2276155517	4.6081949366	15.9034446522
P	6.5450742905	1.9640921225	8.9671881011
P	6.8993218174	5.1141345096	9.2198788001
Fe	1.4332000000	1.4332000000	2.0000000000
Fe	4.2996000000	1.4332000000	2.0000000000
Fe	7.1660000000	1.4332000000	2.0000000000
Fe	10.0324000000	1.4332000000	2.0000000000
Fe	1.4332000000	4.2996000000	2.0000000000
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Fe	10.0324000000	4.2996000000	2.0000000000
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Fe	10.0324000000	7.1660000000	2.0000000000
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Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
Fe	2.8664000000	2.8664000000	3.4332000000
Fe	5.7328000000	2.8664000000	3.4332000000
Fe	8.5992000000	2.8664000000	3.4332000000
Fe	0.0000000000	5.7328000000	3.4332000000
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Fe	5.7328000000	5.7328000000	3.4332000000
Fe	8.5992000000	5.7328000000	3.4332000000
Fe	0.0000000000	8.5992000000	3.4332000000
Fe	2.8664000000	8.5992000000	3.4332000000
Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
Fe	1.2733902614	1.9497512780	5.1545223138
Fe	4.2944354922	1.4879203478	4.3851588666
Fe	7.0869483687	1.5620121786	4.4890324363

Fe	10.3462201812	1.3521966183	5.0896618325
Fe	1.4364118776	4.3661326062	5.1757922166
Fe	4.6084773023	4.5242749205	4.8984457909
Fe	7.0755156358	4.4239154209	5.0087100781
Fe	9.8362266431	4.4212316841	4.6176123308
Fe	1.3367462187	7.2147472336	4.8487464090
Fe	4.6810614327	7.0917422455	4.9312252732
Fe	7.0766634884	6.8499769214	5.0946930426
Fe	9.4793515987	6.9367897029	5.0975995493
Fe	1.3913819440	9.8997209854	4.5450093023
Fe	4.6029068997	10.0021154811	5.0076448490
Fe	7.1017581511	10.0027860659	4.5205472894
Fe	10.2401499600	10.5355120712	4.9359785442
Fe	0.6985290699	-0.0205171961	6.0412730204
Fe	2.9262863887	0.1332585751	5.6645064984
Fe	5.7742828162	0.1832072352	6.0019291509
Fe	8.4779665713	0.2136189187	5.7747432263
Fe	-0.4304830423	3.2738484239	6.1797707923
Fe	3.1362483777	2.9399387496	5.8199282376
Fe	5.7985339033	2.6948977137	5.8173104595
Fe	8.6099191129	2.8388145113	5.7969821645
Fe	-0.1072243795	5.8541387392	5.8581437924
Fe	3.0000353690	5.9019631578	5.7318147628
Fe	5.8068012115	5.5811448125	6.4433522251
Fe	8.6488568148	5.2073452179	6.5542505997
Fe	-0.4983983562	8.4887049642	5.6511709883
Fe	2.9241533927	8.5618975581	5.7586729118
Fe	5.9409411195	8.5860218953	6.0612688869
Fe	8.5311089469	8.9554274063	5.7418525465

(g) 1578 fs

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H	6.6694431506	9.1542139269	8.5894141779
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H	-1.3439423324	3.6026188833	8.2085670913
H	6.9864390431	11.3416190393	10.0477009096
H	11.7848448733	11.3140166224	12.7697570736
H	8.1555731925	1.4756731305	8.0181232419
H	0.0099837376	10.9234751111	8.8182484542
H	11.5924156023	8.9120313964	9.3898109854
H	11.4672816862	9.9583381934	10.6469331333
H	13.1770623375	10.9457855945	11.9347629420
H	5.8840259704	7.7181342861	8.5193898200

H	6.0675861895	8.8475700106	11.9180192550
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H	1.3623355706	11.6965147954	8.7095429186
H	4.7266544392	4.6955581466	10.2631664674
H	11.0085076952	3.8921051489	11.1111274956
H	13.8368882217	7.6349127622	13.5256980659
H	8.3284536060	6.7948204252	10.8555268926
H	11.2718784738	13.5978237120	13.9612642767
H	7.2588409878	9.6327135999	11.4380656572
H	10.2429223051	7.7434327413	11.1162918950
H	10.7286517695	2.5517304802	11.8028496055
H	-0.2084213895	5.0735663024	13.3431527048
H	13.3156198535	8.4591388731	12.3400234299
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H	9.8491490852	8.3264505038	13.5342451642
H	5.4089882754	4.6479327056	11.9063563482
H	4.8280748503	3.1512037932	11.0625932317
H	10.3102072123	6.3790902302	11.8372608439
H	3.4565469739	11.8597810886	9.9370268025
H	8.5128879308	7.8500047567	14.2392644926
H	0.8038967953	6.1073427740	12.7049721571
H	11.2890624073	4.3448389143	15.4048342898
H	10.4799830251	7.1669306776	15.0500825029
H	8.2297357054	0.0857682937	13.3963692141
H	3.4616804560	10.4462670647	9.3570736076
H	14.5072625305	7.0779191381	15.8094938847
H	7.7870798464	4.3286743783	12.7348537614
H	7.6367833383	0.9312991308	12.2657818078
H	14.9458852137	5.1447837658	15.8053695710
H	12.6884007538	4.0907366059	15.1144480864
H	14.9647430583	3.8001367410	14.9010511981
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H	10.8520493361	6.5014499825	16.4559256927
H	7.3083174471	6.1307666423	14.0211785157
H	12.9506201883	7.0984466096	15.4242408546
H	5.0312348753	6.8018545482	17.4973161916
H	5.6288663272	6.6552083823	16.0079273067
C	6.7153522386	3.9095966518	10.2329700522
C	5.3454247074	4.1108466878	10.9458899415
O	8.1625558612	1.9784279056	8.8600667928
O	6.0870300817	5.8640973394	8.4595176265
O	5.8759203955	2.7837700582	7.8866834122

