

Electronic Supplementary Information for

Vacancy Interlayer Migration in Multi-layered Graphene

Lili Liu,^a Junfeng Gao,^b Xiuyun Zhang,^b Tianying Yan^c and Feng Ding ^{a,b*}

^a Beijing Computational Science Research Center, Beijing 100084, Peoples Republic of China

^b Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, Peoples Republic of China

^c Institute of New Energy Material Chemistry, College of Chemistry, Nankai University, P. O. Box 300071, Tianjin, China

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1. The geometries of the cNEB calculations in Fig. 3.
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1. The geometries of the NEB calculations in Fig. 3.(direct coordinates).

The structures of the first set of the calculation in Fig. 3 (a)

(1) The optimized initial1 geometry

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Direct

0.2772970	0.0998140	0.5523270
0.1663615	0.1001506	0.5522895
0.0556611	0.1000080	0.3897870
0.1668928	0.1000072	0.3897929
0.6111719	0.0994131	0.5521674
0.5001017	0.0990641	0.5521992
0.3889920	0.1000096	0.3898102
0.5002196	0.1000096	0.3898510

0.9447454	0.1003152	0.5521858
0.8336500	0.1001575	0.5521375
0.7223140	0.1000109	0.3898450
0.8335698	0.1000065	0.3898345
0.9998429	0.2008870	0.5522382
0.0002195	0.2000032	0.3897385
0.2795319	0.3002652	0.5524556
0.1676898	0.3006792	0.5523838
0.0556404	0.3000032	0.3896102
0.1668660	0.3000053	0.3896187
0.1113462	0.2007647	0.5523302
0.2223166	0.2000137	0.3897106
0.3334228	0.1996752	0.5523518
0.3335627	0.2000253	0.3897768
0.6113261	0.2980195	0.5522850
0.5003569	0.2975528	0.5523546
0.3889926	0.3000176	0.3897914
0.5002108	0.3000163	0.3898811
0.4441001	0.1981503	0.5523167
0.5556467	0.2000203	0.3898386
0.6668656	0.1998032	0.5521891
0.6668900	0.1999849	0.3898229
0.9436280	0.3008997	0.5522844
0.8315585	0.3010513	0.5522401
0.7222981	0.3000040	0.3897781
0.8335080	0.3000021	0.3897356
0.7779883	0.2001107	0.5521827
0.8889726	0.1999833	0.3897521
0.9999159	0.4004463	0.5523389
0.0001669	0.4000068	0.3895703
0.1117736	0.4003033	0.5524080
0.2223091	0.4000186	0.3895216
0.3376081	0.4006619	0.5524988
0.3335281	0.4000280	0.3896910
0.4472112	0.3941165	0.5524364
0.5556169	0.4000105	0.3900035
0.6606708	0.4014393	0.5524507
0.6668163	0.3999928	0.3898841
0.7742591	0.4010495	0.5523727
0.8889421	0.4000016	0.3896286
0.2772970	0.9001860	0.5523270
0.1663615	0.8998494	0.5522895
0.0556611	0.8999920	0.3897870
0.1668928	0.8999928	0.3897929

0.6111719	0.9005869	0.5521674
0.5001017	0.9009359	0.5521992
0.3889920	0.8999904	0.3898102
0.5002196	0.8999904	0.3898510
0.9447454	0.8996848	0.5521858
0.8336500	0.8998425	0.5521375
0.7223140	0.8999891	0.3898450
0.8335698	0.8999935	0.3898345
0.9998429	0.7991130	0.5522382
0.0002195	0.7999968	0.3897385
0.2795319	0.6997348	0.5524556
0.1676898	0.6993208	0.5523838
0.0556404	0.6999968	0.3896102
0.1668660	0.6999947	0.3896187
0.1113462	0.7992353	0.5523302
0.2223166	0.7999863	0.3897106
0.3334228	0.8003248	0.5523518
0.3335627	0.7999747	0.3897768
0.6113261	0.7019805	0.5522850
0.5003569	0.7024472	0.5523546
0.3889926	0.6999824	0.3897914
0.5002108	0.6999837	0.3898811
0.4441001	0.8018497	0.5523167
0.5556467	0.7999797	0.3898386
0.6668656	0.8001968	0.5521891
0.6668900	0.8000151	0.3898229
0.9436280	0.6991003	0.5522844
0.8315585	0.6989487	0.5522401
0.7222981	0.6999960	0.3897781
0.8335080	0.6999979	0.3897356
0.7779883	0.7998893	0.5521827
0.8889726	0.8000167	0.3897521
0.9999159	0.5995537	0.5523389
0.0001669	0.5999932	0.3895703
0.1117736	0.5996967	0.5524080
0.2223091	0.5999814	0.3895216
0.3376081	0.5993381	0.5524988
0.3335281	0.5999720	0.3896910
0.4472112	0.6058835	0.5524364
0.5556169	0.5999895	0.3900035
0.6606708	0.5985607	0.5524507
0.6668163	0.6000072	0.3898841
0.7742591	0.5989505	0.5523727
0.8889421	0.5999984	0.3896286

0.9999411	0.0000000	0.5521683
0.0002232	0.0000000	0.3898539
0.1110158	0.0000000	0.5522596
0.2223319	0.0000000	0.3898045
0.3327978	0.0000000	0.5522699
0.3335548	0.0000000	0.3898338
0.4441549	0.0000000	0.5522320
0.5556721	0.0000000	0.3898397
0.6668927	0.0000000	0.5521219
0.6668834	0.0000000	0.3898638
0.7783580	0.0000000	0.5521164
0.8890022	0.0000000	0.3898457
0.2801110	0.5000000	0.5524841
0.1688429	0.5000000	0.5524395
0.0555997	0.5000000	0.3894931
0.1668551	0.5000000	0.3894759
0.6032247	0.5000000	0.5526074
0.3889521	0.5000000	0.3898125
0.5001777	0.5000000	0.3902034
0.9433435	0.5000000	0.5523627
0.8311887	0.5000000	0.5523672
0.7222482	0.5000000	0.3898079
0.8334773	0.5000000	0.3896708

(2) The structure of TS1

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Direct

0.2788613	0.1003719	0.5564528
0.1676882	0.1003952	0.5569084
0.0545330	0.1000521	0.3854063
0.1658321	0.1000274	0.3860333
0.6118888	0.1002241	0.5546925
0.5009182	0.1006068	0.5556004
0.3881200	0.0998429	0.3873721
0.4990800	0.1001884	0.3864847
0.9454725	0.1004263	0.5565831
0.8341543	0.1004523	0.5559697
0.7211687	0.1000740	0.3855644
0.8323656	0.1000477	0.3850438
0.0009688	0.2007018	0.5569191
0.9989736	0.2003146	0.3850753
0.2800895	0.3008801	0.5507956
0.1685901	0.3008837	0.5548618
0.0548887	0.3002730	0.3851882

0.1664790	0.3003266	0.3868986
0.1125202	0.2007625	0.5567767
0.2214579	0.2000524	0.3875151
0.3344829	0.2005080	0.5527979
0.3327801	0.2002073	0.3900981
0.6117186	0.2995685	0.5451113
0.5007145	0.3007646	0.5410812
0.3880677	0.2992091	0.3964234
0.4991081	0.3003859	0.4002193
0.4453638	0.2009713	0.5512176
0.5545630	0.2005523	0.3906382
0.6671092	0.2006447	0.5518814
0.6654543	0.2002007	0.3890899
0.9449438	0.3006543	0.5568829
0.8333213	0.3007449	0.5550572
0.7198049	0.3005834	0.3909654
0.8313091	0.3005069	0.3871842
0.7784150	0.2004818	0.5545779
0.8874486	0.2004006	0.3852276
0.0010199	0.4004282	0.5566955
0.9988333	0.4000737	0.3851794
0.1125332	0.4004488	0.5547220
0.2225721	0.4003380	0.3893243
0.3363031	0.4006903	0.5404087
0.3344976	0.4005835	0.3964720
0.4450391	0.3971487	0.5261660
0.5547643	0.3968801	0.4145569
0.6652532	0.4009911	0.5449286
0.6635069	0.4005285	0.4007947
0.7771851	0.4007291	0.5522956
0.8873583	0.4000916	0.3872243
0.2788509	0.8999154	0.5566506
0.1676651	0.8999543	0.5570202
0.0545590	0.8995647	0.3852961
0.1658675	0.8996258	0.3859214
0.6118913	0.9002752	0.5548911
0.5009257	0.8998282	0.5557740
0.3881255	0.8998520	0.3873957
0.4990892	0.8994347	0.3864992
0.9454761	0.8999593	0.5566671
0.8341653	0.9000044	0.5561078
0.7211453	0.8996539	0.3856204
0.8323514	0.8996381	0.3850201

0.0009782	0.7996910	0.5570179
0.9990243	0.7993137	0.3849126
0.2800800	0.6993891	0.5511182
0.1685597	0.6994465	0.5549473
0.0549818	0.6993654	0.3850880
0.1665941	0.6993314	0.3867812
0.1124919	0.7995950	0.5568668
0.2215545	0.7996291	0.3873685
0.3344888	0.7997803	0.5531384
0.3328564	0.7994651	0.3901408
0.6117774	0.7009371	0.5454530
0.5007764	0.6996841	0.5415743
0.3881415	0.7004621	0.3967802
0.4991476	0.6993090	0.4007544
0.4453738	0.7994429	0.5515217
0.5545732	0.7990698	0.3908112
0.6671452	0.7998589	0.5521345
0.6654619	0.7995287	0.3892629
0.9449907	0.6997294	0.5568893
0.8333698	0.6996805	0.5551633
0.7198051	0.6991201	0.3912185
0.8313062	0.6991820	0.3872000
0.7784540	0.7999831	0.5548138
0.8874731	0.7992568	0.3851142
0.0010249	0.5999070	0.5566435
0.9988865	0.5996150	0.3851891
0.1125379	0.5998795	0.5547236
0.2226306	0.5992950	0.3893580
0.3363544	0.5995588	0.5408926
0.3345360	0.5990545	0.3966625
0.4451591	0.6031849	0.5269317
0.5547932	0.6029038	0.4154493
0.6653025	0.5995217	0.5450955
0.6634458	0.5992166	0.4012440
0.7772391	0.5997003	0.5523362
0.8873938	0.5996192	0.3872843
0.0009380	0.0001763	0.5566737
0.9991125	0.9998004	0.3852349
0.1121642	0.0001790	0.5571367
0.2212671	0.9998367	0.3861362
0.3342178	0.0001359	0.5574513
0.3325973	0.9998388	0.3862322
0.4453722	0.0001891	0.5576133

0.5546167	0.9998123	0.3846319
0.6674627	0.0002365	0.5558016
0.6657221	0.9998924	0.3847521
0.7787975	0.0002360	0.5558618
0.8878658	0.9998237	0.3848029
0.2793332	0.5000891	0.5427436
0.1688385	0.5001528	0.5512392
0.0548759	0.4998246	0.3852797
0.1664713	0.4998292	0.3876003
0.6120989	0.5003167	0.5370748
0.3877635	0.4997734	0.4047027
0.4991700	0.5001621	0.4709283
0.9449347	0.5001630	0.5564280
0.8332860	0.5001741	0.5540210
0.7205357	0.4998959	0.3987904
0.8310908	0.4998693	0.3905538

(3) The optimized final structure

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Direct

0.2774986	0.1000929	0.5522306
0.1662409	0.1000762	0.5522151
0.0553027	0.1002434	0.3898508
0.1663815	0.1001102	0.3898817
0.6107316	0.1000968	0.5521519
0.4995248	0.1000993	0.5521740
0.3888177	0.0993851	0.3899246
0.4998793	0.0990273	0.3899425
0.9440920	0.1000712	0.5521532
0.8328478	0.1000531	0.5521021
0.7227124	0.0997925	0.3898679
0.8336609	0.1001187	0.3898704
0.9995338	0.2000649	0.5522019
0.0002581	0.2008441	0.3898162
0.2775038	0.3000856	0.5522999
0.1663013	0.3000410	0.5522904
0.0564396	0.3008936	0.3897281
0.1684995	0.3010249	0.3897828
0.1107927	0.2000321	0.5522574
0.2220202	0.2000564	0.3898587
0.3329102	0.2000710	0.5522492
0.3331107	0.1997301	0.3899123
0.6108085	0.3001145	0.5521673
0.4996013	0.3001010	0.5521628

0.3886439	0.2979793	0.3899068
0.4995879	0.2974880	0.3898735
0.4441269	0.2001210	0.5522194
0.5558971	0.1981439	0.3898900
0.6661848	0.2001067	0.5521373
0.6666044	0.1996608	0.3898834
0.9441660	0.3000867	0.5522646
0.8329497	0.3000470	0.5522279
0.7205365	0.3002365	0.3898313
0.8323866	0.3006351	0.3898304
0.7774175	0.2000704	0.5521672
0.8887521	0.2007084	0.3898159
0.9996717	0.4000895	0.5523231
0.0001046	0.4004468	0.3896889
0.1109061	0.4000675	0.5523510
0.2257494	0.4010206	0.3897097
0.3330003	0.4000621	0.5522230
0.3393143	0.4014142	0.3897531
0.4441979	0.4001010	0.5521108
0.5527791	0.3940504	0.3898406
0.6663322	0.4000910	0.5522246
0.6624220	0.4006022	0.3898193
0.7775339	0.4000771	0.5523215
0.8882521	0.4002903	0.3897500
0.2774973	0.9000480	0.5522313
0.1662462	0.9000688	0.5522147
0.0553020	0.8997579	0.3898509
0.1663808	0.8998921	0.3898817
0.6107283	0.9000424	0.5521533
0.4995271	0.9000464	0.5521756
0.3888172	0.9006178	0.3899243
0.4998786	0.9009730	0.3899409
0.9440851	0.9000966	0.5521522
0.8328452	0.9000914	0.5521017
0.7227119	0.9002073	0.3898671
0.8336600	0.8998821	0.3898700
0.9995344	0.8001019	0.5522009
0.0002568	0.7991574	0.3898161
0.2775131	0.7000465	0.5523014
0.1663045	0.7001169	0.5522909
0.0564382	0.6991086	0.3897282
0.1684977	0.6989782	0.3897824
0.1107968	0.8001178	0.5522570
0.2220187	0.7999464	0.3898584

0.3329094	0.8000677	0.5522513
0.3331096	0.8002738	0.3899118
0.6108036	0.7000163	0.5521701
0.4996078	0.7000352	0.5521656
0.3886410	0.7020257	0.3899076
0.4995847	0.7025121	0.3898800
0.4441340	0.8000066	0.5522223
0.5558958	0.8018556	0.3898892
0.6661849	0.8000317	0.5521389
0.6666026	0.8003388	0.3898827
0.9441737	0.7000745	0.5522640
0.8329555	0.7001124	0.5522280
0.7205324	0.6997615	0.3898322
0.8323837	0.6993647	0.3898292
0.7774188	0.8000735	0.5521675
0.8887504	0.7992920	0.3898149
0.9996738	0.6000815	0.5523228
0.0001043	0.5995545	0.3896892
0.1109022	0.6000964	0.5523512
0.2257464	0.5989835	0.3897087
0.3329984	0.6000689	0.5522240
0.3393097	0.5985928	0.3897522
0.4442016	0.6000351	0.5521124
0.5527678	0.6059434	0.3898621
0.6663336	0.6000423	0.5522262
0.6624155	0.5993941	0.3898277
0.7775268	0.6000827	0.5523223
0.8882515	0.5997108	0.3897502
-0.0004153	0.0000827	0.5521230
0.0000411	0.0000009	0.3898945
0.1108184	0.0000683	0.5521891
0.2216898	0.0000011	0.3899111
0.3329046	0.0000745	0.5522161
0.3331294	0.0000014	0.3899309
0.4440906	0.0000648	0.5522109
0.5558349	0.0000002	0.3899202
0.6661525	0.0000741	0.5521007
0.6671930	0.0000001	0.3899067
0.7773620	0.0000669	0.5520895
0.8889974	0.0000001	0.3898658
0.2775729	0.5000765	0.5522889
0.1663530	0.5000855	0.5523423
0.0566627	0.5000009	0.3896230
0.1688602	0.5000011	0.3896547

0.6109104	0.5000707	0.5521768
0.3967337	0.5000079	0.3896803
0.4996883	0.5000701	0.5518933
0.9442377	0.5000785	0.5523570
0.8329796	0.5000853	0.5523419
0.7198728	0.5000000	0.3898444
0.8311839	0.5000004	0.3897904

The structures of the first set of the calculation in Fig. 2(b)(Direct coordinates)

(4) The optimized initial2 geometry.

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Direct

0.2759935	0.1520906	0.5813121
0.1647892	0.1514313	0.5812690
0.0531646	0.1511728	0.4186663
0.1648252	0.1514322	0.4186103
0.6073428	0.1523524	0.5815499
0.4966225	0.1544836	0.5814777
0.9976161	0.2508678	0.5812575
0.2750314	0.3529793	0.5813494
0.1637915	0.3517357	0.5812707
0.0524724	0.3505405	0.4188316
0.1631786	0.3506446	0.4189734
0.1087849	0.2512848	0.5812709
0.2203679	0.2517295	0.4187603
0.3310801	0.2537442	0.5813850
0.3322481	0.2533521	0.4186815
0.6078680	0.3542347	0.5809615
0.4964186	0.3643758	0.5812490
0.4418136	0.2584888	0.5814315
0.9969088	0.4506895	0.5811719
0.1069617	0.4506723	0.5813343
0.2167376	0.4510353	0.4192535
0.3289076	0.4548006	0.5814461
0.3276096	0.4518661	0.4196739
0.4375416	0.4677353	0.5813261
0.7185193	0.1520934	0.4186881
0.8297216	0.1514279	0.4187306
0.9413456	0.1511712	0.5813339
0.8296900	0.1514330	0.5813898
0.3871645	0.1523485	0.4184500
0.4978831	0.1544835	0.4185222
0.9968876	0.2508659	0.4187424

0.7194821	0.3529791	0.4186505
0.8307170	0.3517311	0.4187288
0.9420331	0.3505398	0.5811686
0.8313298	0.3506435	0.5810281
0.8857230	0.2512801	0.4187282
0.7741465	0.2517280	0.5812396
0.6634326	0.2537459	0.4186149
0.6622673	0.2533520	0.5813183
0.3866360	0.3542364	0.4190385
0.4980832	0.3643749	0.4187510
0.5526926	0.2584884	0.4185685
0.9975925	0.4506891	0.4188282
0.8875482	0.4506711	0.4186655
0.7777687	0.4510312	0.5807473
0.6656044	0.4548003	0.4185539
0.6668976	0.4518642	0.5803270
0.5569647	0.4677332	0.4186730
0.7185164	0.9505934	0.4186886
0.8297217	0.9512564	0.4187306
0.9413458	0.9515095	0.5813339
0.8296899	0.9512543	0.5813898
0.3871636	0.9503274	0.4184499
0.4978825	0.9481945	0.4185223
0.9968892	0.8518155	0.4187426
0.7194841	0.7496891	0.4186511
0.8307191	0.7509488	0.4187287
0.9420340	0.7521399	0.5811682
0.8313299	0.7520386	0.5810276
0.8857237	0.8514037	0.4187283
0.7741456	0.8509569	0.5812392
0.6634341	0.8489240	0.4186156
0.6622630	0.8493202	0.5813180
0.3866380	0.7484349	0.4190388
0.4980856	0.7382922	0.4187509
0.5526921	0.8441808	0.4185686
0.9975938	0.6519924	0.4188285
0.8875499	0.6520112	0.4186658
0.7777701	0.6516508	0.5807471
0.6656056	0.6478679	0.4185540
0.6669017	0.6508172	0.5803270
0.5569664	0.6349557	0.4186731
0.2759964	0.9505911	0.5813124
0.1647897	0.9512590	0.5812690
0.0531651	0.9515114	0.4186663

0.1648257	0.9512561	0.4186103
0.6073403	0.9503272	0.5815499
0.4966204	0.9481960	0.5814777
0.9976160	0.8518134	0.5812572
0.2750343	0.7496888	0.5813492
0.1637921	0.7509509	0.5812703
0.0524746	0.7521412	0.4188319
0.1631801	0.7520410	0.4189728
0.1087851	0.8514067	0.5812710
0.2203690	0.8509560	0.4187603
0.3310821	0.8489250	0.5813850
0.3322489	0.8493190	0.4186814
0.6078653	0.7484346	0.5809605
0.4964175	0.7382944	0.5812491
0.4418166	0.8441804	0.5814314
0.9969108	0.6519903	0.5811715
0.1069638	0.6520124	0.5813341
0.2167368	0.6516506	0.4192535
0.3289083	0.6478643	0.5814458
0.3276060	0.6508183	0.4196746
0.4375408	0.6349578	0.5813263
0.9973100	0.0513406	0.5812827
0.1089600	0.0513449	0.5812736
0.2205133	0.0513435	0.4185085
0.3310666	0.0513433	0.5813059
0.3320150	0.0513399	0.4184573
0.4419791	0.0513454	0.5814804
0.9971958	0.0513415	0.4187172
0.8855489	0.0513416	0.4187256
0.7740047	0.0513442	0.5814913
0.6634483	0.0513468	0.4186947
0.6624926	0.0513419	0.5815426
0.5525310	0.0513455	0.4185196
0.2692471	0.5513356	0.5815237
0.1608699	0.5513412	0.5814643
0.0520902	0.5513412	0.4189390
0.1621551	0.5513427	0.4191797
0.6190198	0.5513424	0.5793281
0.7252568	0.5513380	0.4184763
0.8336318	0.5513417	0.4185356
0.9424146	0.5513406	0.5810610
0.8323499	0.5513409	0.5808209
0.3754814	0.5513438	0.4206721

(5) The optimized intermediate2 geometry

118

Direct

0.3381389	0.1029231	0.5521639
0.2270615	0.1019583	0.5518017
0.9958714	0.0997892	0.3893751
0.1071496	0.0979078	0.3888418
0.6709523	0.0965708	0.5539091
0.5600487	0.0996620	0.5537642
0.3301914	0.0963985	0.3883747
0.4410803	0.0995078	0.3884942
0.0052275	0.0998594	0.5529813
0.8939508	0.0979846	0.5534911
0.6629747	0.1027139	0.3899526
0.7740310	0.1018420	0.3903309
0.0616233	0.2007340	0.5523686
0.9394853	0.2007015	0.3899186
0.3452054	0.3066644	0.5498399
0.2314750	0.3039448	0.5505860
0.9960420	0.2997807	0.3895523
0.1077959	0.2980264	0.3890657
0.1738731	0.2029190	0.5514465
0.1620229	0.1971664	0.3887464
0.3954730	0.2035859	0.5516162
0.2731072	0.1954543	0.3885523
0.6737739	0.2932362	0.5531125
0.5637138	0.3001775	0.5518050
0.3274101	0.2930889	0.3890708
0.4374911	0.3000321	0.3904021
0.5058814	0.2009956	0.5522643
0.4952859	0.2008187	0.3900168
0.7280455	0.1956151	0.5536782
0.6057179	0.2034195	0.3905793
0.0051108	0.2998376	0.5527904
0.8933360	0.2981486	0.5532242
0.6559724	0.3065008	0.3923049
0.7696589	0.3038613	0.3915783
0.8391472	0.1973184	0.5535095
0.8272374	0.2028520	0.3907650
0.0604475	0.4003177	0.5525950
0.9406818	0.4002599	0.3896914
0.1729039	0.4019210	0.5514548
0.1651559	0.3970589	0.3890920
0.4064748	0.4092103	0.5470400

0.2770942	0.3949098	0.3891927
0.5218404	0.4056403	0.5495120
0.4794634	0.4054532	0.3927311
0.7240071	0.3950704	0.5530007
0.5947164	0.4090590	0.3951702
0.8359162	0.3972016	0.5531483
0.8282249	0.4019060	0.3907429
0.3354836	0.9023123	0.5517875
0.2239330	0.9010663	0.5527134
0.9991902	0.8989023	0.3887031
0.1104883	0.8971467	0.3883836
0.6689599	0.8970469	0.5537106
0.5580131	0.8994843	0.5545198
0.3321038	0.8968877	0.3885184
0.4430391	0.8993392	0.3876566
0.0018801	0.8989630	0.5535795
0.8905678	0.8972099	0.5539104
0.6655560	0.9020878	0.3903722
0.7771226	0.9009494	0.3895121
0.0556741	0.7986097	0.5536979
0.9453942	0.7985460	0.3886180
0.3327817	0.7040216	0.5466714
0.2225072	0.7015429	0.5522849
0.0016918	0.6974141	0.3891786
0.1143768	0.6950447	0.3893180
0.1670293	0.8008282	0.5535917
0.1673194	0.7963736	0.3886105
0.3898682	0.8032565	0.5482866
0.2784833	0.7954863	0.3895204
0.6645583	0.6957862	0.5476627
0.5560208	0.7011456	0.5396666
0.3363839	0.6956584	0.3945108
0.4449143	0.7009767	0.4023000
0.5011075	0.8005133	0.5497561
0.4998912	0.8003622	0.3923041
0.7225361	0.7956266	0.5526803
0.6111245	0.8030533	0.3937442
0.9993622	0.6974645	0.5531980
0.8866695	0.6951419	0.5529433
0.6682415	0.7038910	0.3953662
0.7785546	0.7014983	0.3899118
0.8337021	0.7964796	0.5536249
0.8340446	0.8007663	0.3886869
0.0572301	0.5988582	0.5525547

0.9438384	0.5988165	0.3898307
0.1693878	0.6003874	0.5512260
0.1724784	0.5937787	0.3899533
0.3871332	0.6077612	0.5332508
0.2883702	0.5894747	0.3917916
0.4912293	0.6194288	0.5063145
0.5097572	0.6192971	0.4356694
0.7126080	0.5896013	0.5503997
0.6138879	0.6076192	0.4087488
0.8285579	0.5938903	0.5523242
0.8316971	0.6003990	0.3909944
0.0588836	0.9994517	0.5530541
0.9422041	0.9993722	0.3892697
0.1700962	0.0012168	0.5524830
0.1641928	0.9975861	0.3885743
0.3922174	0.0022943	0.5530633
0.2754597	0.9966950	0.3882793
0.5033140	0.0003199	0.5543308
0.4977808	0.0001359	0.3879101
0.7256327	0.9968505	0.5539447
0.6088785	0.0020780	0.3891527
0.8368648	0.9976882	0.5536808
0.8309755	0.0011169	0.3897175
0.3409426	0.5052644	0.5428578
0.2284531	0.5019902	0.5496878
0.9988412	0.4988431	0.3896168
0.1115290	0.4971938	0.3893609
0.6574394	0.4853724	0.5516259
0.3435227	0.4853012	0.3906049
0.0022336	0.4988907	0.5527445
0.8895345	0.4973142	0.5530018
0.6601800	0.5051600	0.3992782
0.7726395	0.5019630	0.3924563

(6) The structure of TS2

118

Direct

0.3378882	0.0965091	0.552903
0.2266108	0.0958619	0.553323
-0.0036775	0.1056084	0.390609
0.1074702	0.1036923	0.390767
0.6709616	0.0901830	0.551437

0.5597567	0.0940807	0.551437
0.3303541	0.1029638	0.388718
0.4414004	0.1067107	0.387688
1.0050253	0.0937699	0.553376
0.8937803	0.0917419	0.5527
0.6635981	0.1093942	0.388073
0.7747458	0.1078962	0.38934
0.0612881	0.1947735	0.55491
0.9401910	0.2067132	0.391347
0.3452191	0.3000153	0.557879
0.2314081	0.2977930	0.557999
-0.0028576	0.3058573	0.392199
0.1090864	0.3043572	0.39349
0.1734857	0.1967388	0.555697
0.1626209	0.2031561	0.392671
0.3953307	0.1970141	0.555227
0.2731542	0.2013963	0.391991
0.6739030	0.2866391	0.553472
0.5638382	0.2947117	0.554415
0.3276655	0.2993318	0.393499
0.4376475	0.3062433	0.391069
0.5057966	0.1953322	0.553529
0.4958970	0.2076286	0.389765
0.7281198	0.1890499	0.552348
0.6062237	0.2097863	0.389334
1.0045799	0.2939635	0.555311
0.8929188	0.2922204	0.553976
0.6562889	0.3130301	0.39154
0.7704161	0.3099562	0.391796
0.8390673	0.1910668	0.552825
0.8281524	0.2088816	0.390969
0.0600546	0.3944553	0.556701
0.9417533	0.4060348	0.391804
0.1727348	0.3956753	0.558627
0.1670905	0.4034461	0.394338
0.4067096	0.4027184	0.556697
0.2790892	0.4011127	0.396188
0.5245761	0.4014010	0.555579
0.4775913	0.4124190	0.390486
0.7232928	0.3885516	0.554416
0.5955829	0.4149909	0.393858
0.8351885	0.3912354	0.554382
0.8289991	0.4075802	0.392223

0.3347552	0.8958641	0.546355
0.2237323	0.8948158	0.548006
0.9992512	0.9047441	0.388249
0.1102085	0.9033368	0.387044
0.6683548	0.8904940	0.551235
0.5575207	0.8942987	0.549668
0.3322430	0.9043215	0.384128
0.4431725	0.9084185	0.381816
1.0018829	0.8924244	0.551774
0.8903611	0.8906587	0.55214
0.6667610	0.9092905	0.385848
0.7777061	0.9071805	0.387199
0.0560892	0.7920796	0.550929
0.9454458	0.8040685	0.38789
0.3352128	0.6965955	0.537052
0.2248861	0.6947056	0.54562
1.0019333	0.7031672	0.388363
0.1150501	0.7012375	0.387102
0.1681434	0.7940783	0.548401
0.1671000	0.8026700	0.38553
0.3888286	0.7960459	0.541828
0.2783033	0.8025120	0.38468
0.6614471	0.6879026	0.553323
0.5538569	0.6981125	0.552049
0.3360376	0.7038665	0.388423
0.4470010	0.7131530	0.394323
0.5003246	0.7947011	0.547156
0.5010646	0.8105652	0.383697
0.7212349	0.7888599	0.552176
0.6119441	0.8100945	0.386353
0.9991616	0.6913689	0.551673
0.8859815	0.6888040	0.552796
0.6669779	0.7101201	0.390124
0.7779374	0.7071806	0.388381
0.8329224	0.7898683	0.552387
0.8339506	0.8062930	0.387302
0.0580826	0.5928853	0.552552
0.9438867	0.6046397	0.390145
0.1698383	0.5940507	0.550639
0.1744606	0.6002309	0.388213
0.3892968	0.5930521	0.524617
0.2896633	0.5978945	0.388106
0.4501260	0.5639685	0.469241