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O	5.8923383462	1.2819272538	9.9553291353
O	6.9999601371	8.9964373907	12.1742586419
O	10.4430827246	3.1115780399	11.0502977315
O	9.6862113476	7.1697325407	11.7168165471
O	10.9663458953	12.9902253413	13.2259088040
O	7.7329151569	3.5322166390	11.2404015651
O	13.6160792699	7.5683451345	12.5600187078
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O	11.1356715301	6.4984787934	15.5457169626
O	11.8402939068	3.6054410809	15.0729390404
O	8.1426735762	0.9974585648	13.0713495208
O	13.8284018336	7.5907961637	15.3255879269
O	7.0977772526	7.0948732339	14.2642048276
O	7.9622710176	4.4499184036	13.7208379370
O	14.4301962062	4.4231689172	15.3967169945
O	4.8979253832	6.3806861706	16.6349294975
P	6.5914854516	2.4179396631	9.1860772041
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Fe	4.2996000000	1.4332000000	2.0000000000
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Fe	4.2996000000	4.2996000000	2.0000000000
Fe	7.1660000000	4.2996000000	2.0000000000
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Fe	10.0324000000	10.0324000000	2.0000000000

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Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
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Fe	8.5992000000	2.8664000000	3.4332000000
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Fe	8.5992000000	5.7328000000	3.4332000000
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Fe	8.5992000000	8.5992000000	3.4332000000
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Fe	4.2364362959	1.4713715110	4.6595047065
Fe	6.9624480409	1.4340347583	4.4211625456
Fe	10.2034994599	1.2373665369	4.9529997174
Fe	1.3606070293	4.0852268008	4.9757158052
Fe	4.6684004267	4.5086174349	5.0098905809
Fe	7.0924635413	4.5515579671	5.0467058584
Fe	9.6635633683	4.4283553733	4.9076551899
Fe	1.3767805149	7.1241398797	4.3586776844
Fe	4.5429298811	7.2249794024	5.1156747115
Fe	7.1691919471	6.9173779151	5.0337360621
Fe	9.7721251060	6.7414806756	5.1140574656
Fe	1.2318183769	10.0893691750	5.0511634957
Fe	4.4101947992	9.7166616274	5.0071006016
Fe	7.3055472608	10.1177176469	4.4617320404
Fe	10.1187416684	10.3542204780	5.0989019333
Fe	0.1578933352	0.2095276176	6.2823926676
Fe	2.9761495629	-0.2389319835	5.6705074397
Fe	5.7680021640	-0.0571961527	5.8294674598
Fe	8.2526395848	0.1298097789	5.8424701808
Fe	-0.1977756817	2.9258217937	5.9512971011
Fe	3.2247406170	3.1066461111	5.7815303401
Fe	5.8282770047	2.5437388329	6.0222462850
Fe	8.3569698200	2.7783430978	5.6840669878
Fe	0.2412397073	5.5010804260	5.7866344536
Fe	2.8546875004	5.7243482069	5.7805014052
Fe	5.8043274976	5.8889021211	6.4550350388
Fe	8.3807403565	5.5955392003	6.4914748640

Fe	-0.1042464421	8.3200178915	5.6880099891
Fe	2.7834539152	8.4481884147	5.7697542350
Fe	6.1130768922	8.8216085575	6.1250356384
Fe	8.7495348771	8.5020311021	5.8371814956

(h) 2161 fs

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H	5.7859553545	9.2599566956	8.5409120315
H	12.9310862963	5.4276104679	7.0496557984
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H	6.4312142118	10.9823834037	10.0233292667
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H	0.0706002731	9.4704092035	8.5638869308
H	11.4822486436	7.2980713695	7.8920198381
H	12.2982408729	7.2800352410	9.2120161596
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H	10.0441328745	7.6897522487	9.8557490475
H	11.1375252819	2.9137760299	11.0324349759
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H	14.5100999769	4.2426043024	14.9079142281
H	16.8626463358	4.0828697915	14.5179775780
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O	5.1515103832	8.7198741511	7.9579605278
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O	6.6958540304	10.0763897686	10.0529293856
O	0.1756706051	10.4099370587	8.3344829684
O	7.1903511174	6.6443746081	10.2945976152
O	6.5193464309	1.3474249922	9.9884411188
O	9.0294054496	9.5442606997	12.5497060474
O	10.8818142124	3.6097097737	10.4243381398
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O	8.0310962476	3.7897115945	10.9312629611
O	12.6292400635	8.2774453457	12.0697289817
O	0.9016974546	5.4721194638	12.2495786574
O	10.5728757941	8.4944240954	14.9220551880
O	3.6773110582	12.0495328564	8.1370927242
O	12.4550840861	9.6564690170	16.3359653714
O	13.6408154962	4.3714686414	14.4422624444
O	9.7795148822	0.5077199525	11.9338660855
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O	8.1628961723	6.6338614900	15.2789424705
O	9.3663837414	5.6927692127	12.8573535741
O	16.3240815924	3.5632842533	15.1345356078

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Fe	4.2590559043	1.5759685797	4.9708565044
Fe	7.2103606532	1.5113880346	4.3073988711
Fe	10.0547003137	1.2032586024	4.9575550588
Fe	1.4111681243	4.1932266280	4.3856841963
Fe	4.5552549458	4.3930536503	4.9006047277
Fe	6.9451381838	4.4264318343	4.9355947779
Fe	9.8427530291	4.4533148213	4.8927323014
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Fe	4.4866861744	6.8193363086	4.9329585762
Fe	7.1959125531	6.9988181447	5.0499127968
Fe	9.7369725661	6.9877862988	4.9869625531
Fe	1.2827126064	10.3387772535	4.9727339226
Fe	4.2511262717	10.3305254770	4.9939114152
Fe	7.0283315257	9.8913931851	4.4779287031
Fe	10.1886739847	10.2111686930	4.8692931777
Fe	-0.2625909193	-0.2279836226	6.4787630942
Fe	2.8184928766	0.3828920976	5.9918615588
Fe	6.0342356491	-0.0056501013	5.6665784131
Fe	8.3171177654	-0.0649852765	5.8805433665
Fe	-0.0821506461	3.0903526513	5.8723794295
Fe	2.7788659993	2.9819809963	5.7264760143
Fe	5.7212387670	2.7941749835	6.0713864419
Fe	8.4880353785	2.8161519006	5.7404738605
Fe	0.3548709509	5.9024789875	5.8117442384
Fe	2.7196561550	5.4592760842	5.8166881788
Fe	5.6665361201	5.7727958367	6.3243471214
Fe	8.3773384564	5.5043807195	6.3089344187
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Fe	3.0517051064	8.4723636046	5.6840221819
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(i) 2774 fs