0.5041853	0.6255801	0.420087
0.7103577	0.5820078	0.555008
0.6106514	0.6135734	0.403239
0.8268028	0.5873714	0.55412
0.8318338	0.6061585	0.391431
0.0587323	0.9933495	0.552242
0.9425708	1.0053913	0.389312
0.1696971	-0.0047945	0.551162
0.1641035	1.0037639	0.388412
0.3916706	-0.0040812	0.549806
0.2755763	1.0032855	0.386901
0.5029029	0.9948953	0.549855
0.4982439	0.0082003	0.384328
0.7254291	0.9905036	0.551456
0.6096869	0.0090358	0.385647
0.8367355	0.9913306	0.551987
0.8314928	0.0074149	0.38869
0.3410858	0.4963437	0.551946
0.2290244	0.4954766	0.556021
1.0002441	0.5046982	0.391204
0.1126993	0.5034279	0.391311
0.6537035	0.4774516	0.555449
0.3506997	0.4905873	0.395468
1.0019729	0.4929553	0.554966
0.8890430	0.4914080	0.554666
0.6603790	0.5100846	0.398945
0.7725458	0.5074733	0.394052

(7) The optimized final2 geometry

118

Direct

0.3390656	0.1056929	0.5528747
0.2277753	0.1037745	0.5530518
0.9966328	0.1007674	0.3899138
0.1078510	0.1007813	0.3897194
0.6720213	0.0927318	0.5524098
0.5610704	0.0980102	0.5525255
0.3299745	0.1007068	0.3890372
0.4411906	0.1006385	0.3887519
1.0061992	0.0993080	0.5529482
0.8950175	0.0951995	0.5527094
0.6632987	0.1007254	0.3891532
0.7744983	0.1007925	0.3895292
0.0640417	0.2012606	0.5530768

0.9412337	0.2007731	0.3897951
0.3510664	0.3109118	0.5530545
0.2367165	0.3072979	0.5531370
0.9966713	0.3007437	0.3896206
0.1078971	0.3007437	0.3894944
0.1766108	0.2054447	0.5530858
0.1633013	0.2007811	0.3895127
0.3980944	0.2058919	0.5528801
0.2745370	0.2007400	0.3891486
0.6772688	0.2885267	0.5524094
0.5678474	0.2975796	0.5526277
0.3300132	0.3006884	0.3887359
0.4412323	0.3006174	0.3883742
0.5082404	0.2001905	0.5526318
0.4966520	0.2006212	0.3885561
0.7307383	0.1912164	0.5524221
0.6078849	0.2006906	0.3887378
1.0087188	0.3007110	0.5530530
0.8963589	0.2967009	0.5527901
0.6633315	0.3007204	0.3888012
0.7745192	0.3007682	0.3892334
0.8417309	0.1948735	0.5525926
0.8299642	0.2007867	0.3896020
0.0654170	0.4021337	0.5532970
0.9412281	0.4007328	0.3893764
0.1805174	0.4064598	0.5532216
0.1633749	0.4007630	0.3892640
0.4172402	0.4133712	0.5531926
0.2745567	0.4007285	0.3888640
0.5324079	0.4061382	0.5529546
0.4966971	0.4005981	0.3881588
0.7261170	0.3903627	0.5526860
0.6078928	0.4006597	0.3883038
0.8376853	0.3948676	0.5528491
0.8299957	0.4007535	0.3891539
0.3333841	0.9065800	0.5528510
0.2225111	0.9029162	0.5530436
0.9965942	0.9007430	0.3897048
0.1078371	0.9007727	0.3895439
0.6659050	0.8919444	0.5526472
0.5556948	0.8975814	0.5526517
0.3299047	0.9007110	0.3889256
0.4411610	0.9006251	0.3887607
1.0001082	0.8964588	0.5531519

0.8874664	0.8923639	0.5529562
0.6632535	0.9007096	0.3891519
0.7744809	0.9007698	0.3894242
0.0554937	0.7970576	0.5532262
0.9411858	0.8007359	0.3894568
0.3381682	0.7073557	0.5529555
0.2266078	0.7028953	0.5531556
0.9966278	0.7007319	0.3893244
0.1078534	0.7007361	0.3892432
0.1678968	0.8010494	0.5531152
0.1632926	0.8007535	0.3893260
0.3869059	0.8092119	0.5527548
0.2744762	0.8007253	0.3889912
0.6467447	0.6843740	0.5530674
0.5314124	0.6912866	0.5529333
0.3299685	0.7007126	0.3887103
0.4411790	0.7006187	0.3885035
0.4962249	0.8001373	0.5527137
0.4965878	0.8006264	0.3886877
0.7129030	0.7868917	0.5528996
0.6078067	0.8006866	0.3888502
0.9988326	0.6956206	0.5532719
0.8836606	0.6913345	0.5531501
0.6632756	0.7006893	0.3888903
0.7744707	0.7007494	0.3891027
0.8273388	0.7904601	0.5529618
0.8299298	0.8007411	0.3893681
0.0599152	0.5987674	0.5534840
0.9412118	0.6007298	0.3891660
0.1745339	0.6018478	0.5533891
0.1633465	0.6007654	0.3891410
0.4114449	0.6211476	0.5530827
0.2745494	0.6007358	0.3888189
0.4412481	0.5006051	0.3882040
0.4966457	0.6006110	0.3883880
0.7047787	0.5825655	0.5532311
0.6078779	0.6006517	0.3884387
0.8245397	0.5903135	0.5532126
0.8299578	0.6007361	0.3890210
0.0579594	0.9984086	0.5531282
0.9411876	0.0007530	0.3898491
0.1691240	0.0025638	0.5530909
0.1632679	1.0007673	0.3895532
0.3919579	0.0051091	0.5528139

0.2744710	1.0007108	0.3892271
0.5028876	0.9998011	0.5526091
0.4966115	0.0006175	0.3888111
0.7249150	0.9921598	0.5525405
0.6078273	0.0006849	0.3889623
0.8362694	0.9940270	0.5526760
0.8299419	0.0007623	0.3896790
0.3595693	0.5153423	0.5532558
0.2397270	0.5074409	0.5533272
0.9966462	0.5007287	0.3892893
0.1079253	0.5007272	0.3892131
0.6532591	0.4767104	0.5529629
0.3300093	0.5006909	0.3885716
1.0044135	0.4989800	0.5533819
0.8897131	0.4958756	0.5532512
0.6633247	0.5006891	0.3885199
0.7745435	0.5007452	0.3888628

The structures of the first set of the calculation in Fig. 3 (c)

(8) The optimized initial3 geometry

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Direct

0.2769610	0.0994055	0.5518204
0.1663658	0.1000233	0.5519856
0.0552647	0.1002157	0.3900606
0.1663620	0.1000926	0.3897839
0.6118920	0.1004266	0.5511918
0.4990823	0.1009205	0.5513052
0.3887767	0.0993942	0.3893203
0.4998644	0.0990194	0.3893353
0.9449844	0.0999990	0.5519483
0.8340380	0.0997129	0.5516342
0.7227019	0.0997513	0.3896729
0.8336454	0.1000844	0.3899925
0.0000126	0.2000550	0.5519345
0.0001680	0.2007735	0.3898466
0.2744539	0.2948877	0.5509517
0.1675623	0.3001093	0.5514409
0.0562460	0.3008371	0.3895111
0.1682798	0.3009625	0.3895027
0.1109600	0.1997838	0.5518820
0.2219288	0.2000531	0.3895437
0.3335520	0.2010690	0.5513399

0.3330290	0.1997211	0.3894502
0.3884719	0.2979577	0.3899151
0.4994859	0.2974427	0.3901618
0.4416568	0.1942653	0.5509732
0.5558694	0.1980988	0.3896579
0.6706336	0.1926805	0.5507965
0.6665856	0.1996095	0.3896807
0.9444247	0.2999534	0.5518441
0.8327659	0.3007093	0.5515214
0.7205547	0.3001301	0.3897257
0.8323661	0.3005464	0.3894623
0.7778165	0.1994846	0.5512983
0.8887009	0.2006764	0.3898070
0.9992365	0.4000960	0.5518268
0.9999310	0.4004061	0.3892021
0.1109768	0.4006133	0.5514147
0.2253439	0.4009596	0.3896468
0.3388990	0.4013035	0.3901042
0.5528956	0.3938610	0.3903485
0.6625459	0.4005198	0.3900431
0.7831363	0.3996308	0.5512093
0.8881173	0.4002359	0.3891701
0.2769610	0.9005945	0.5518204
0.1663658	0.8999767	0.5519856
0.0552647	0.8997843	0.3900606
0.1663620	0.8999074	0.3897839
0.6118920	0.8995734	0.5511918
0.4990823	0.8990795	0.5513052
0.3887767	0.9006058	0.3893203
0.4998644	0.9009806	0.3893353
0.9449844	0.9000010	0.5519483
0.8340380	0.9002871	0.5516342
0.7227019	0.9002487	0.3896729
0.8336454	0.8999156	0.3899925
0.0000126	0.7999450	0.5519345
0.0001680	0.7992265	0.3898466
0.2744539	0.7051123	0.5509517
0.1675623	0.6998907	0.5514409
0.0562460	0.6991629	0.3895111
0.1682798	0.6990375	0.3895027
0.1109600	0.8002162	0.5518820
0.2219288	0.7999469	0.3895437
0.3335520	0.7989310	0.5513399
0.3330290	0.8002789	0.3894502

0.3884719	0.7020423	0.3899151
0.4994859	0.7025573	0.3901618
0.4416568	0.8057347	0.5509732
0.5558694	0.8019012	0.3896579
0.6706336	0.8073195	0.5507965
0.6665856	0.8003905	0.3896807
0.9444247	0.7000466	0.5518441
0.8327659	0.6992907	0.5515214
0.7205547	0.6998699	0.3897257
0.8323661	0.6994536	0.3894623
0.7778165	0.8005154	0.5512983
0.8887009	0.7993236	0.3898070
0.9992365	0.5999040	0.5518268
0.9999310	0.5995939	0.3892021
0.1109768	0.5993867	0.5514147
0.2253439	0.5990404	0.3896468
0.3388990	0.5986965	0.3901042
0.5528956	0.6061390	0.3903485
0.6625459	0.5994802	0.3900431
0.7831363	0.6003692	0.5512093
0.8881173	0.5997641	0.3891701
0.0002760	0.0000000	0.5520523
0.0000638	0.0000000	0.3902374
0.1109271	0.0000000	0.5520911
0.2216448	0.0000000	0.3896838
0.3328817	0.0000000	0.5518207
0.3331145	0.0000000	0.3893698
0.4436774	0.0000000	0.5515927
0.5557826	0.0000000	0.3893810
0.6674887	0.0000000	0.5514179
0.6672447	0.0000000	0.3895781
0.7782318	0.0000000	0.5515548
0.8889783	0.0000000	0.3901919
0.1586830	0.5000000	0.5508968
0.0563963	0.5000000	0.3891295
0.1685277	0.5000000	0.3894666
0.3958700	0.5000000	0.3902005
0.9448865	0.5000000	0.5518635
0.8312089	0.5000000	0.5515707
0.7199049	0.5000000	0.3896657
0.8311306	0.5000000	0.3891275

(9)The structure of TS3

Direct

0.2759856	0.1013734	0.5510947
0.1646467	0.1001843	0.5515369
0.0568140	0.0980273	0.3890753
0.1681020	0.0968227	0.3891565
0.6107858	0.0965918	0.5506025
0.4989489	0.0988819	0.5511231
0.3902367	0.0992393	0.3886084
0.5012401	0.1023424	0.3891135
0.9423189	0.0990975	0.5510762
0.8315406	0.0978646	0.5511072
0.7239035	0.1015642	0.3895013
0.8351283	0.0998759	0.3894094
0.9984680	0.1992265	0.5513009
0.0003334	0.1984089	0.3894233
0.2742307	0.2949954	0.5513774
0.1671475	0.2992357	0.5514749
0.0546433	0.2986011	0.3897124
0.1656121	0.2971280	0.3903288
0.1092438	0.1994271	0.5514018
0.2223114	0.1974926	0.3897287
0.3344239	0.2022350	0.5510991
0.3335626	0.1981775	0.3899098
0.3883945	0.2983407	0.3923632
0.4995046	0.3015274	0.3929758
0.4426245	0.1930458	0.5519383
0.5559373	0.2022951	0.3909489
0.6686567	0.1910178	0.5500922
0.6672758	0.2015879	0.3906952
0.9435688	0.2993663	0.5513816
0.8315714	0.2996441	0.5510736
0.7216536	0.3019528	0.3911133
0.8327112	0.3005241	0.3900687
0.7754211	0.1980671	0.5509179
0.8892504	0.2000734	0.3895604
0.9993395	0.3990510	0.5513821
0.9982275	0.3990762	0.3895640
0.1114071	0.3998891	0.5513561
0.2206308	0.3969819	0.3917328
0.3314812	0.3966387	0.3936590
0.5540131	0.4030585	0.3936189
0.6653781	0.4024020	0.3922892

0.7833044	0.3988956	0.5506562
0.8868223	0.4008987	0.3898043
0.2708493	0.9086726	0.5518608
0.1624094	0.9020553	0.5540764
0.0605298	0.8967130	0.3887121
0.1741957	0.8943150	0.3904949
0.6076822	0.8937726	0.5474339
0.4987690	0.8996176	0.5415561
0.3945153	0.8998764	0.3922720
0.5037066	0.9053912	0.3875343
0.9442770	0.8981326	0.5512039
0.8336002	0.8979895	0.5507038
0.7231981	0.9012741	0.3887470
0.8346622	0.9000204	0.3890408
0.0014812	0.7979170	0.5517710
0.0021947	0.7987590	0.3886186
0.2829022	0.7078857	0.5386246
0.1721988	0.6978906	0.5490940
0.0579690	0.6991473	0.3891760
0.1700360	0.6983430	0.3920111
0.1129325	0.7978542	0.5527597
0.2336707	0.7930273	0.3943914
0.3176924	0.8105322	0.5400353
0.3528800	0.7938704	0.4040289
0.3941361	0.7628414	0.5020761
0.4917406	0.7110804	0.3864806
0.4975233	0.5023182	0.3937822
0.5548526	0.8035257	0.3861967
0.6695404	0.8018117	0.5487900
0.6666128	0.8018707	0.3881707
0.9458790	0.6985198	0.5512230
0.8335095	0.6973636	0.5508542
0.7206147	0.7017585	0.3896573
0.8328863	0.7006989	0.3893619
0.7764698	0.7979930	0.5504904
0.8899411	0.7997592	0.3887647
0.0014643	0.5990938	0.5514864
1.0002075	0.5995861	0.3888561
0.1143334	0.5990517	0.5508340
0.2210006	0.5955868	0.3922019
0.3273519	0.5894415	0.3955756
0.5460446	0.6071510	0.3908968
0.6608960	0.6043746	0.3908901
0.7842869	0.5990238	0.5506868

0.8884497	0.6006373	0.3892110
0.9973954	0.9996495	0.5512672
0.0031722	0.9974035	0.3886276
0.1075107	1.0010429	0.5523889
0.2252282	0.9969540	0.3896936
0.3303461	0.0031617	0.5499626
0.3360678	0.9981923	0.3895095
0.4422134	0.9949631	0.5478151
0.5581472	0.0038280	0.3877529
0.6654483	0.9959281	0.5504857
0.6688828	0.0021279	0.3885280
0.7764985	0.9972039	0.5509699
0.8911835	0.9992393	0.3888792
0.1605625	0.4984885	0.5506445
0.0538742	0.4983441	0.3893846
0.1645353	0.4962092	0.3906646
0.3864937	0.4971016	0.3952184
0.9461425	0.4993059	0.5514406
0.8325261	0.4987646	0.5510614
0.7185121	0.5034550	0.3912733
0.8310023	0.5017045	0.3900419

(10) The optimized final3 geometry

106

Direct

0.2742766	0.0961759	0.5512173
0.1641027	0.1028839	0.5512758
0.0557304	0.0997816	0.3891918
0.1669944	0.0997498	0.3893982
0.6084796	0.0921806	0.5506666
0.4961040	0.0898512	0.5508363
0.3890730	0.0998386	0.3896808
0.5003065	0.0998746	0.3896727
0.9404063	0.1023854	0.5512752
0.8287815	0.0990314	0.5510526
0.7223797	0.0998968	0.3891023
0.8335959	0.0998344	0.3889810
0.9990668	0.2026321	0.5515504
0.0003448	0.1998331	0.3893473
0.2772889	0.2917750	0.5513016
0.1709094	0.3026104	0.5516841
0.0558320	0.2998064	0.3896727
0.1670482	0.2997850	0.3902909

0.1105689	0.2032397	0.5515819
0.2224788	0.1997591	0.3900603
0.3334100	0.1960116	0.5512211
0.3336472	0.1998005	0.3905448
0.3891033	0.2997952	0.3922853
0.5003397	0.2998329	0.3926982
0.4406101	0.1841252	0.5508429
0.5557831	0.1998738	0.3908590
0.6664892	0.1875573	0.5504141
0.6669929	0.1999432	0.3903038
0.9465183	0.3035744	0.5516527
0.8330404	0.3022256	0.5513114
0.7225031	0.2999363	0.3908486
0.8337336	0.2998833	0.3897914
0.7736454	0.2000820	0.5510237
0.8890995	0.1998894	0.3893216
0.0058950	0.4034436	0.5517493
0.0003879	0.3998487	0.3895654
0.1185349	0.4064474	0.5518264
0.2224250	0.3997635	0.3913418
0.3336606	0.3997734	0.3929674
0.5558023	0.3998800	0.3936319
0.6670883	0.3999095	0.3924645
0.7899688	0.4036155	0.5509917
0.8891359	0.3999176	0.3896825
0.2674975	0.8989236	0.5511497
0.1593886	0.9078911	0.5509435
0.0557443	0.8998147	0.3887955
0.1669614	0.8997899	0.3889777
0.6016402	0.8863131	0.5507842
0.4847035	0.8818852	0.5510059
0.3890490	0.8998364	0.3891118
0.5002642	0.8998700	0.3891583
0.9431737	0.9011782	0.5508574
0.8319282	0.8988079	0.5506981
0.7224329	0.8999467	0.3887232
0.8336413	0.8999092	0.3886371
0.0019094	0.8024819	0.5509213
0.0003393	0.7997831	0.3887080
0.3890604	0.6999012	0.3913077
0.1867880	0.7190916	0.5513431
0.0557657	0.6997994	0.3890018
0.1669809	0.6997741	0.3895867
0.1127908	0.8049046	0.5510660

0.2224011	0.7998021	0.3892412
0.3014570	0.7872391	0.5514165
0.3335882	0.7998503	0.3896242
0.4124309	0.7895004	0.5512451
0.5003078	0.6999478	0.3917315
0.5003580	0.4999065	0.3940760
0.5557470	0.7999276	0.3899647
0.6684870	0.7989126	0.5503176
0.6669733	0.7999322	0.3895717
0.9507627	0.7018976	0.5510534
0.8375652	0.6995298	0.5506917
0.7224619	0.6999709	0.3902786
0.8336904	0.6999171	0.3892715
0.7771226	0.7980141	0.5505157
0.8891176	0.7998210	0.3887014
0.0135105	0.6065616	0.5514238
0.0003476	0.5998296	0.3891867
0.1323563	0.6118710	0.5516518
0.2224232	0.5998141	0.3907962
0.3336301	0.5998777	0.3922967
0.5557801	0.5999410	0.3930928
0.6670548	0.5999591	0.3920985
0.7907006	0.6004171	0.5505497
0.8891152	0.5998756	0.3893603
0.9952327	0.0031088	0.5510173
0.0003149	-0.0001992	0.3888567
0.1056294	0.0052026	0.5510271
0.2224110	-0.0002106	0.3891216
0.3278175	0.9945722	0.5511104
0.3336441	-0.0001666	0.3891128
0.4379930	0.9879799	0.5510362
0.5556885	-0.0000932	0.3890146
0.6608911	0.9904368	0.5507684
0.6669838	-0.0000586	0.3888157
0.7731734	0.9965405	0.5508006
0.8890390	-0.0001529	0.3887042
0.1700765	0.5057291	0.5516185
0.0557857	0.4998172	0.3896164
0.1670374	0.4998055	0.3906596
0.3890839	0.4998586	0.3937039
0.9566188	0.5055364	0.5515418
0.8420101	0.5025822	0.5511134
0.7224866	0.4999438	0.3917236
0.8337213	0.4998845	0.3900841

2. The geometries of the evolution process in Fig. 4.(Direct coordinates, the order of the structure is from left to right)

(1) The optimized geometry of V6+V8

106

Direct

0.2750773	0.0968231	0.5523152
0.1642179	0.0978702	0.5524659
0.0641630	0.1015448	0.3898576
0.1778995	0.1029916	0.3902507
0.6088035	0.1007070	0.5499254
0.4967211	0.1050025	0.5500991
0.3960392	0.0996891	0.3907457
0.5060882	0.0956622	0.3907937
0.9433544	0.0987078	0.5515649
0.8324746	0.0982745	0.5509065
0.7260101	0.0996200	0.3897601
0.8377767	0.0994646	0.3896368
0.0000101	0.1986686	0.5520054
0.0038693	0.2004676	0.3898023
0.2757454	0.2965479	0.5518717
0.1673430	0.2985025	0.5523897
0.0581697	0.3004856	0.3897995
0.1730712	0.3012893	0.3900408
0.1105025	0.1983233	0.5524503
0.2388459	0.2052052	0.3903303
0.3278356	0.1955007	0.5518035
0.3537082	0.2051297	0.3906504
0.4471421	0.3274827	0.5493790
0.4822759	0.2867563	0.3908244
0.4379991	0.2078474	0.5504711
0.5546492	0.1966636	0.3904296
0.6705234	0.1926883	0.5498350
0.6661487	0.1989551	0.3901705
0.9476329	0.2998929	0.5520052
0.8351646	0.3000997	0.5514898
0.7176994	0.2999294	0.3901706

0.8310673	0.2998689	0.3897394
0.7775869	0.1991743	0.5507608
0.8911940	0.2006661	0.3896777
0.0054639	0.3997797	0.5522214
0.9985133	0.3994757	0.3896305
0.1180154	0.4008904	0.5521732
0.2176673	0.4014494	0.3901883
0.3477736	0.3870684	0.5504198
0.5388078	0.3850487	0.3908739
0.6524588	0.3965762	0.3906504
0.7867277	0.3989542	0.5514128
0.8848026	0.4000186	0.3896208
0.2750612	0.9000013	0.5522103
0.1642089	0.8990862	0.5523528
0.0639395	0.8974531	0.3897065
0.1776639	0.8959951	0.3901494
0.6087879	0.8963180	0.5498253
0.4967448	0.8919192	0.5500311
0.3959148	0.8990982	0.3907304
0.5059964	0.9028792	0.3907432
0.9434081	0.8983178	0.5514607
0.8325158	0.8988413	0.5507795
0.7258481	0.8987329	0.3896688
0.8375704	0.8991694	0.3895189
0.0000636	0.7983353	0.5518143
0.0035292	0.7985170	0.3895384
0.2757484	0.7003354	0.5516802
0.1673359	0.6984419	0.5522067
0.0578176	0.6985691	0.3895365
0.1726752	0.6977440	0.3898293
0.1105434	0.7986527	0.5522626
0.2384257	0.7938008	0.3901986
0.3278612	0.8013766	0.5516111
0.3532014	0.7938528	0.3906155
0.4380263	0.7890632	0.5503474
0.4825241	0.7115816	0.3907553
0.4471151	0.6694772	0.5493444
0.5545316	0.8018518	0.3902799
0.6705448	0.8043747	0.5496199
0.6659714	0.7993839	0.3900275
0.9476744	0.6971145	0.5517729
0.8351815	0.6969492	0.5512294
0.7174612	0.6983782	0.3900319
0.8308033	0.6986645	0.3895454

0.7776197	0.7979409	0.5505283
0.8908832	0.7979990	0.3894489
0.0054684	0.5971843	0.5520931
-0.0016958	0.5995096	0.3894717
0.1180178	0.5960472	0.5520685
0.2175285	0.5977075	0.3900488
0.3477605	0.6098076	0.5503291
0.5388661	0.6133029	0.3909070
0.6524012	0.6015862	0.3906332
0.7867334	0.5980783	0.5512376
0.8846254	0.5986009	0.3894910
-0.0018969	-0.0014829	0.5518115
0.0087588	0.9994935	0.3896355
0.1087047	-0.0015223	0.5522994
0.2295637	0.9994550	0.3903479
0.3319672	0.9983944	0.5518197
0.3393513	-0.0005618	0.3906734
0.4430839	0.9984213	0.5507570
0.5623015	-0.0007597	0.3904726
0.6640319	0.9985054	0.5501116
0.6727399	-0.0008108	0.3898930
0.7755686	-0.0014526	0.5505258
0.8951644	-0.0006639	0.3895190
0.1810762	0.4984509	0.5517755
0.0527584	0.4995617	0.3895458
0.1663650	0.4995550	0.3898624
0.3005191	0.4984098	0.5506815
0.9497625	0.4984880	0.5521353
0.8361740	0.4985102	0.5517885
0.7090731	0.4990964	0.3903626
0.8246366	0.4992372	0.3897116

(2) The structure of TS between V6+V8 and Intermediate

106

Direct

0.2978497	0.0814018	0.5532345
0.1870217	0.0824044	0.5556189
0.0424930	0.1156907	0.3909417
0.1564178	0.1171650	0.3908678
0.6315088	0.0853745	0.5484331
0.5194789	0.0895798	0.5474036
0.3744591	0.1138590	0.3881119
0.4844210	0.1098125	0.3867618
0.9660211	0.0832191	0.5561515

0.8551042	0.0828741	0.5542187
0.7042688	0.1140379	0.3878162
0.8160390	0.1137097	0.3892898
0.0228151	0.1832541	0.5568701
0.9819824	0.2145528	0.3913285
0.2983533	0.2812079	0.5526850
0.1900161	0.2831839	0.5550806
0.0361298	0.3145982	0.3912348
0.1511392	0.3153245	0.3908722
0.1332540	0.1829412	0.5565614
0.2172621	0.2194405	0.3909571
0.3505260	0.1801573	0.5520232
0.3324369	0.2194959	0.3902154
0.4695638	0.3119216	0.5466627
0.4598783	0.3002603	0.3904126
0.4605606	0.1926428	0.5485844
0.5327830	0.2107204	0.3885687
0.6932906	0.1774788	0.5506711
0.6442249	0.2132991	0.3894948
0.9704384	0.2845502	0.5565698
0.8579293	0.2847638	0.5558939
0.6955101	0.3143699	0.3915460
0.8089252	0.3142144	0.3914994
0.8002166	0.1838594	0.5539019
0.8691973	0.2149569	0.3909556
0.0282094	0.3844767	0.5557106
0.9763676	0.4136013	0.3909024
0.1407383	0.3855751	0.5543393
0.1956181	0.4155091	0.3897436
0.3701809	0.3716483	0.5489195
0.5163275	0.3985306	0.3914904
0.6298981	0.4109828	0.3918855
0.8096232	0.3836348	0.5558851
0.8625266	0.4144419	0.3913579
0.2978542	0.8845964	0.5502503
0.1870971	0.8836718	0.5529160
0.0425952	0.9114963	0.3894926
0.1564912	0.9100272	0.3894840
0.6315336	0.8810266	0.5467132
0.5195217	0.8765034	0.5455034
0.3744914	0.9134611	0.3865279
0.4844019	0.9175208	0.3843030
0.9659909	0.8829251	0.5545084
0.8551292	0.8835252	0.5527377

0.7042746	0.9131532	0.3853041
0.8160603	0.9134259	0.3872975
0.0228026	0.7829036	0.5537789
0.9820757	0.8126137	0.3889460
0.2984136	0.6849169	0.5472408
0.1900843	0.6830301	0.5506960
0.0362546	0.7126131	0.3889359
0.1512523	0.7119273	0.3885693
0.1332923	0.7831862	0.5526146
0.2173632	0.8078314	0.3886738
0.3506063	0.7858950	0.5468801
0.3325632	0.8076725	0.3879747
0.4607751	0.7733706	0.5449629
0.4596453	0.7272387	0.3869206
0.4697775	0.6537933	0.5439241
0.5327424	0.8165190	0.3842732
0.6933368	0.7889721	0.5475764
0.6442367	0.8139392	0.3851542
0.9704119	0.6817457	0.5536875
0.8578411	0.6815794	0.5530679
0.6955227	0.7129873	0.3880560
0.8089761	0.7130363	0.3885854
0.8001947	0.7825924	0.5510427
0.8693032	0.8122585	0.3881921
0.0282266	0.5818635	0.5539360
0.9764712	0.6136273	0.3895056
0.1407265	0.5806746	0.5520759
0.1956979	0.6117049	0.3883128
0.3705090	0.5943155	0.5457034
0.5161067	0.6291707	0.3902199
0.6299564	0.6165891	0.3902414
0.8095279	0.5827869	0.5541094
0.8626270	0.6129065	0.3898082
0.0208162	0.9830362	0.5558050
0.9872606	0.0135576	0.3899020
0.1315127	0.9830282	0.5553247
0.2081723	0.0136385	0.3897411
0.3546563	0.9830058	0.5501245
0.3179359	0.0136196	0.3880771
0.4657971	0.9830530	0.5472728
0.5407296	0.0136781	0.3847196
0.6867203	0.9831935	0.5488478
0.6511634	0.0136606	0.3852835
0.7981996	0.9832223	0.5518394

0.8735734	0.0135377	0.3887604
0.2037732	0.4830711	0.5514886
0.0307081	0.5135811	0.3898967
0.1443863	0.5136015	0.3891670
0.3231016	0.4829077	0.5482119
0.9725297	0.4831603	0.5552583
0.8589396	0.4831929	0.5555779
0.6863424	0.5138319	0.3914500
0.8022901	0.5137159	0.3909114

(3) The structure of intermediate between V6+V8 and V5+V9

106

Direct

0.3399873	0.0520877	0.5590543
0.2293618	0.0524013	0.5625364
0.0037289	0.1431145	0.3931486
0.1173680	0.1444388	0.3942148
0.6742300	0.0616089	0.5475764
0.5616525	0.0678800	0.5459363
0.3358044	0.1420761	0.3899474
0.4455875	0.1390713	0.3849910
0.0092183	0.0539895	0.5611415
0.8986251	0.0553090	0.5575882
0.6651806	0.1421772	0.3857942
0.7770423	0.1415977	0.3885848
0.0643017	0.1538399	0.5638221
0.9433096	0.2420744	0.3938169
0.3368390	0.2507234	0.5570116
0.2290715	0.2528610	0.5618088
-0.0024009	0.3420813	0.3947237
0.1124237	0.3428685	0.3951659
0.1743182	0.1525115	0.5647098
0.1782128	0.2466698	0.3958043
0.3912702	0.1515314	0.5569966
0.2926164	0.2469651	0.3959183
0.5054011	0.2854626	0.5376326
0.4247216	0.3315556	0.3968139
0.5006349	0.1685146	0.5464870
0.4938453	0.2410554	0.3882754
0.7363987	0.1521052	0.5517328
0.6057493	0.2418298	0.3891526
0.0110386	0.2552852	0.5626529
0.8994322	0.2568067	0.5601638
0.6574587	0.3424665	0.3942982