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H	11.8032830268	12.3439544989	10.8112631527
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H	12.6663338011	2.4003512407	13.7303779029
H	13.0252920918	9.1674052719	14.4532888725
H	8.7026807384	-0.3451053731	11.7956482755
H	3.8674102664	11.6890097782	8.6574499587
H	16.2740366126	7.2548849255	14.2895902875
H	8.9330376580	4.8683103101	12.3666243240
H	8.0149598633	0.9060102092	10.7631750345
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H	14.9888247392	8.2735141300	14.4516288418
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H	6.5435316650	6.0854643470	15.8259065328
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C	5.5632091491	3.9993189111	10.8861743448
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Fe	10.1377674816	1.2576327998	5.0774815939
Fe	1.2855333102	4.2583274332	4.4520122349
Fe	4.6986730833	4.5311437929	4.9970847827
Fe	7.3007215367	4.5181330319	4.9321051931
Fe	9.9335208971	4.6505485951	5.0674582454
Fe	1.3533338011	7.2830553567	4.4109014951
Fe	4.6981356418	6.8589519014	4.9936621282
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Fe	9.7701317016	6.9890543471	5.0870400854
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Fe	9.9794949685	10.1606888524	4.5337300827
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Fe	3.1230401991	0.4992163237	6.1883373291
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Fe	3.0543925129	8.2901477530	5.6721737676
Fe	5.6341695417	8.7936400456	5.9642926420
Fe	8.4406963378	8.7457826015	5.8476469377

(j) 2808 fs

H	8.3336702295	-1.4172147470	6.8445027923
H	0.2875540329	3.6156861696	8.7431893511
H	6.2822339519	9.3928372252	8.7024559980
H	13.1802463980	5.8964090448	6.9735829697
H	1.4440083699	4.2079282248	7.7722640891
H	6.8877981177	11.3238992930	9.1940240107
H	9.9483733776	12.2565659802	10.8191302729
H	8.3378937545	1.6111873544	7.8442357412
H	0.1579984863	9.9317287744	8.4708532726
H	10.0725114040	7.8640454192	7.8538645494
H	11.5639296244	7.4965860472	8.2300879416
H	11.3170308757	11.8315660850	11.4966165926
H	5.7634812109	7.8502994830	8.4942841207
H	8.5164222162	9.1100196068	13.9277475662
H	7.9136804494	10.2857382785	8.7018592454
H	-0.1192915217	11.3843221251	9.1922417945
H	4.7594850541	4.2392650819	10.4606801165
H	11.8366119681	3.9985313063	10.7935197235
H	15.3099354847	6.9342646724	11.4484413182
H	8.1402525682	6.9514603206	10.6062778960
H	12.5948097521	10.6076787449	13.5409960057
H	9.1300200775	8.4234634691	12.6901909018
H	10.0905622988	7.6461794973	10.1846310387
H	11.0111711503	2.6641057105	10.4820578097
H	1.6533855692	4.0465243749	12.1717890561
H	15.6729916366	6.2824845697	10.0643201931
H	11.0729542927	10.5202936267	13.3243567493
H	8.9447775112	3.8635446208	10.3414034381
H	12.1723632605	5.8467009640	13.1933921702
H	5.7649227301	5.2695258753	11.3788730616
H	5.8286474949	3.4979379922	11.7420743907
H	10.4844039067	6.7825814199	11.3680393190
H	4.2234563308	11.9070473931	8.4379823962
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H	2.3372906672	5.2370906838	11.1741347518
H	14.0584946849	1.9602796920	12.7499252543
H	12.4638254220	7.8473457831	14.7306427535
H	8.0897402557	-0.2562799760	11.6638618418
H	3.8493886118	10.4306499348	8.0056236071
H	16.1727701207	7.4903387719	13.3178088566
H	8.7652233564	4.2167494844	12.9214043054
H	7.5934584114	1.0243976113	10.8240174622
H	13.2083261650	4.7054053689	15.6192514888
H	12.7703718943	1.4933726662	13.2358818036

H	14.0807806743	3.7166978193	14.9508449006
H	9.6530625663	3.4770044414	13.9734448791
H	8.1132300366	5.6721997184	16.5402034315
H	13.3716870238	8.7427035328	15.6442226453
H	7.9763910396	4.9843989158	15.1411859603
H	14.8408067100	8.1504992998	13.3707268138
H	4.2541718641	6.1043811625	15.1755078013
H	5.7631453968	6.2110575261	15.2169203969
C	6.9620573881	4.1263084013	10.0295794416
C	5.7225793453	4.2685885263	10.9912065793
O	8.2594008180	2.4346397782	8.4140630088
O	5.8463593445	6.0452253848	8.3825673354
O	5.7463087498	2.9008414972	7.8381200651
O	10.9425716358	12.2511498294	10.6736686881
O	8.4182842659	5.8507380433	8.2654176441
O	10.8441340409	8.0951083458	8.4754901723
O	5.7658939547	8.7179224639	8.0358936493
O	0.7925622812	3.4393095112	7.8699837794
O	7.2607117422	10.4025410085	9.3671909709
O	0.1356390829	10.9227662732	8.3112574947
O	7.2078142640	6.8254289796	10.3150464427
O	6.3908853503	1.4067348363	9.7688272893
O	9.2729017197	9.1178065366	13.3228850433
O	11.0149454050	3.6580137754	10.3428642791
O	9.8252558413	7.4769693901	11.0871358926
O	11.8384019359	11.1242567485	13.2173901037
O	8.0906618598	3.8889144666	10.8955869354
O	14.9194994024	6.6030232033	10.5796810368
O	1.5197488807	4.8166883814	11.5653309028
O	11.6733507448	6.1451224382	13.9505593960
O	3.5484130935	11.3628840019	7.9774880592
O	13.1608975017	8.5540365435	14.7462565122
O	13.1787159222	2.3544032582	13.0528222476
O	8.2276736524	0.7256957271	11.5574231264
O	15.5137742953	7.8845545661	12.7272775034
O	7.4837880918	5.4779125015	15.8136128676
O	9.0649451558	4.2396142712	13.8480577409
O	14.1164761434	4.3116206301	15.7055310239
O	4.9827141186	6.7056684432	14.9271869117
P	6.7238236927	2.6220382696	8.9882933624
P	7.1456659457	5.7649925577	9.0890544898
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Fe	4.2996000000	1.4332000000	2.0000000000
Fe	7.1660000000	1.4332000000	2.0000000000