0.7708977	0.3419504	0.3943165
0.8432293	0.1560712	0.5570454
0.8306753	0.2425041	0.3923536
0.0671765	0.3551195	0.5605324
0.9382786	0.4412230	0.3941451
0.1782351	0.3542569	0.5580324
0.1570936	0.4429128	0.3933022
0.4037959	0.3410323	0.5414416
0.4774826	0.4350277	0.4074126
0.5941993	0.4390419	0.4000118
0.8509914	0.3560333	0.5587896
0.8247757	0.4419843	0.3953110
0.3437055	0.8530918	0.5482050
0.2326955	0.8528881	0.5529787
0.0037995	0.9392755	0.3904388
0.1175346	0.9377843	0.3915901
0.6763617	0.8585664	0.5454529
0.5636989	0.8608272	0.5425492
0.3358181	0.9408633	0.3874893
0.4456152	0.9444460	0.3823905
0.0099847	0.8539400	0.5560963
0.8986010	0.8560392	0.5538448
0.6652208	0.9408861	0.3828528
0.7771416	0.9411752	0.3856301
0.0672474	0.7537139	0.5536850
0.9434303	0.8403935	0.3893065
0.3437101	0.6515438	0.5250242
0.2355237	0.6523869	0.5404805
-0.0022625	0.7403928	0.3902691
0.1126136	0.7394629	0.3908461
0.1788998	0.7526400	0.5505386
0.1784718	0.8355830	0.3915287
0.3992547	0.7518011	0.5357527
0.2930546	0.8355344	0.3915701
0.5067114	0.7667527	0.5361897
0.4242314	0.7522426	0.3920537
0.4369459	0.5434906	0.4347556
0.4938690	0.8423744	0.3836097
0.7355395	0.7650633	0.5470189
0.6057036	0.8411815	0.3839486
0.0127122	0.6539996	0.5528636
0.8997798	0.6546248	0.5531962
0.6574511	0.7405504	0.3888321
0.7709293	0.7407681	0.3889719

0.8426092	0.7561360	0.5513545
0.8307918	0.8400830	0.3874441
0.0697748	0.5536375	0.5523721
0.9383391	0.6414165	0.3912930
0.1810358	0.5513050	0.5449894
0.1572379	0.6392995	0.3907784
0.3861592	0.5465052	0.4963859
0.4771462	0.6494108	0.4041790
0.5941479	0.6445838	0.3968627
0.8510495	0.5559624	0.5548818
0.8248607	0.6408487	0.3922188
0.0647603	0.9535124	0.5594012
0.9482252	0.0411926	0.3906140
0.1756581	0.9524985	0.5592984
0.1694987	0.0411608	0.3924242
0.3977854	0.9541621	0.5515972
0.2793575	0.0413709	0.3895549
0.5083852	0.9637242	0.5465538
0.5012680	0.0418234	0.3813677
0.7309245	0.9592322	0.5486170
0.6120011	0.0416438	0.3819030
0.8420428	0.9565976	0.5533072
0.8345600	0.0413349	0.3879422
0.2383534	0.4499996	0.5458334
-0.0074863	0.5412484	0.3923306
0.1060357	0.5411071	0.3914368
0.3499401	0.4441707	0.5303662
0.0133149	0.4549369	0.5571931
0.8999857	0.4558046	0.5577299
0.6503499	0.5418018	0.3994671
0.7653321	0.5415394	0.3959528

(4) The structure of TS between intermediate and V5+V9

106

Direct

0.3155997	0.0679536	0.5577675
0.2050999	0.0685263	0.5601806
0.0266428	0.1276319	0.3914993
0.1406478	0.1291237	0.3926520
0.6501718	0.0782618	0.5489956
0.5377043	0.0843061	0.5483041
0.3585889	0.1259246	0.3901543
0.4677940	0.1225838	0.3871295
0.9850936	0.0704944	0.5589528

0.8745742	0.0719133	0.5561845
0.6872295	0.1268680	0.3872283
0.7993467	0.1261312	0.3886030
0.0401678	0.1704139	0.5609470
0.9657516	0.2266037	0.3921033
0.3130263	0.2660460	0.5556319
0.2051614	0.2688616	0.5594743
0.0201416	0.3265408	0.3927170
0.1353081	0.3272702	0.3934007
0.1501471	0.1688237	0.5616437
0.2021367	0.2316515	0.3943087
0.3672503	0.1669218	0.5562393
0.3176048	0.2330142	0.3946856
0.4821698	0.3020434	0.5419876
0.4417478	0.3125209	0.3966841
0.4767151	0.1839973	0.5488229
0.5147824	0.2254356	0.3907451
0.7122194	0.1690177	0.5515960
0.6269284	0.2265075	0.3908030
0.9870576	0.2717965	0.5600718
0.8753999	0.2734314	0.5577962
0.6785604	0.3274535	0.3941467
0.7924241	0.3266334	0.3929743
0.8191037	0.1727368	0.5553944
0.8528606	0.2271963	0.3913102
0.0432148	0.3715344	0.5590287
0.9604282	0.4255533	0.3917547
0.1542597	0.3705439	0.5574160
0.1795109	0.4274185	0.3913376
0.3816166	0.3557202	0.5444154
0.4947866	0.4215969	0.4021716
0.6145422	0.4241912	0.3972111
0.8269754	0.3724932	0.5563563
0.8465235	0.4265977	0.3927246
0.3198975	0.8696056	0.5482706
0.2087308	0.8691964	0.5524407
0.0269302	0.9233107	0.3890609
0.1409971	0.9216713	0.3900482
0.6524965	0.8755146	0.5471079
0.5400884	0.8778818	0.5448252
0.3587996	0.9255966	0.3872482
0.4678807	0.9297075	0.3838815
0.9859072	0.8703127	0.5554915
0.8745092	0.8725349	0.5537119

0.6873219	0.9251596	0.3843905
0.7994553	0.9254880	0.3860388
0.0432964	0.7699408	0.5540299
0.9661032	0.8245041	0.3880722
0.3228744	0.6656138	0.5323608
0.2119960	0.6679161	0.5448178
0.0205218	0.7244782	0.3885465
0.1357999	0.7235633	0.3887479
0.1549548	0.7684770	0.5509630
0.2027903	0.8190184	0.3896245
0.3764939	0.7691698	0.5381854
0.3184925	0.8179291	0.3896853
0.4833756	0.7830884	0.5393744
0.4419828	0.7401879	0.3906513
0.4522031	0.5284999	0.4125364
0.5150430	0.8268877	0.3852198
0.7113912	0.7817071	0.5484585
0.6271810	0.8255767	0.3854530
0.9887378	0.6701303	0.5539869
0.8756137	0.6710013	0.5536524
0.6789979	0.7248693	0.3887729
0.7928054	0.7251265	0.3883332
0.8184471	0.7725898	0.5518602
0.8531903	0.8243255	0.3871236
0.0455636	0.5700833	0.5542190
0.9606160	0.6256637	0.3892941
0.1580682	0.5676914	0.5496511
0.1798494	0.6232107	0.3884942
0.3719680	0.5632443	0.5202193
0.4957971	0.6328462	0.3980088
0.6149964	0.6288390	0.3935323
0.8270385	0.5723999	0.5542263
0.8467115	0.6250743	0.3900986
0.0405047	0.9698960	0.5579521
0.9711833	0.0255064	0.3893338
0.1515479	0.9685501	0.5578278
0.1922294	0.0254676	0.3912236
0.3738040	0.9705172	0.5519287
0.3021168	0.0257041	0.3893201
0.4844663	0.9799476	0.5485665
0.5238646	0.0262354	0.3837000
0.7069372	0.9761157	0.5496723
0.6345185	0.0261322	0.3841748
0.8181037	0.9731603	0.5531470

0.8570761	0.0257247	0.3876185
0.2147365	0.4668768	0.5500954
0.0146564	0.5255100	0.3900833
0.1282893	0.5253812	0.3894181
0.3291564	0.4620750	0.5383897
0.9893227	0.4714907	0.5569605
0.8758558	0.4722943	0.5563303
0.6707292	0.5262989	0.3955215
0.7869383	0.5259213	0.3928332

(5) The structure of V5+V9

106

Direct

0.2745051	0.0958960	0.5526806
0.1640119	0.0962748	0.5530136
0.0646372	0.1018998	0.3900944
0.1788187	0.1035455	0.3905526
0.6094628	0.1050583	0.5489005
0.4970657	0.1116311	0.5488048
0.3963585	0.0997289	0.3913974
0.5056606	0.0956798	0.3917606
0.9442992	0.0978101	0.5516997
0.8338353	0.0990414	0.5506341
0.7250426	0.1004189	0.3902422
0.8372399	0.0998972	0.3899143
-0.0007118	0.1978085	0.5524924
0.0038304	0.2006346	0.3901770
0.2725937	0.2933848	0.5519991
0.1644403	0.2962003	0.5530369
0.0582737	0.3005237	0.3903198
0.1734386	0.3013714	0.3906688
0.1092697	0.1963914	0.5532251
0.2404175	0.2060238	0.3909034
0.3264042	0.1944452	0.5519342
0.3563615	0.2072956	0.3912685
0.4428911	0.3297772	0.5463158
0.4783971	0.2846093	0.3919563
0.4366122	0.2112912	0.5489989
0.5523655	0.1985003	0.3914605
0.6716102	0.1956861	0.5490210
0.6648553	0.1999282	0.3908783
0.9462133	0.2990150	0.5523133
0.8345248	0.3006896	0.5513194
0.7167277	0.3007498	0.3907133

0.8305235	0.3002109	0.3901579
0.7785482	0.1998337	0.5503363
0.8907731	0.2010189	0.3900325
0.0024180	0.3987469	0.5525901
0.9985283	0.3995714	0.3900924
0.1135578	0.3978264	0.5524967
0.2176031	0.4016553	0.3909817
0.3426990	0.3834959	0.5486781
0.5324612	0.3941115	0.3915796
0.6527298	0.3972747	0.3911676
0.7858477	0.3996219	0.5509890
0.8846295	0.4004132	0.3900417
0.2789646	0.8979494	0.5514650
0.1674696	0.8970556	0.5519256
0.0645231	0.8975257	0.3896355
0.1786624	0.8958873	0.3900382
0.6116746	0.9024902	0.5490971
0.4993586	0.9052820	0.5492331
0.3962617	0.8995372	0.3910031
0.5056116	0.9033435	0.3912065
0.9448106	0.8976076	0.5513250
0.8334243	0.8995613	0.5505164
0.7250948	0.8986768	0.3899949
0.8372933	0.8993127	0.3896107
0.0020060	0.7974674	0.5516189
0.0037952	0.7987084	0.3894821
0.2828899	0.6947159	0.5496902
0.1707598	0.6960323	0.5512414
0.0581836	0.6987369	0.3895670
0.1732909	0.6979457	0.3898558
0.1135800	0.7965164	0.5517483
0.2400111	0.7934360	0.3900764
0.3360941	0.7977745	0.5499932
0.3558183	0.7922541	0.3907407
0.4428549	0.8100822	0.5493139
0.4787988	0.7142206	0.3912866
0.4899757	0.4994624	0.3917499
0.5523966	0.8004788	0.3909941
0.6702666	0.8086290	0.5490295
0.6649730	0.7991286	0.3905278
0.9477459	0.6973016	0.5516624
0.8346399	0.6980672	0.5509663
0.7167599	0.6983415	0.3903151
0.8306264	0.6989252	0.3896963

0.7775045	0.7995707	0.5501802
0.8908494	0.7982173	0.3894681
0.0045111	0.5973215	0.5521093
-0.0014632	0.5996647	0.3896673
0.1175228	0.5953321	0.5517127
0.2175761	0.5976605	0.3904661
0.3336899	0.5944373	0.5477899
0.5324776	0.6051104	0.3914016
0.6527394	0.6018666	0.3909666
0.7858918	0.5994746	0.5508458
0.8846745	0.5987736	0.3897050
-0.0005659	-0.0027406	0.5518533
0.0090475	0.9996665	0.3896926
0.1103381	-0.0037277	0.5524118
0.2299848	0.9996639	0.3904644
0.3329665	0.9984508	0.5515310
0.3397838	-0.0003176	0.3909740
0.4436439	0.0072018	0.5500709
0.5617420	-0.0005978	0.3911421
0.6661426	0.0029898	0.5493217
0.6723769	-0.0005207	0.3904294
0.7773229	0.0002104	0.5500587
0.8949263	0.9996089	0.3896295
0.1744558	0.4946385	0.5513756
0.0526445	0.4996011	0.3899330
0.1663723	0.4996527	0.3903964
0.2908185	0.4907138	0.5490777
0.9483491	0.4987135	0.5522759
0.8348223	0.4994891	0.5515497
0.7083355	0.4995718	0.3907490
0.8251199	0.4995700	0.3900744

(6) The structure of TS between V5+V9 and intermediate

106

Direct

0.2724413	0.0921617	0.5554322
0.1620002	0.0929719	0.5576889
0.0655431	0.1041260	0.3917449
0.1793776	0.1054749	0.3928102
0.6071838	0.1020803	0.5437566
0.4943354	0.1074038	0.5416643
0.3973049	0.1030181	0.3931823
0.5072782	0.1001585	0.3943995
0.9420411	0.0948465	0.5547441

0.8315026	0.0962061	0.5514778
0.7266175	0.1037165	0.3913534
0.8387678	0.1028241	0.3906600
0.9971370	0.1948267	0.5563405
0.0051572	0.2030919	0.3920973
0.2707976	0.2900569	0.5481423
0.1624702	0.2930387	0.5537986
0.0595716	0.3030680	0.3922914
0.1742718	0.3037472	0.3930189
0.1073063	0.1933474	0.5575044
0.2399979	0.2077446	0.3943877
0.3245052	0.1905333	0.5506178
0.3548608	0.2084805	0.3947966
0.4386046	0.3207524	0.5199577
0.4809956	0.2902629	0.4045498
0.4327613	0.2054825	0.5388980
0.5544720	0.2019672	0.3987026
0.6689049	0.1930385	0.5459477
0.6666443	0.2032770	0.3950666
0.9438433	0.2959538	0.5547729
0.8320311	0.2975568	0.5528871
0.7189436	0.3041303	0.3942325
0.8322749	0.3032078	0.3922447
0.7758743	0.1968690	0.5505288
0.8923505	0.2037888	0.3917481
1.0000752	0.3955217	0.5533151
0.0002749	0.4023582	0.3911360
0.1112781	0.3942409	0.5510431
0.2192772	0.4037476	0.3916815
0.3387138	0.3778314	0.5327112
0.5365975	0.3999414	0.3962618
0.6556707	0.4012982	0.3943719
0.7835285	0.3966019	0.5518759
0.8865718	0.4034359	0.3913204
0.2768671	0.8938650	0.5518733
0.1655177	0.8935643	0.5536088
0.0661844	0.9000427	0.3895830
0.1802293	0.8983055	0.3900432
0.6095958	0.8994819	0.5457144
0.4973110	0.9019635	0.5458678
0.3979754	0.9026670	0.3897487
0.5075511	0.9071453	0.3888504
0.9427212	0.8945674	0.5525111
0.8313445	0.8967085	0.5502344

0.7268930	0.9020179	0.3881320
0.8389609	0.9022178	0.3884142
0.9999797	0.7942569	0.5519677
0.0057835	0.8013053	0.3887530
0.2809115	0.6901363	0.5435565
0.1687332	0.6924858	0.5480860
0.0603146	0.7013745	0.3886167
0.1753807	0.7003893	0.3886194
0.1116078	0.7929162	0.5516672
0.2417495	0.7960959	0.3892093
0.3344045	0.7938983	0.5469676
0.3577527	0.7956028	0.3895775
0.4407267	0.8070457	0.5453685
0.4815216	0.7178484	0.3898955
0.4932604	0.5036488	0.3939883
0.5546630	0.8043507	0.3883608
0.6681616	0.8056398	0.5467900
0.6670829	0.8027071	0.3881174
0.9456902	0.6941876	0.5512110
0.8325057	0.6951606	0.5504672
0.7191055	0.7019307	0.3888729
0.8327935	0.7020471	0.3886935
0.7753937	0.7967061	0.5490764
0.8928078	0.8011413	0.3883519
0.0024413	0.5941108	0.5509947
0.0006728	0.6023514	0.3890715
0.1154115	0.5917396	0.5483188
0.2197484	0.5999482	0.3891099
0.3299066	0.5899923	0.5352174
0.5353666	0.6095243	0.3913510
0.6553342	0.6055669	0.3907243
0.7838006	0.5964976	0.5507131
0.8869251	0.6018118	0.3893975
0.9973128	0.9942439	0.5548087
0.0102900	0.0020778	0.3902354
0.1083519	0.9929518	0.5561557
0.2313697	0.0021448	0.3914686
0.3308188	0.9946795	0.5519656
0.3411702	0.0025478	0.3912381
0.4412688	0.0033780	0.5470895
0.5634727	0.0032331	0.3903515
0.6640012	0.0001508	0.5459544
0.6739265	0.0029574	0.3897433
0.7751250	0.9973637	0.5490925

0.8964337	0.0024294	0.3894951
0.1719916	0.4907077	0.5455989
0.0546707	0.5021979	0.3897631
0.1683131	0.5019823	0.3896951
0.2876283	0.4857888	0.5363180
0.9462054	0.4955896	0.5520826
0.8326870	0.4964103	0.5518722
0.7110877	0.5032353	0.3918531
0.8274908	0.5027775	0.3907192

(7) The structure of intermediate between V5+V9 and V3+V11

106

Direct

0.2662498	0.0975681	0.5608946
0.1561460	0.0969202	0.5658786
0.0679633	0.0974957	0.3872156
0.1793009	0.0963492	0.3918475
0.5992724	0.1047450	0.5353826
0.4851461	0.1084800	0.5319469
0.3996379	0.1013168	0.3946360
0.5106853	0.1050159	0.3931024
0.9348480	0.0981156	0.5595358
0.8244091	0.0993534	0.5518449
0.7332260	0.1035834	0.3848661
0.8449778	0.1005255	0.3843120
0.9898746	0.1980899	0.5629275
0.0106692	0.1984421	0.3863671
0.2585373	0.2913648	0.5319469
0.1548090	0.2956417	0.5526932
0.0648793	0.2983137	0.3901032
0.1746158	0.2963009	0.4049531
0.1005748	0.1970124	0.5644572
0.2335456	0.1960211	0.4044055
0.3161201	0.1965170	0.5429119
0.3434824	0.1964455	0.4130172
0.4073079	0.2816518	0.4555920
0.5103027	0.3027377	0.4203198
0.4189686	0.2002446	0.5174307
0.5642662	0.2063448	0.3996472
0.6612274	0.1951028	0.5401377
0.6755379	0.2044480	0.3901345
0.9359476	0.2986800	0.5585396
0.8242708	0.3002136	0.5533991
0.7298620	0.3041019	0.3917884

0.8416624	0.3014584	0.3879068
0.7681196	0.1995835	0.5490351
0.8991164	0.2008421	0.3855243
-0.0077324	0.3986337	0.5561803
0.0078942	0.3985681	0.3894309
0.1026418	0.3973053	0.5512216
0.2238957	0.3913748	0.4263674
0.3021649	0.3779984	0.4848991
0.5601339	0.4054881	0.4106417
0.6723089	0.4042219	0.3971675
0.7760177	0.3996290	0.5504854
0.8957287	0.4016077	0.3881362
0.2700317	0.8973317	0.5567441
0.1587535	0.8968220	0.5595988
0.0727120	0.8947015	0.3861852
0.1871696	0.8914848	0.3873792
0.6026765	0.9024540	0.5407775
0.4899919	0.9044472	0.5440203
0.4044761	0.9008893	0.3856506
0.5136396	0.9089670	0.3836480
0.9360263	0.8980353	0.5546368
0.8246207	0.9001046	0.5491171
0.7322235	0.9021383	0.3830310
0.8445621	0.8999401	0.3834031
-0.0069352	0.7976033	0.5542585
0.0134706	0.7967033	0.3857643
0.2734252	0.6936955	0.5453311
0.1618475	0.6958000	0.5507719
0.0696721	0.6967044	0.3880075
0.1845225	0.6928737	0.3918278
0.1046288	0.7963265	0.5556076
0.2506095	0.7891963	0.3888510
0.3269573	0.7966319	0.5494643
0.3674456	0.7916039	0.3889514
0.4336144	0.8097613	0.5447738
0.4880264	0.7196115	0.3909778
0.5089147	0.5071756	0.4100271
0.5614834	0.8058699	0.3852992
0.6615922	0.8090830	0.5421080
0.6738813	0.8028586	0.3846987
0.9384514	0.6976487	0.5518517
0.8256733	0.6985337	0.5486040
0.7278683	0.7023987	0.3867149
0.8417068	0.7004114	0.3853669

0.7688578	0.8001401	0.5459996
0.9002293	0.7989998	0.3843899
-0.0051591	0.5972932	0.5528494
0.0113968	0.5978982	0.3876713
0.1075995	0.5950459	0.5504760
0.2267234	0.5914527	0.4025056
0.3200933	0.5916555	0.5303222
0.5454477	0.6115114	0.3971152
0.6658028	0.6066575	0.3916411
0.7766631	0.5998109	0.5482742
0.8977458	0.6002872	0.3863302
0.9907507	0.9976082	0.5600278
0.0146586	0.9962843	0.3851891
0.1018649	0.9964629	0.5636168
0.2359583	0.9957199	0.3888062
0.3237655	-0.0008700	0.5557726
0.3461560	0.9994228	0.3876433
0.4337754	0.0059388	0.5460371
0.5674288	0.0071257	0.3849853
0.6569847	0.0032454	0.5404172
0.6787930	0.0040409	0.3836721
0.7681481	0.0006089	0.5466862
0.9015197	0.9990435	0.3837853
0.1628473	0.4940842	0.5444406
0.0651294	0.4964539	0.3916887
0.1765483	0.4923543	0.4058070
0.2755133	0.4913858	0.5251811
0.9384476	0.4988419	0.5537529
0.8250305	0.4995567	0.5513607
0.7244352	0.5055448	0.3918084
0.8386992	0.5026198	0.3881839

(8) The structure of TS between intermediate and V3+V11

106

Direct

0.2752176	0.1035961	0.5516647
0.1643717	0.1015475	0.5527661
0.0607996	0.0950983	0.3874475
0.1719632	0.0938188	0.3891893
0.6082651	0.1006010	0.5481840
0.4961611	0.1019128	0.5476829
0.3939891	0.0975211	0.3902384
0.5046301	0.1019812	0.3903295
0.9422074	0.1006501	0.5529202

0.8309575	0.1003248	0.5512440
0.7273585	0.1006943	0.3879432
0.8388130	0.0980477	0.3873812
0.9975492	0.2008198	0.5527988
0.0037282	0.1959396	0.3875882
0.2738740	0.3059163	0.5392074
0.1649812	0.3014078	0.5475113
0.0575303	0.2961162	0.3896573
0.1681991	0.2937859	0.3957767
0.1089712	0.2011994	0.5518192
0.2254076	0.1938755	0.3947715
0.3311454	0.2073749	0.5468093
0.3366155	0.1952876	0.3976007
0.3902303	0.2943393	0.4123102
0.5005315	0.3006786	0.4042034
0.4393521	0.1964454	0.5457040
0.5580927	0.2024261	0.3944024
0.6664146	0.1938955	0.5491598
0.6698982	0.2011879	0.3913803
0.9414321	0.3001028	0.5517997
0.8295006	0.3010197	0.5513109
0.7240232	0.3013540	0.3929261
0.8354539	0.2991372	0.3899590
0.7739156	0.2000454	0.5507893
0.8924884	0.1984452	0.3880330
0.9965830	0.4001050	0.5516532
0.0012644	0.3968715	0.3904879
0.1068045	0.3996816	0.5504632
0.2223803	0.3911748	0.4099797
0.3233880	0.3776018	0.4364422
0.5544058	0.4038221	0.4011070
0.6668883	0.4021576	0.3960641
0.7806804	0.4002511	0.5506074
0.8895849	0.3995544	0.3898475
0.2747895	0.9011492	0.5532974
0.1640099	0.9004525	0.5541871
0.0663353	0.8928957	0.3873632
0.1808331	0.8897949	0.3878379
0.6088761	0.9001576	0.5468329
0.4962036	0.9003657	0.5476762
0.3984862	0.8977713	0.3868839
0.5079858	0.9059376	0.3860254
0.9428275	0.9003967	0.5525581
0.8316024	0.9007275	0.5504705

0.7267227	0.8996208	0.3860037
0.8387450	0.8976459	0.3861239
0.9982608	0.8000240	0.5530518
0.0074373	0.7951188	0.3874436
0.2773720	0.6976565	0.5520027
0.1654213	0.6989353	0.5537100
0.0634550	0.6951972	0.3895395
0.1780626	0.6919976	0.3924688
0.1094663	0.7997626	0.5541028
0.2441412	0.7878735	0.3894262
0.3307890	0.7998212	0.5517239
0.3604895	0.7896457	0.3891540
0.4382704	0.8071862	0.5489111
0.4844712	0.7163330	0.3906255
0.5038667	0.5042762	0.3982029
0.5564347	0.8032771	0.3873930
0.6678148	0.8076193	0.5465701
0.6687776	0.8006443	0.3870451
0.9427137	0.7001584	0.5522017
0.8305370	0.6997107	0.5503944
0.7228582	0.7005599	0.3884754
0.8360895	0.6986352	0.3874797
0.7751172	0.8010409	0.5489634
0.8944797	0.7971224	0.3865906
0.9977503	0.5999775	0.5526283
0.0048091	0.5966883	0.3897266
0.1092162	0.5994457	0.5533405
0.2206795	0.5906709	0.4008160
0.3241312	0.5932214	0.5486457
0.5416275	0.6096613	0.3936655
0.6610904	0.6046389	0.3917985
0.7810407	0.6009831	0.5498570
0.8917282	0.5986522	0.3884095
0.9978207	1.0006083	0.5534337
0.0079816	0.9939753	0.3867464
0.1090282	1.0008908	0.5539045
0.2297742	0.9933422	0.3879339
0.3300397	0.0022056	0.5517708
0.3400482	0.9959719	0.3873956
0.4403988	0.0012216	0.5490385
0.5621025	0.0034401	0.3868407
0.6646795	0.0004986	0.5480860
0.6730431	0.0011007	0.3866557
0.7754960	0.0004265	0.5497605

0.8954006	0.9967400	0.3864562
0.1629761	0.4977953	0.5524768
0.0579454	0.4954430	0.3928966
0.1695247	0.4924508	0.4021591
0.2724534	0.5037807	0.5519728
0.9426002	0.5005033	0.5520517
0.8292416	0.5006101	0.5510429
0.7193808	0.5035244	0.3924401
0.8331661	0.5007231	0.3899511

(9) The structure of V3+V11

106

Direct

0.2791694	0.1074780	0.5517476
0.1687053	0.1013187	0.5516093
0.0595356	0.0995944	0.3892232
0.1703752	0.0996211	0.3894341
0.6111002	0.1009390	0.5505309
0.4977951	0.1045507	0.5507933
0.3924135	0.0994544	0.3898603
0.5028932	0.0993691	0.3899797
0.9466560	0.0982456	0.5511166
0.8354627	0.0981354	0.5508269
0.7268894	0.0994158	0.3894846
0.8380810	0.0994831	0.3892857
0.0006477	0.1990999	0.5513229
0.0050521	0.2017304	0.3895245
0.2739450	0.3223767	0.5519736
0.1654264	0.3024465	0.5519140
0.0615907	0.3027023	0.3899107
0.1762034	0.3041057	0.3902707
0.1122217	0.2004634	0.5516207
0.2264908	0.2009161	0.3900079
0.3340624	0.2182247	0.5517511
0.3370606	0.2003780	0.3904698
0.3939506	0.2997135	0.3915603
0.5036065	0.2952127	0.3922159
0.4416297	0.2005814	0.5511779
0.5592320	0.1981500	0.3909867
0.6711481	0.1920120	0.5502319
0.6703472	0.1992425	0.3905693
0.9426852	0.2975489	0.5513335
0.8315822	0.2989954	0.5509975
0.7215519	0.3011544	0.3909805

0.8339359	0.3008462	0.3900782
0.7780890	0.1975611	0.5507181
0.8924653	0.2013588	0.3895640
-0.0045229	0.3981339	0.5515545
0.0012338	0.4010267	0.3899446
0.1038750	0.3975294	0.5518311
0.2383978	0.4055349	0.3909329
0.3544836	0.4076940	0.3916681
0.5488298	0.3998161	0.3925125
0.6610535	0.4010299	0.3919192
0.7819630	0.3981945	0.5505725
0.8879560	0.4016984	0.3900140
0.2801402	0.8968647	0.5516580
0.1692927	0.8970411	0.5516095
0.0614124	0.8965159	0.3890532
0.1760469	0.8951649	0.3891841
0.6120247	0.8998017	0.5501270
0.4989745	0.9006834	0.5503914
0.3937893	0.8991595	0.3893738
0.5034610	0.9034709	0.3893784
0.9477091	0.8980305	0.5510297
0.8359165	0.8991984	0.5506151
0.7214102	0.8977368	0.3890954
0.8337847	0.8981366	0.3890303
0.0032343	0.7970967	0.5512583
0.0010799	0.7981534	0.3891957
0.2823825	0.6833762	0.5515649
0.1703246	0.6927104	0.5518651
0.0577738	0.6992445	0.3895667
0.1719313	0.6991859	0.3899214
0.1149377	0.7954707	0.5516220
0.2381575	0.7937444	0.3895610
0.3361044	0.7912454	0.5513352
0.3541275	0.7912829	0.3898061
0.4428203	0.8054425	0.5506905
0.4717053	0.7124357	0.3906638
0.4718842	0.4862151	0.3921073
0.5486406	0.7989559	0.3898614
0.6714565	0.8074198	0.5496406
0.6608819	0.7978156	0.3896659
0.9462404	0.6977332	0.5511890
0.8338880	0.6982218	0.5506719
0.7124292	0.6963883	0.3900919
0.8281158	0.6976466	0.3895711