Fe	10.0324000000	1.4332000000	2.0000000000
Fe	1.4332000000	4.2996000000	2.0000000000
Fe	4.2996000000	4.2996000000	2.0000000000
Fe	7.1660000000	4.2996000000	2.0000000000
Fe	10.0324000000	4.2996000000	2.0000000000
Fe	1.4332000000	7.1660000000	2.0000000000
Fe	4.2996000000	7.1660000000	2.0000000000
Fe	7.1660000000	7.1660000000	2.0000000000
Fe	10.0324000000	7.1660000000	2.0000000000
Fe	1.4332000000	10.0324000000	2.0000000000
Fe	4.2996000000	10.0324000000	2.0000000000
Fe	7.1660000000	10.0324000000	2.0000000000
Fe	10.0324000000	10.0324000000	2.0000000000
Fe	0.0000000000	0.0000000000	3.4332000000
Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
Fe	2.8664000000	2.8664000000	3.4332000000
Fe	5.7328000000	2.8664000000	3.4332000000
Fe	8.5992000000	2.8664000000	3.4332000000
Fe	0.0000000000	5.7328000000	3.4332000000
Fe	2.8664000000	5.7328000000	3.4332000000
Fe	5.7328000000	5.7328000000	3.4332000000
Fe	8.5992000000	5.7328000000	3.4332000000
Fe	0.0000000000	8.5992000000	3.4332000000
Fe	2.8664000000	8.5992000000	3.4332000000
Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
Fe	1.1342172882	1.2600278570	4.9691616720
Fe	4.5205814330	1.4880781065	4.5345717360
Fe	7.0990414567	1.5018363409	4.4705252243
Fe	10.1387791396	1.2371500903	4.9813514421
Fe	1.4377503317	4.2403435782	4.3817399101
Fe	4.6206988003	4.4361833271	5.1041809318
Fe	7.3008140794	4.4104698587	4.9517008607
Fe	9.9825239275	4.5413139654	4.9926013188
Fe	1.4108495910	7.2563280643	4.3308725125
Fe	4.5419308362	6.8888524250	5.1316131826
Fe	7.2117870055	6.8990738919	4.7836455339
Fe	9.8505967693	6.9786608140	4.9246737429
Fe	1.5909470865	10.1200561126	4.9778082658
Fe	4.2006328927	9.9258591465	4.9635457954
Fe	7.2384067186	9.9509787477	4.4169371877

Fe	10.3035808390	10.2720542081	4.8211486984
Fe	0.0611007688	-0.2542119466	6.3399372805
Fe	3.0915776145	0.2037294557	5.8495708579
Fe	5.8876193404	-0.1011759504	5.7250381493
Fe	8.4385862930	-0.0530665266	5.8433299391
Fe	0.1173547647	3.1257074924	5.8740324684
Fe	2.9247896829	2.7890103544	5.6349919218
Fe	5.8734535872	2.7688243517	5.9135063501
Fe	8.5942269798	2.7010033561	5.6965879204
Fe	0.2736730081	5.9677760147	5.8286252066
Fe	2.6377951031	5.6819047213	5.6855172478
Fe	5.9574862217	5.5888427347	6.4171572453
Fe	8.5364055862	5.7626485635	6.3215995877
Fe	-0.0600424220	8.4012037008	5.7279360324
Fe	2.7645462673	8.2997656364	5.7028157899
Fe	5.8617787957	8.7233049057	5.9328198388
Fe	8.3823789898	8.7272037026	5.7311368548

(k) 4000 fs

H	7.8795175046	-1.2735256618	6.6345979456
H	-0.8162554633	3.1430708524	8.6412670140
H	5.4722598610	9.5075417407	8.5610846803
H	12.9678067081	5.4079397385	6.8869105323
H	0.2635768377	4.1107501619	8.1621215685
H	5.3583413499	11.6011487412	9.7833750480
H	10.1301665028	12.3088485215	11.4803579346
H	7.5403277373	2.2555083463	7.6409351822
H	-0.2261641020	9.9484191900	8.6826295227
H	11.1263988489	7.6872599876	7.9519965940
H	12.2953868576	7.8648210316	8.8654215280
H	11.5583714082	11.5819502120	11.4911538658
H	5.3475079539	7.8489617005	8.2862811480
H	6.9700707455	9.8533611058	11.0654974890
H	6.6722218091	11.0667157674	8.8811348169
H	-0.2263835372	11.4957221469	9.1301593363
H	4.5676815845	4.8618181042	10.3682418771
H	10.7830332395	3.8980667106	10.6331496903
H	14.6049154623	6.9978696712	10.2772740783
H	8.0089640142	6.9166031251	10.6451493592
H	12.7599491785	9.8270023693	13.0409416817
H	8.3485987907	9.2809586994	11.3689258672
H	10.1731242876	7.9544235760	10.3092474073
H	10.7751999560	2.3497790459	10.7218478604
H	1.3693689019	4.0960143291	11.1928910892

H	14.7441719962	6.2755151476	8.8539546815
H	11.7070009655	10.7544420868	13.5976746151
H	8.5401322798	3.5689788870	10.4303789611
H	11.5344409785	5.6760745331	12.3842092157
H	5.6749247644	5.3365694717	11.6970751937
H	5.0480455647	3.6151514780	11.5746347280
H	9.8331823868	7.4347559584	11.8013281351
H	3.3785524841	12.7286540728	8.3368594415
H	10.4024229877	5.5384350657	13.3825998545
H	1.4434682920	5.5067150702	10.3944857805
H	14.6768291167	1.9984545735	11.8634586003
H	12.4021242382	7.6385515219	13.8017016623
H	8.4585391693	-0.0186582457	12.3398957482
H	3.8746200668	11.2454042730	8.2814098890
H	15.5193424575	7.5256126734	12.3326189285
H	7.9560934796	4.9535307311	12.4766334301
H	8.4300946005	1.4096589079	12.2359132563
H	14.0880214606	5.3117365112	13.2824477881
H	14.0297306942	1.4057941713	13.0397737545
H	14.3192993300	3.8210758527	13.5948656388
H	7.8625684027	4.6422883737	14.0118954711
H	6.9182125395	8.5079909984	13.9695715551
H	13.9658161671	7.6470053646	13.8355538806
H	7.3118411189	6.9766757353	13.8522130149
H	14.9681269023	8.7244434940	11.6098687053
H	4.2398899484	5.8503330467	14.1400919200
H	5.1855852893	7.0759257339	14.0796798823
C	6.5099920265	4.0400325576	10.1067426481
C	5.3718427620	4.5210715202	11.0582516448
O	7.2982907665	1.9259954611	8.5792228742
O	5.7673075452	6.0748249790	8.3165878148
O	5.2171825641	3.0500481940	7.8024978224
O	10.9239254102	12.0692091468	10.8723846214
O	8.2727449159	5.4373658946	8.3956011051
O	11.3329251974	8.0123738314	8.8803381287
O	5.2284109986	8.7116267529	7.9051618162
O	-0.1423257762	3.2415473503	7.9333607659
O	5.9062583373	10.6903408777	9.4098642045
O	-0.0393472079	10.8432950879	8.4302006464
O	7.1495626812	6.5994332232	10.3711605080
O	5.1842840061	1.7098111660	10.0433594430
O	7.6094673852	9.7450388043	11.7763097662
O	10.2850677504	3.0935546466	10.4570552394
O	9.4678028585	7.6998809575	10.9508313745