0.7788499	0.7998886	0.5502957
0.8878302	0.7973519	0.3891597
0.0002389	0.5969112	0.5515312
0.0009830	0.5995319	0.3897763
0.1123108	0.5944842	0.5519109
0.2180879	0.5996922	0.3909534
0.3251454	0.5723784	0.5513284
0.5185452	0.5993084	0.3914244
0.6476139	0.5994108	0.3910894
0.7828423	0.6001565	0.5504955
0.8865053	0.5994934	0.3897279
0.0031510	-0.0017492	0.5512033
0.0050071	0.9974425	0.3889835
0.1145133	-0.0014265	0.5514671
0.2264130	0.9982750	0.3892558
0.3335274	0.0025165	0.5515129
0.3369815	0.9985648	0.3893533
0.4438747	0.0022790	0.5509882
0.5591358	0.0005807	0.3893567
0.6677183	0.0000599	0.5504419
0.6702786	-0.0004521	0.3892214
0.7791701	-0.0010987	0.5505932
0.8923893	0.9977170	0.3889859
0.1635197	0.4923585	0.5520413
0.0579080	0.4999319	0.3901225
0.1721330	0.5000595	0.3907526
0.2739938	0.4710918	0.5519638
0.9428449	0.4988301	0.5513861
0.8297372	0.4991876	0.5509011
0.7124693	0.5025203	0.3910823
0.8281988	0.5013617	0.3901703

(10) The structure of TS between V3+V11 and V2+V12

106

Direct

0.2779320	0.0968971	0.5495512
0.1676834	0.1011364	0.5500100
0.0597487	0.0983150	0.3881560
0.1708260	0.0983436	0.3885413
0.6119149	0.0995608	0.5505979
0.4988761	0.0972866	0.5501809
0.3924739	0.0994652	0.3912734

0.5031260	0.0998730	0.3913862
0.9463742	0.1018400	0.5511312
0.8349029	0.1003507	0.5508701
0.7269587	0.0994419	0.3897237
0.8383138	0.0987890	0.3892335
0.0031676	0.2021837	0.5509182
0.0047103	0.2002166	0.3878479
0.2799871	0.2984994	0.5433700
0.1724096	0.3045488	0.5476803
0.0606571	0.3011779	0.3869739
0.1748208	0.3022278	0.3872850
0.1143830	0.2030526	0.5497718
0.2262616	0.1993476	0.3892665
0.3341593	0.1998413	0.5471553
0.3366792	0.2000901	0.3927765
0.3930655	0.2999605	0.3965254
0.5026879	0.2962470	0.3951645
0.4419689	0.1906847	0.5481171
0.5589864	0.1987575	0.3927558
0.6713833	0.1922959	0.5505222
0.6701330	0.1994332	0.3911448
0.9491717	0.3027648	0.5514247
0.8361240	0.3015118	0.5511725
0.7218717	0.3010574	0.3910616
0.8340102	0.3002266	0.3892676
0.7791058	0.2002361	0.5508427
0.8924256	0.2003717	0.3887762
0.0054979	0.4039785	0.5521107
0.0009548	0.3997936	0.3872106
0.1192059	0.4083819	0.5501608
0.2343524	0.4029993	0.3883688
0.3510886	0.4075424	0.3962948
0.5497038	0.4005774	0.3927403
0.6620411	0.4010966	0.3916284
0.7850388	0.3992159	0.5506956
0.8878537	0.4009220	0.3881804
0.2766245	0.8926831	0.5495393
0.1658727	0.8997200	0.5517539
0.0627557	0.8949849	0.3897937
0.1771685	0.8932546	0.3901386
0.6099186	0.8978263	0.5487558
0.4965370	0.8938158	0.5478924
0.3947727	0.8988788	0.3891469
0.5044208	0.9037865	0.3889281

0.9437539	0.9018663	0.5520578
0.8330695	0.9011738	0.5507749
0.7227990	0.8977560	0.3889078
0.8351650	0.8974526	0.3890706
0.9972946	0.8018146	0.5542542
0.0033008	0.7964630	0.3899603
0.2675247	0.6866408	0.5464563
0.1601951	0.7027708	0.5547950
0.0601938	0.6971341	0.3914850
0.1749804	0.6952906	0.3959570
0.1077552	0.8024928	0.5547663
0.2396656	0.7914081	0.3923967
0.3304658	0.7860466	0.5460721
0.3554692	0.7911294	0.3903090
0.4388348	0.7986325	0.5448270
0.4746448	0.7128900	0.3903994
0.4765460	0.4885103	0.3905930
0.5503411	0.7996469	0.3893872
0.6696278	0.8065159	0.5485712
0.6626411	0.7981891	0.3892800
0.9418000	0.7017697	0.5542541
0.8307199	0.6998905	0.5514885
0.7140703	0.6967988	0.3896792
0.8295314	0.6974577	0.3895490
0.7765758	0.8011921	0.5501791
0.8895345	0.7965581	0.3893698
0.9958704	0.6017323	0.5556435
0.0015898	0.5985362	0.3901972
0.1047056	0.6037109	0.5565973
0.2218541	0.5948620	0.4015693
0.2757908	0.5632722	0.5372958
0.5224782	0.6007571	0.3905250
0.6492430	0.5999688	0.3903579
0.7827949	0.5999743	0.5506129
0.8873973	0.5989883	0.3894068
0.0007043	0.0013101	0.5515531
0.0058321	0.9962905	0.3889055
0.1117449	0.0009499	0.5513002
0.2271134	0.9968461	0.3892727
0.3321950	0.9945826	0.5497741
0.3375060	0.9982058	0.3896432
0.4428533	0.9954137	0.5497467
0.5597685	0.0009953	0.3896216
0.6665756	0.9989404	0.5500779

0.6709043	0.9996799	0.3893203
0.7777304	0.0005024	0.5505016
0.8932236	0.9971128	0.3890134
0.1700318	0.5127180	0.5522928
0.0574969	0.4986931	0.3886422
0.1707504	0.4981488	0.3909364
0.3291396	0.5157267	0.4864286
0.9453395	0.5007764	0.5533283
0.8319909	0.5000045	0.5515357
0.7133622	0.5025423	0.3901638
0.8288214	0.5009931	0.3889644

(11) The structure of V2+V12

106

Direct

0.2779674	0.0950489	0.5512875
0.1678965	0.1004519	0.5513142
0.0571952	0.0945262	0.3889561
0.1684772	0.0926227	0.3891329
0.6123638	0.0993384	0.5505362
0.4997106	0.0969423	0.5507061
0.3904835	0.1006287	0.3895637
0.5013845	0.1059863	0.3896934
0.9465277	0.1013987	0.5512268
0.8350582	0.1001844	0.5509826
0.7243703	0.1034042	0.3896017
0.8354794	0.0991117	0.3893689
0.0034194	0.2021924	0.5513280
-0.0016457	0.1958062	0.3891265
0.2787941	0.2933761	0.5513354
0.1722506	0.3045999	0.5514402
0.0516358	0.2954789	0.3895454
0.1624987	0.2917948	0.3903637
0.1142965	0.2024595	0.5514077
0.2212905	0.1934070	0.3900014
0.3349908	0.1973615	0.5513119
0.3321530	0.1987886	0.3906359
0.3848584	0.3010552	0.3925318
0.4950914	0.3067884	0.3927525
0.4426681	0.1901861	0.5509801
0.5542108	0.2066690	0.3911108
0.6720619	0.1923798	0.5503160

0.6655476	0.2046929	0.3907512
0.9500212	0.3029860	0.5513675
0.8367940	0.3017837	0.5511719
0.7167309	0.3062756	0.3910891
0.8293452	0.3019998	0.3899339
0.7794862	0.2002836	0.5509115
0.8872742	0.2000812	0.3893966
0.0064495	0.4043629	0.5512924
-0.0029630	0.3973222	0.3897559
0.1206606	0.4092582	0.5512031
0.2158768	0.3891819	0.3918959
0.3251936	0.3983053	0.3934099
0.5419637	0.4119416	0.3931753
0.6564551	0.4082227	0.3921280
0.7854005	0.3990085	0.5508811
0.8846346	0.4014136	0.3897601
0.2769252	0.8917799	0.5511771
0.1660746	0.8995326	0.5511915
0.0662647	0.8909808	0.3892635
0.1806689	0.8873114	0.3893109
0.6099759	0.8978770	0.5501561
0.4971949	0.8941785	0.5502952
0.3973118	0.9010227	0.3888990
0.5066236	0.9102508	0.3886877
0.9435111	0.9016418	0.5509960
0.8330876	0.9011134	0.5506708
0.7256081	0.9019179	0.3888758
0.8380129	0.8978135	0.3890285
0.9968558	0.8013066	0.5509374
0.0098933	0.7917379	0.3895910
0.2700018	0.6835095	0.5508020
0.1592625	0.7026684	0.5508261
0.0690511	0.6907765	0.3901588
0.1890579	0.6828721	0.3909056
0.1076666	0.8014977	0.5510524
0.2469913	0.7847827	0.3899774
0.3317230	0.7852244	0.5508823
0.3623562	0.7919685	0.3898016
0.4389597	0.7985997	0.5502664
0.4816654	0.7223404	0.3906898
0.4756396	0.5144673	0.3931794
0.5552330	0.8082698	0.3894159
0.6696132	0.8063886	0.5496273
0.6667674	0.8037616	0.3893340

0.9413955	0.7016834	0.5508750
0.8301799	0.6995253	0.5504983
0.7187956	0.7027114	0.3899360
0.8334631	0.6995099	0.3895650
0.7763495	0.8009634	0.5502453
0.8947015	0.7962386	0.3892935
0.9960035	0.6019056	0.5510828
0.0036297	0.5965298	0.3899553
0.1043478	0.6045580	0.5509072
0.2407353	0.5771102	0.3921622
0.2755469	0.5673070	0.5501334
0.5334656	0.6163035	0.3918369
0.6534311	0.6084132	0.3911469
0.7823189	0.5996988	0.5503739
0.8890829	0.5996941	0.3897243
0.0005610	0.0011120	0.5511736
0.0060945	0.9928489	0.3889884
0.1119850	0.0001321	0.5512312
0.2275187	0.9924869	0.3889985
0.3326030	0.9933933	0.5510712
0.3377001	0.9982982	0.3889217
0.4434162	0.9950631	0.5507305
0.5600915	0.0075249	0.3888699
0.6668877	0.9989793	0.5505346
0.6711140	0.0037868	0.3890131
0.7778787	0.0004697	0.5507057
0.8933689	0.9971697	0.3890388
0.1729679	0.5138163	0.5508611
0.0557596	0.4954532	0.3902730
0.1671640	0.4909724	0.3914534
0.3601068	0.5073995	0.3936453
0.9454775	0.5007746	0.5511547
0.8321974	0.4999863	0.5509090
0.7127297	0.5073400	0.3911365
0.8279038	0.5028777	0.3900637

(12) The structure of the TS between V2+V12 and intermediate

106

Direct

0.2840076	0.0841800	0.5553894
0.1738569	0.0897216	0.5546815
0.0517389	0.1047312	0.3868314
0.1630093	0.1030812	0.3878794

0.6186808	0.0881276	0.5524869
0.5059130	0.0861843	0.5540635
0.3849310	0.1097109	0.3903190
0.4958338	0.1141203	0.3907670
0.9525652	0.0901056	0.5534131
0.8411028	0.0885687	0.5527472
0.7186679	0.1117453	0.3886654
0.8298382	0.1083464	0.3874809
0.0096750	0.1908884	0.5535087
0.9934362	0.2057853	0.3870348
0.2850469	0.2821253	0.5547879
0.1787151	0.2938475	0.5508887
0.0471229	0.3054963	0.3870856
0.1579623	0.3021876	0.3889068
0.1205305	0.1917168	0.5536063
0.2162413	0.2037106	0.3897163
0.3411510	0.1862121	0.5569277
0.3271580	0.2083774	0.3920896
0.3800918	0.3102767	0.3969323
0.4905925	0.3148209	0.3978318
0.4489029	0.1793851	0.5574469
0.5490870	0.2146651	0.3936322
0.6784950	0.1810789	0.5535290
0.6604738	0.2129038	0.3920273
0.9569300	0.2920098	0.5534923
0.8437460	0.2902421	0.5540767
0.7122369	0.3143458	0.3931063
0.8247492	0.3108545	0.3896986
0.7860471	0.1889263	0.5536170
0.8822262	0.2092613	0.3879333
0.0139155	0.3933355	0.5506700
0.9925094	0.4071167	0.3872012
0.1280619	0.3985460	0.5451049
0.2115145	0.3997454	0.3918310
0.3203656	0.4078798	0.3986816
0.5383974	0.4195737	0.4000015
0.6526593	0.4161216	0.3967345
0.7926028	0.3875894	0.5532446
0.8801632	0.4104076	0.3885736
0.2829628	0.8813987	0.5479611
0.1722167	0.8889470	0.5510590
0.0594652	0.9015839	0.3864023
0.1736984	0.8981732	0.3878810
0.6159822	0.8865499	0.5460151

0.5029949	0.8839283	0.5438388
0.3909265	0.9097153	0.3903113
0.5004353	0.9179782	0.3902344
0.9496449	0.8900445	0.5520065
0.8390505	0.8891486	0.5506622
0.7194913	0.9103556	0.3872713
0.8318390	0.9071208	0.3857661
0.0035948	0.7899680	0.5513617
0.0032609	0.8022011	0.3861873
0.2757175	0.6745647	0.5346559
0.1666854	0.6921753	0.5453885
0.0622700	0.7013260	0.3875846
0.1812073	0.6942137	0.3904822
0.1143847	0.7907616	0.5501557
0.2390510	0.7956577	0.3902480
0.3372966	0.7761744	0.5382112
0.3543545	0.8015567	0.3922807
0.4446262	0.7895434	0.5362740
0.4773074	0.7294123	0.3966560
0.4728053	0.5220853	0.4020117
0.5494455	0.8161042	0.3927558
0.6755640	0.7948099	0.5457474
0.6611442	0.8119504	0.3906173
0.9484633	0.6900941	0.5510761
0.8370205	0.6876925	0.5501235
0.7138712	0.7111442	0.3914929
0.8280019	0.7085847	0.3878271
0.7824537	0.7889199	0.5488119
0.8884806	0.8058806	0.3858633
0.0037557	0.5906683	0.5509908
0.9979971	0.6064187	0.3871264
0.1121361	0.5935695	0.5464129
0.2335428	0.5886947	0.3936049
0.2814100	0.5588665	0.5243475
0.5300778	0.6235181	0.3993943
0.6496540	0.6162891	0.3962499
0.7895355	0.5877377	0.5507379
0.8838672	0.6089053	0.3877442
0.0065017	0.9896465	0.5531981
-0.0001091	0.0032296	0.3860668
0.1178368	0.9893657	0.5535777
0.2214901	0.0027868	0.3880038
0.3386466	0.9827390	0.5521188
0.3317429	0.0075718	0.3889434

0.4494335	0.9845944	0.5506365
0.5540737	0.0153581	0.3890811
0.6728706	0.9874808	0.5498437
0.6650714	0.0120727	0.3879288
0.7838819	0.9886954	0.5510845
0.8872882	0.0067014	0.3859183
0.1801858	0.5033912	0.5377716
0.0507227	0.5055710	0.3875513
0.1621909	0.5014434	0.3899455
0.3563640	0.5165253	0.4032037
0.9530924	0.4895532	0.5514805
0.8397363	0.4882369	0.5520986
0.7088726	0.5154001	0.3948493
0.8235322	0.5116220	0.3900511

(13) The structure of intermediate between V2+V12 and V0+V14

106

Direct

0.2941511	0.0648342	0.5620323
0.1836048	0.0673292	0.5607431
0.0422306	0.1235977	0.3827627
0.1535999	0.1233950	0.3849705
0.6287803	0.0672204	0.5564404
0.5162790	0.0654819	0.5606267
0.3752195	0.1241606	0.3919410
0.4863792	0.1252342	0.3922382
0.9621190	0.0677253	0.5575645
0.8507887	0.0673068	0.5560686
0.7084667	0.1248583	0.3872927
0.8196784	0.1242791	0.3837351
0.0177553	0.1680168	0.5579580
0.9861991	0.2238472	0.3830218
0.2927470	0.2612420	0.5621176
0.1860886	0.2687420	0.5574885
0.0415077	0.3236855	0.3833232
0.1530902	0.3237200	0.3877286
0.1288123	0.1678494	0.5592951
0.2085947	0.2235165	0.3889315
0.3509197	0.1665346	0.5648654
0.3197464	0.2247971	0.3937122
0.3745294	0.3254205	0.4015641
0.4855963	0.3258901	0.4050313

0.4588163	0.1583391	0.5663469
0.5412182	0.2254066	0.3973725
0.6875817	0.1599138	0.5594465
0.6526093	0.2248296	0.3944188
0.9628503	0.2684599	0.5569052
0.8508417	0.2689124	0.5582122
0.7072384	0.3250907	0.3957895
0.8183184	0.3242762	0.3886009
0.7948987	0.1674835	0.5580947
0.8746170	0.2243749	0.3847205
0.0182801	0.3687681	0.5532629
0.9849137	0.4233393	0.3818287
0.1303578	0.3701949	0.5507617
0.2079657	0.4233424	0.3938647
0.3187509	0.4262504	0.4054321
0.5400779	0.4268937	0.4121264
0.6513594	0.4255161	0.4033742
0.8020221	0.3681951	0.5576715
0.8734379	0.4240806	0.3856405
0.2948198	0.8656969	0.5483652
0.1839971	0.8675421	0.5527504
0.0425372	0.9228669	0.3805672
0.1540457	0.9223974	0.3836025
0.6260307	0.8678937	0.5384887
0.5127790	0.8688279	0.5321024
0.3765095	0.9211061	0.3911246
0.4888616	0.9244834	0.3938179
0.9617262	0.8675743	0.5545217
0.8504237	0.8678967	0.5510867
0.7090059	0.9247859	0.3807507
0.8200598	0.9240940	0.3786976
0.0173988	0.7677768	0.5519114
0.9864224	0.8230829	0.3787296
0.2860903	0.6827900	0.4999504
0.1840030	0.6723554	0.5296256
0.0417935	0.7224639	0.3809810
0.1520043	0.7210366	0.3887747
0.1287466	0.7680728	0.5478541
0.2105901	0.8208978	0.3871855
0.3474521	0.7723429	0.5207579
0.3197773	0.8241826	0.3871971
0.4538297	0.7829446	0.5014867
0.5015119	0.7363383	0.4392158
0.4844524	0.5276096	0.4251146

0.5471347	0.8266332	0.4031472
0.6861268	0.7756768	0.5387776
0.6544423	0.8246945	0.3875668
0.9615688	0.6685041	0.5489781
0.8493539	0.6676781	0.5491451
0.7084600	0.7240381	0.3913517
0.8188170	0.7234301	0.3834821
0.7933460	0.7686811	0.5467102
0.8750639	0.8233919	0.3787683
0.0178058	0.5691664	0.5467662
0.9852485	0.6226818	0.3805925
0.1296778	0.5702836	0.5374590
0.2039797	0.6204117	0.4008238
0.3020766	0.6176763	0.4374305
0.5425308	0.6283974	0.4241416
0.6510086	0.6259365	0.4033639
0.8009944	0.5682836	0.5517246
0.8740254	0.6231727	0.3833829
0.0172500	0.9674827	0.5573673
0.9869848	0.0234416	0.3808085
0.1283283	0.9670932	0.5584548
0.2093739	0.0225818	0.3854067
0.3495809	0.9654474	0.5559784
0.3204195	0.0230886	0.3890361
0.4602302	0.9646780	0.5529313
0.5423430	0.0246901	0.3890583
0.6834108	0.9671888	0.5491583
0.6536387	0.0247470	0.3854453
0.7944750	0.9675461	0.5520804
0.8755238	0.0240322	0.3801246
0.1771988	0.4697533	0.5404860
0.0406069	0.5228051	0.3804932
0.1516327	0.5221417	0.3877352
0.3711489	0.5255619	0.4241895
0.9640143	0.4688933	0.5515841
0.8502339	0.4684943	0.5544340
0.7065065	0.5252341	0.3982425
0.8175206	0.5241852	0.3880795

(14) The structure of the TS between intermediate and V0+V14

106

Direct

0.2978205	0.0722672	0.5572670
0.1877282	0.0765654	0.5527619
0.0385529	0.1160214	0.3798255
0.1501129	0.1159495	0.3826431
0.6322326	0.0767558	0.5602137
0.5197994	0.0734740	0.5631526
0.3713365	0.1150417	0.3939112
0.4823875	0.1159383	0.3966536
0.9660536	0.0783697	0.5516438
0.8547310	0.0780870	0.5539071
0.7039447	0.1161107	0.3895325
0.8152622	0.1160890	0.3842130
0.0219887	0.1785070	0.5524175
0.9828158	0.2160309	0.3823634
0.2965983	0.2695067	0.5585943
0.1904804	0.2784915	0.5529506
0.0389741	0.3159059	0.3830654
0.1505910	0.3162529	0.3866880
0.1329607	0.1775927	0.5528089
0.2056937	0.2160314	0.3880880
0.3542448	0.1742696	0.5620777
0.3166032	0.2163549	0.3941766
0.3714753	0.3173905	0.4033896
0.4826431	0.3178504	0.4080204
0.4617575	0.1664076	0.5660988
0.5378028	0.2169940	0.4007414
0.6911579	0.1703221	0.5605136
0.6489989	0.2162670	0.3974009
0.9670486	0.2794102	0.5537705
0.8547180	0.2797773	0.5565519
0.7043509	0.3166419	0.3986737
0.8153609	0.3160940	0.3904629
0.7983004	0.1781455	0.5573165
0.8710646	0.2161239	0.3852081
0.0225080	0.3792993	0.5505000
0.9827052	0.4155607	0.3820633
0.1351079	0.3809506	0.5472142
0.2063848	0.4163668	0.3916598
0.3163050	0.4185846	0.4056164
0.5376237	0.4191423	0.4163346
0.6490258	0.4169599	0.4073726
0.8066272	0.3792402	0.5570323
0.8711764	0.4158625	0.3869542
0.2988901	0.8729060	0.5407879

0.1879011	0.8777164	0.5399052
0.0371974	0.9160582	0.3728580
0.1481318	0.9164488	0.3760836
0.6314851	0.8766023	0.5486800
0.5203413	0.8738742	0.5440369
0.3692348	0.9117707	0.4028868
0.4823707	0.9138905	0.4045219
0.9649128	0.8786957	0.5461030
0.8542840	0.8787720	0.5488433
0.7048577	0.9161755	0.3835769
0.8156515	0.9160189	0.3782697
0.0199673	0.7786278	0.5415088
0.9818087	0.8154202	0.3728599
0.3179200	0.7223154	0.4565856
0.1859897	0.6834173	0.5230502
0.0375213	0.7147007	0.3745627
0.1471892	0.7145600	0.3816333
0.1306131	0.7783020	0.5340801
0.2009590	0.8160765	0.3841051
0.3590770	0.7783214	0.5169379
0.3033867	0.8154118	0.4094418
0.4659663	0.7810257	0.5151633
0.5100117	0.7287777	0.4530973
0.4829768	0.5204134	0.4299276
0.5456116	0.8175832	0.4125812
0.6910388	0.7839192	0.5457758
0.6513977	0.8159763	0.3925424
0.9661699	0.6786823	0.5434726
0.8538961	0.6774521	0.5475913
0.7065115	0.7156246	0.3954837
0.8157786	0.7151140	0.3838065
0.7979209	0.7785361	0.5475554
0.8709322	0.8154136	0.3766430
0.0231128	0.5800422	0.5430436
0.9820089	0.6144612	0.3770059
0.1365091	0.5820756	0.5333416
0.2039682	0.6149771	0.3915892
0.3045910	0.6157540	0.4241347
0.5444167	0.6197026	0.4337934
0.6505957	0.6170289	0.4093512
0.8055675	0.5790400	0.5518595
0.8712537	0.6148581	0.3826981
0.0209494	0.9780507	0.5479168
0.9822431	0.0163673	0.3763580

0.1325051	0.9767397	0.5472173
0.2050718	0.0153854	0.3827936
0.3533282	0.9717141	0.5536383
0.3161383	0.0134066	0.3911646
0.4647806	0.9711402	0.5564132
0.5370989	0.0148349	0.3954285
0.6878038	0.9771729	0.5547352
0.6485242	0.0157443	0.3891904
0.7986137	0.9782358	0.5527628
0.8709722	0.0163453	0.3785986
0.1824972	0.4794571	0.5369853
0.0386670	0.5150799	0.3786638
0.1503684	0.5152002	0.3837225
0.3684460	0.5197956	0.4237347
0.9690122	0.4798241	0.5492999
0.8551656	0.4791671	0.5534599
0.7048673	0.5164159	0.4017642
0.8152694	0.5156682	0.3895778

(15) The structure of V0+V14

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Direct

0.2732741	0.1037442	0.5510956
0.1626835	0.1015961	0.5512797
0.0555083	0.0997324	0.3892582
0.1667527	0.0996409	0.3893362
0.6076325	0.0920142	0.5504283
0.4960489	0.0965595	0.5505920
0.3888101	0.0997967	0.3895098
0.5000649	0.0999546	0.3895182
0.9401096	0.0971523	0.5513226
0.8280000	0.0942593	0.5510404
0.7221342	0.0999606	0.3892216
0.8333476	0.0998294	0.3892283
-0.0038994	0.1987359	0.5515915
-0.0000029	0.1997761	0.3896319
0.2732705	0.2962290	0.5514966
0.1660619	0.3002166	0.5516923
0.0554564	0.2997606	0.3898758
0.1666568	0.2996672	0.3902701
0.1070325	0.2003859	0.5516312
0.2221693	0.1996625	0.3899450
0.3329943	0.2037842	0.5512749

0.3333703	0.1997365	0.3903533
0.3887445	0.2997438	0.3918965
0.4999563	0.2999165	0.3923860
0.4406846	0.1916168	0.5508111
0.5554565	0.1999841	0.3907108
0.6672237	0.1855635	0.5501207
0.6666570	0.1999969	0.3904278
0.9428022	0.2994988	0.5516359
0.8303888	0.2987284	0.5512572
0.7220923	0.3000233	0.3910398
0.8333224	0.2998807	0.3901621
0.7736367	0.1960067	0.5509207
0.8887905	0.1998850	0.3897671
0.0004786	0.3995703	0.5516515
-0.0000270	0.3997938	0.3897384
0.1122993	0.4017567	0.5516230
0.2220305	0.3996389	0.3911172
0.3332697	0.3996869	0.3925000
0.5553607	0.3999682	0.3932412
0.6666516	0.4000215	0.3923193
0.7851690	0.3993870	0.5508784
0.8887051	0.3999013	0.3898839
0.2788948	0.9064050	0.5508125
0.1682647	0.9019938	0.5509310
0.0555697	0.8997801	0.3886722
0.1667839	0.8996807	0.3887057
0.5924334	0.8836416	0.5507309
0.4734316	0.8883986	0.5507119
0.3888396	0.8998200	0.3886415
0.5000289	0.8999960	0.3887512
0.9430874	0.8972293	0.5509534
0.8303127	0.8954678	0.5507479
0.7221613	0.8999926	0.3885534
0.8333537	0.8998971	0.3885534
0.0030959	0.7990735	0.5509922
0.0000818	0.7997495	0.3886347
0.2958846	0.7222127	0.5511995
0.1822324	0.7058988	0.5512038
0.0554797	0.6997433	0.3888978
0.1667304	0.6996618	0.3892890
0.1164155	0.8007519	0.5510859
0.2222130	0.7996911	0.3888624
0.3543458	0.8189596	0.5509846
0.3334039	0.7998112	0.3889921

0.3887205	0.6998236	0.3904322
0.4999581	0.7000536	0.3909449
0.4999249	0.5000007	0.3934399
0.5554362	0.8000389	0.3894554
0.6629556	0.7978297	0.5503979
0.6666702	0.8000303	0.3892343
0.9480532	0.6995898	0.5511005
0.8340286	0.6974378	0.5507869
0.7220600	0.7000412	0.3899513
0.8333377	0.6999170	0.3891269
0.7725167	0.7960354	0.5506231
0.8888267	0.7998199	0.3885860
0.0067619	0.6015607	0.5513261
-0.0000199	0.5997726	0.3891556
0.1224681	0.6037185	0.5513629
0.2220632	0.5996796	0.3904118
0.3332610	0.5997935	0.3916201
0.5553505	0.6000601	0.3924485
0.6666257	0.6000754	0.3916838
0.7869270	0.5981827	0.5505758
0.8887309	0.5998648	0.3892868
-0.0025285	0.9982880	0.5511121
0.0001307	-0.0002395	0.3888383
0.1092421	0.0004185	0.5510717
0.2222044	-0.0003186	0.3889158
0.3280292	0.0071332	0.5507095
0.3334344	-0.0002196	0.3888903
0.4377130	0.9965145	0.5506581
0.5554679	0.0000128	0.3887756
0.6565605	-0.0118247	0.5506564
0.6667357	0.0000158	0.3886994
0.7703855	0.9927808	0.5507878
0.8888157	-0.0001673	0.3887289
0.1636465	0.5005403	0.5512021
0.0553808	0.4997567	0.3896153
0.1666309	0.4996819	0.3904659
0.3886666	0.4997919	0.3930384
0.9501085	0.5011095	0.5514367
0.8361216	0.4989237	0.5510479
0.7220499	0.5000594	0.3915191
0.8332822	0.4999217	0.3900737

3. The total energy table of the configurations in Fig. 3 and Fig. 4.

Table 1. Table Title The total energies of the vacancy migration processes in Fig. 3

Structures	Relative energy (eV)	
	GGA-PBE (eV)	DFTB (eV)
Initial 1	0.00	0.00
TS1	7.33	5.51
Final 1	0.00	0.00
Initial 2	0.00	0.00
Intermediate 2	-2.13	-1.53
TS2	1.73	2.71
Final 2	-8.14	-7.20
Initial 3	0.00	0.00
TS3	3.66	3.95
Final 3	-7.19	-5.65

Table 2. The total energies of the evolution of two holes in bilayer graphene (BLG) by interlayer atomic migration in Fig. 4

Structures	Relative energy (eV)	
	GGA-PBE (eV)	DFTB (eV)
V6+V8	14.08	14.31
TS	14.25	14.40
Intermediate	10.45	9.31
TS	13.16	9.79
V5+V9	12.62	13.40
TS	12.84	12.92
Intermediate	9.54	8.65
TS	11.24	14.07
V3+V11	8.48	8.60
TS	11.79	10.12
V2+V12	6.44	5.79
TS	6.99	5.91
Intermediate	3.40	0.55
TS	4.71	2.08
V0+V14	0.00	0.00