O	12.2589687930	10.6699749875	12.8131044016
O	7.7323209409	3.8524935943	10.9147058811
O	14.0914345121	6.6664321684	9.4526068687
O	0.8470032118	4.8515148598	10.8435323597
O	11.0351771415	6.1886193653	13.0532071432
O	3.2063788849	11.8788217079	7.9171179197
O	13.1475098791	8.2315768267	13.6342883792
O	14.1136552864	2.2656080722	12.5844416445
O	9.0186236871	0.7120353153	12.5934535385
O	15.3290898520	7.8540498449	11.4457025704
O	6.6047617645	7.6001723070	14.2275649262
O	8.2577466393	5.2733788826	13.3880887240
O	14.2075575933	4.6972340118	14.0669104730
O	4.2537088464	6.7971175936	13.8639293634
P	5.9155838319	2.5911305099	9.0478518857
P	6.9511216047	5.6183802126	9.2054087751
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Fe	4.2996000000	1.4332000000	2.0000000000
Fe	7.1660000000	1.4332000000	2.0000000000
Fe	10.0324000000	1.4332000000	2.0000000000
Fe	1.4332000000	4.2996000000	2.0000000000
Fe	4.2996000000	4.2996000000	2.0000000000
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Fe	7.1660000000	10.0324000000	2.0000000000
Fe	10.0324000000	10.0324000000	2.0000000000
Fe	0.0000000000	0.0000000000	3.4332000000
Fe	2.8664000000	0.0000000000	3.4332000000
Fe	5.7328000000	0.0000000000	3.4332000000
Fe	8.5992000000	0.0000000000	3.4332000000
Fe	0.0000000000	2.8664000000	3.4332000000
Fe	2.8664000000	2.8664000000	3.4332000000
Fe	5.7328000000	2.8664000000	3.4332000000
Fe	8.5992000000	2.8664000000	3.4332000000
Fe	0.0000000000	5.7328000000	3.4332000000
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Fe	5.7328000000	5.7328000000	3.4332000000
Fe	8.5992000000	5.7328000000	3.4332000000

Fe	0.0000000000	8.5992000000	3.4332000000
Fe	2.8664000000	8.5992000000	3.4332000000
Fe	5.7328000000	8.5992000000	3.4332000000
Fe	8.5992000000	8.5992000000	3.4332000000
Fe	1.1734633713	1.2387141502	4.9826220282
Fe	4.3678088083	1.3654379101	4.4918098825
Fe	7.1624421120	1.3860752706	4.3855391196
Fe	10.2253673410	1.2376164414	5.1036418603
Fe	1.3351524105	4.1807792666	4.4230481277
Fe	4.6784666990	4.5907843927	5.0471047317
Fe	7.4063207293	4.4713234729	4.9623896354
Fe	9.8590196343	4.3404857790	4.9022250287
Fe	1.3683237722	7.2403787013	4.3985664109
Fe	4.6047894233	6.8808832488	5.1339781724
Fe	7.3028733800	6.7548590431	4.9697640722
Fe	9.7564566886	6.8473761017	5.0742716008
Fe	1.3194589437	10.1859495315	4.9869953427
Fe	4.2166690277	9.8103354357	4.9370989148
Fe	7.1583238759	9.9182764254	4.4656116814
Fe	10.0720416633	10.2996350455	4.8364136136
Fe	-0.0786697243	-0.2981331312	6.4288290953
Fe	2.9746846210	0.4169363160	5.8195154700
Fe	5.7100696953	-0.1581379459	5.6509305379
Fe	8.4307291865	0.0368669802	5.7262667822
Fe	-0.0337402744	2.9836725835	5.8444376593
Fe	2.9904205524	3.0147647024	5.5969491304
Fe	5.7589432019	2.7376158379	5.8267197337
Fe	8.5750930650	2.5999929947	5.7700364023
Fe	0.2358564292	5.7244935009	5.7608991868
Fe	2.7839721453	5.7745611948	5.6999326920
Fe	6.0133305176	5.7575051450	6.3933071133
Fe	8.5660366891	5.4887820977	6.4589779548
Fe	-0.0607514619	8.4761700511	5.5751410372
Fe	2.7483204844	8.4816736658	5.7514205146
Fe	5.8392989191	8.4981434317	5.9797196226
Fe	8.6630968232	8.6951191400	5.7732234731

(l) 5000 fs

H	7.3819666815	-0.1670426122	6.7728810453
H	0.2681473225	3.1466114143	8.9822063775
H	6.2106306547	9.1763872211	8.3863654317
H	12.8307001886	5.7201339887	6.9316615630
H	1.4018171372	2.2916473017	8.1662132724
H	6.9873193438	11.0257788286	9.2029009240

H	9.9504648378	12.2765830452	10.9798808138
H	8.0479966486	1.5359852948	7.4602252062
H	-0.3547899108	11.4297143593	9.3128482959
H	12.5768627717	7.3960364104	8.6019221585
H	12.6220805741	7.7680840306	10.1175152989
H	11.5055442463	12.1136946963	11.3822182581
H	5.7370971279	7.6034201909	8.1031868940
H	7.7857986046	9.8657046308	11.2735161537
H	7.9419379366	10.1846864270	8.4598541675
H	-0.3075779042	9.8448406910	8.8500946336
H	5.1319871555	4.6328504850	10.6280056692
H	12.2120357708	3.6245229347	10.9941959119
H	15.1185454887	4.7701981874	8.8743275634
H	8.4341413977	6.5705734739	10.3106642044
H	12.0126130879	10.6000982580	12.9533535268
H	8.6241387275	8.7505483449	11.9393284738
H	10.3866703220	7.5277891407	10.1862246474
H	11.3254779418	2.3429341948	10.6170931993
H	2.5044965479	4.2482849089	12.4006215761
H	13.6702097821	4.5114685871	8.6320829974
H	11.5281750383	11.9196987033	13.7863426079
H	9.0960197200	3.6554972909	10.1073561779
H	12.2324951593	5.8346833332	12.6466863569
H	6.5090768364	4.9370299219	11.7353041582
H	5.7810336424	3.2872744820	11.7052618966
H	10.4805746471	6.8557398085	11.6353129956
H	3.5368478897	12.8608332874	8.2035290893
H	10.9305742447	5.5080324371	13.3887250043
H	2.4444861574	4.8560974859	10.9365966002
H	15.9642607323	0.8338771635	10.7865880819
H	11.7576325673	8.0429813276	12.8847089902
H	8.6987774267	-0.1099629323	12.3788130346
H	2.8081927136	11.4918786362	8.8487639741
H	14.4602010234	9.5023745403	10.2774598743
H	9.8998392274	4.0489466289	12.0035835135
H	7.9247885484	0.9863939503	11.5429910547
H	14.0811637372	2.3630952837	13.6985525081
H	14.7189633297	0.1707270496	11.0142823838
H	15.1855874891	2.2729653817	12.5981852906
H	9.5228009161	3.1464428770	13.1656462656
H	5.9245976840	10.1348323187	12.6469873191
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H	3.9416627016	7.5504177116	11.9232488867
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C	7.0986948466	3.8499810348	9.9864258646
C	6.0097630098	4.1835805102	11.1230484163
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O	10.8706078022	12.2622813200	10.6163801953
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O	12.0477082349	7.8916403272	9.2878648927
O	5.5424251627	8.5920580337	7.9442300606
O	0.7869610305	3.0612594779	8.0654794968
O	7.2940592866	10.0648655607	9.1898991295
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O	7.4772940858	6.5345193990	10.0134298664
O	6.2155065316	1.1378367459	10.1660875356
O	8.1507781542	9.6033847001	12.1054429892
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O	2.7841385423	12.2495161950	8.1823392344
O	12.1007477435	8.8622000679	12.5015942597
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O	4.9657257918	10.1863960729	12.6803609402
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P	7.3290122231	5.4151816221	8.8916657982
Fe	1.4332000000	1.4332000000	2.0000000000
Fe	4.2996000000	1.4332000000	2.0000000000
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Fe	4.2996000000	4.2996000000	2.0000000000
Fe	7.1660000000	4.2996000000	2.0000000000
Fe	10.0324000000	4.2996000000	2.0000000000
Fe	1.4332000000	7.1660000000	2.0000000000

Fe	4.2996000000	7.1660000000	2.0000000000
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Fe	4.1187158532	10.1870716703	5.0144197163
Fe	7.1269580128	9.8985124908	4.3675906448
Fe	10.1129126847	10.1290710301	4.6014831053
Fe	-0.4585982993	-0.6821973421	6.5397250113
Fe	2.9455267970	0.2694398359	6.1228088863
Fe	5.9739825623	-0.1075862471	5.8025326733
Fe	8.5555260071	-0.0581243355	5.8057201713
Fe	0.0821713556	3.0605630632	5.9139275505

Fe	2.7113074533	2.8257630587	5.5450132593
Fe	5.0132191847	2.7449749100	6.2679966554
Fe	8.7775335027	2.8987767539	5.7541742119
Fe	0.1076823836	5.8180765699	5.7938821786
Fe	2.5581543011	5.5243690448	5.7827777989
Fe	5.9523519144	5.9831555287	6.0759247112
Fe	8.6447820637	5.3521000254	6.1321573131
Fe	-0.0603998980	8.4820071932	5.7845652579
Fe	2.6600345247	8.4029337955	5.8111391759
Fe	5.7197669665	8.8358952949	5.8231571865
Fe	8.6703432236	8.8198793433	5.6860221713

3. The IRI isosurfaces of the model shown in Fig. 1

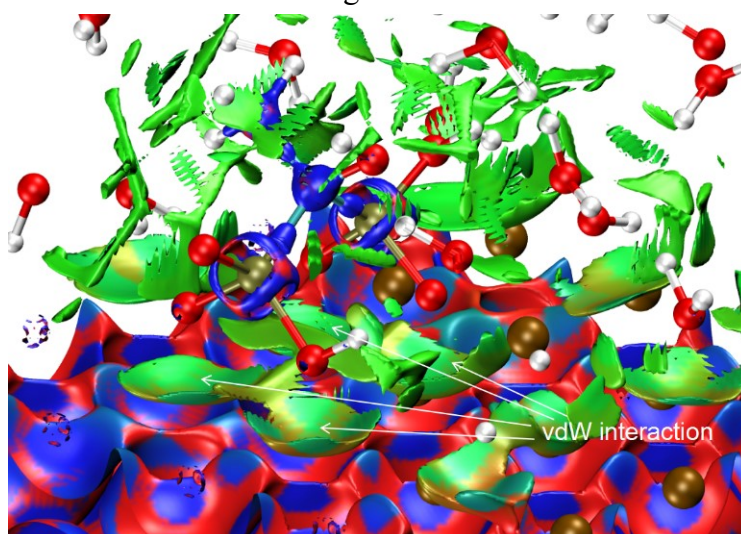


Figure S2. The IRI isosurfaces of the model at 0 fs

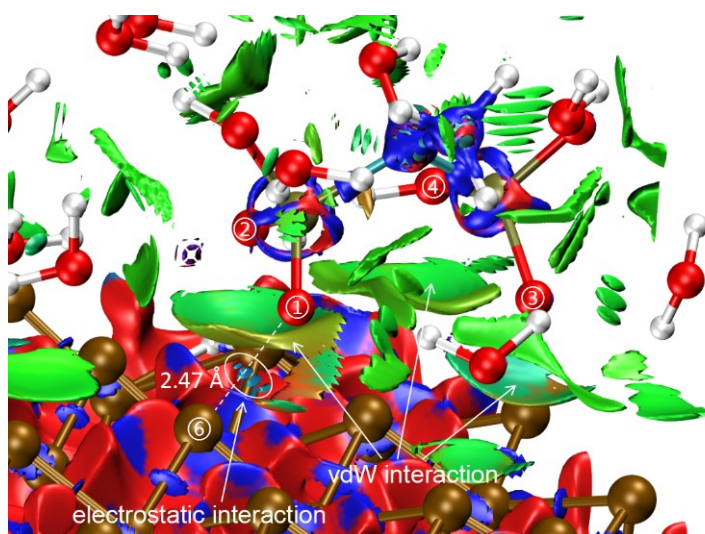


Figure S3. The IRI isosurfaces of the model at 75 fs

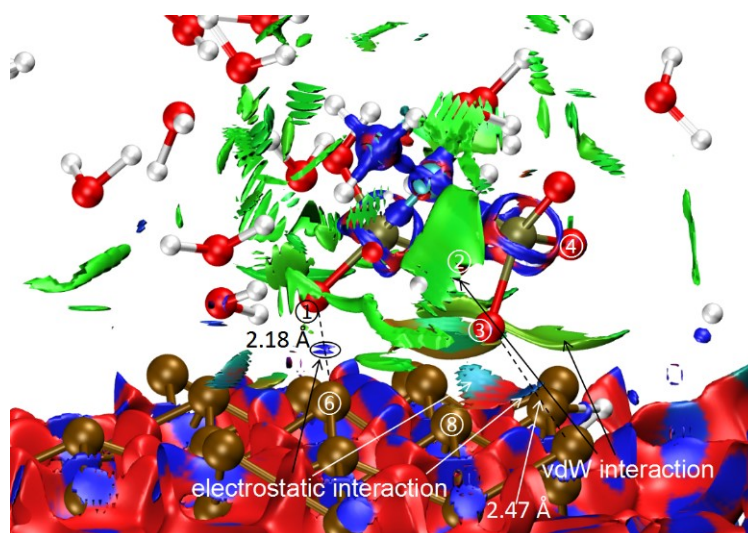


Figure S4. The IRI isosurfaces of the model at 107 fs

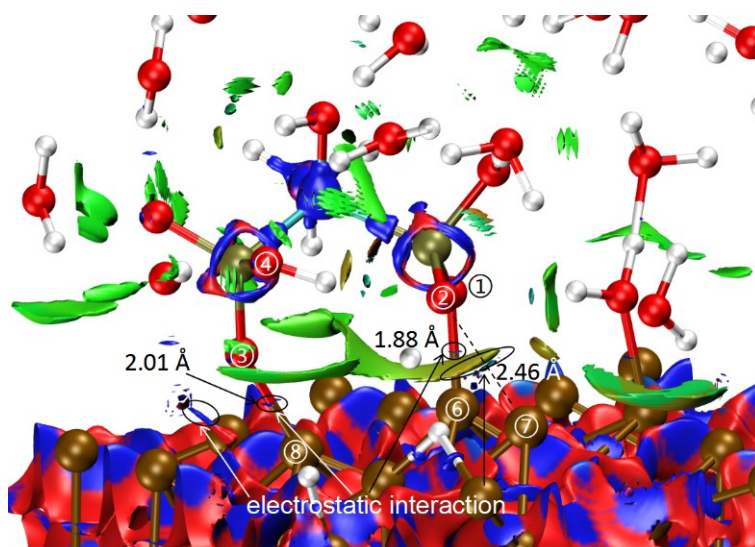


Figure S5. The IRI isosurfaces of the model at 265 fs

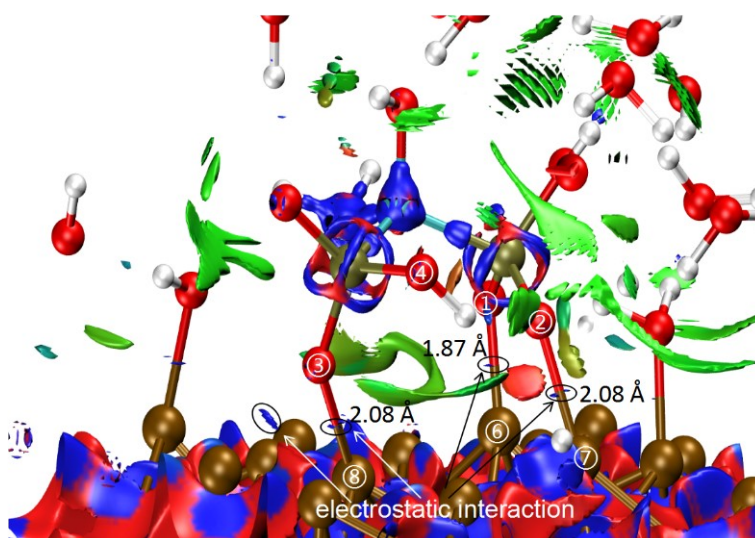


Figure S6. The IRI isosurfaces of the model at 524 fs

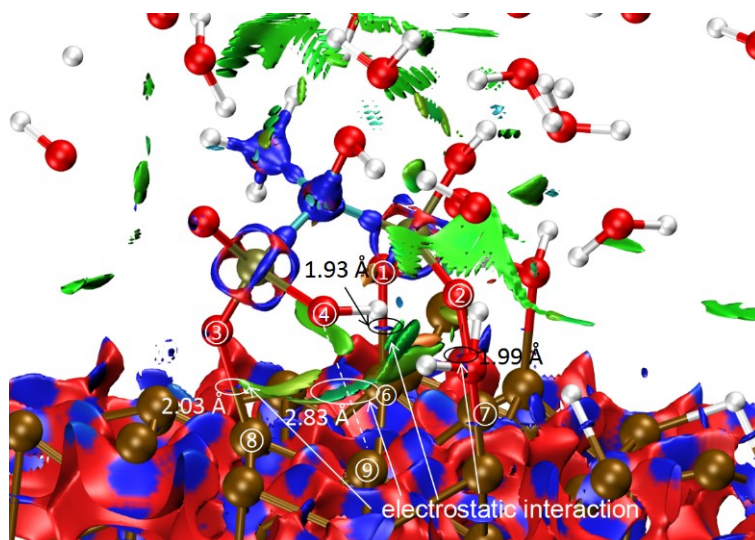


Figure S7. The IRI isosurfaces of the model at 671 fs

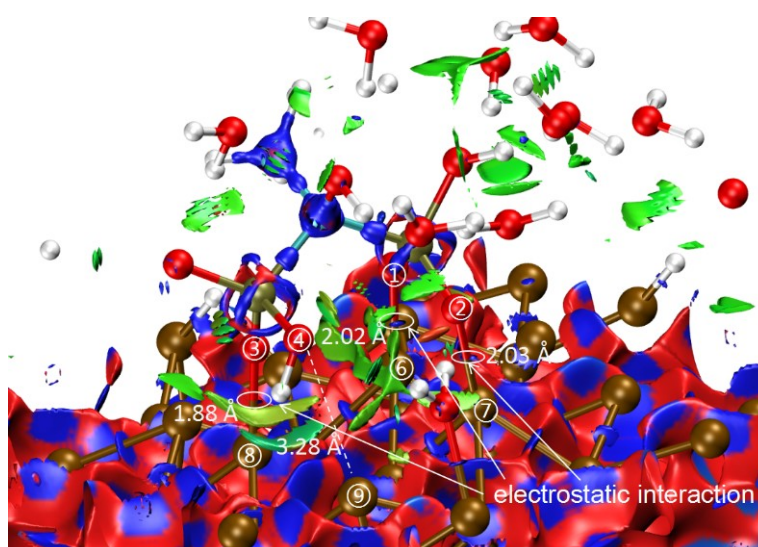


Figure S8. The IRI isosurfaces of the model at 1578 fs

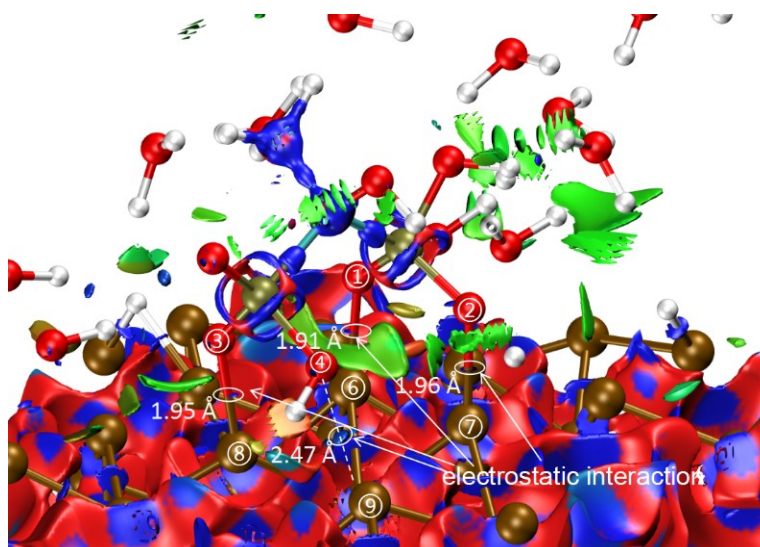


Figure S9. The IRI isosurfaces of the model at 2161 fs

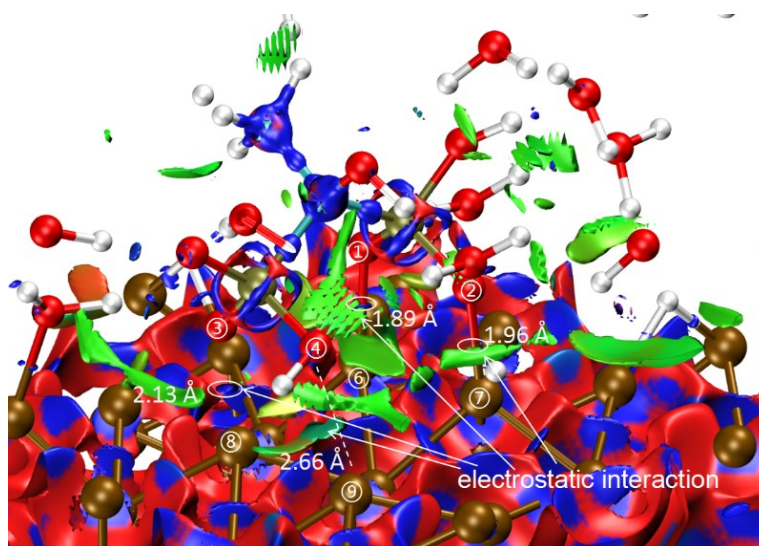


Figure S10. The IRI isosurfaces of the model at 2774 fs

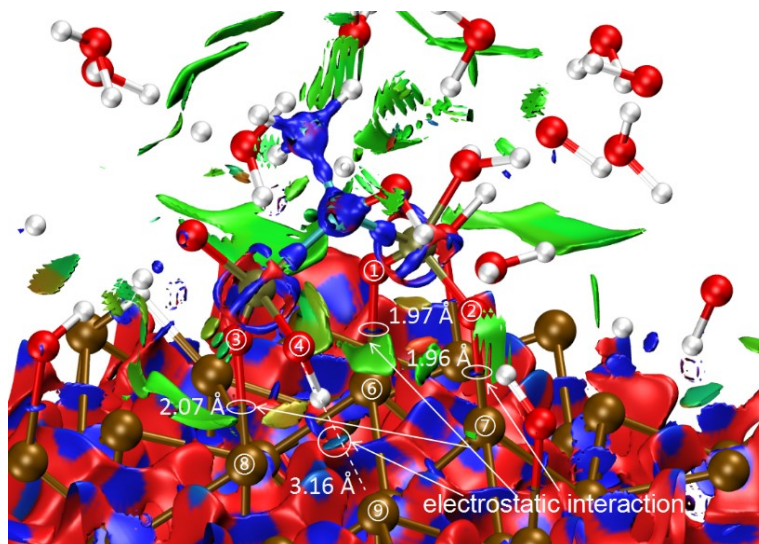


Figure S11. The IRI isosurfaces of the model at 4000 fs

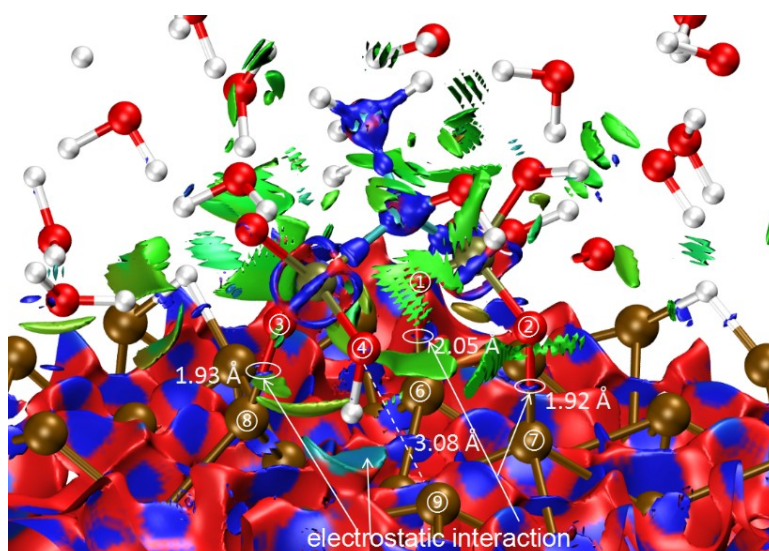


Figure S12. The IRI isosurfaces of the model at 5000 fs