

Supplementary Data

Optimized Geometries (VASP_POSCAR format)

Reaction mechanism and kinetics for N₂ reduction to ammonia on Fe-Ru dual atom catalyst

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1: Fe-Ru/C₃N-C₂N (n = 0)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru

36 16 1 1

Direct

0.3084964072343134 0.9297945815120688 0.5075387576609428

0.3711058597501361 0.1728064011234624 0.5067886228540196

0.4340090147447151 0.4246891177244849 0.5063739723982509

0.4955876328851939 0.6732023984640907 0.5057091786007990

0.3705483726105843 0.6732541784736020 0.5076929058181812

0.8683747756866547 0.1722972370187154 0.5056315246122609

0.7484469485201843 0.1724101476392951 0.5046772524430631

0.9343956267119355 0.4313103866910917 0.5066520771317374

0.9962260614681026 0.6692439304171004 0.5071312923931093

0.3084834652289761 0.5848976526390365 0.5075203147285492

0.3711020925541239 0.3418765180071385 0.5067793385897973

0.4340155707815243 0.0899958831750772 0.5063793400481225

0.4955903651906838 0.8414695665438593 0.5057094148378308

0.3705508989459420 0.8414221162995091 0.5077008610085135

0.8683639870613383 0.3425475340795328 0.5056311627694711

0.7484403233393448 0.3423088765625510 0.5046878057213982

0.9344050279214322 0.0835859106492726 0.5066587292274377

0.9962300306720843 0.8456684445453065 0.5071343870624492

0.6826467671112977 0.0838061674068289 0.5044919147789722

0.6221803867972070 0.8437685190603965 0.5044924635894488

0.5577928179020023 0.5905032282818489 0.5050131947194446

0.4962670442117538 0.3411925790186779 0.5056124955386010

0.6207248772260783 0.3401044007127811 0.5047407993197510

0.1245456958446029 0.8435050507981929 0.5086028140096157

0.2445917910032155 0.8432240434421193 0.5078027480576025

0.0598038084633544 0.5846396506684678 0.5088642400761079

0.9964567662015255 0.3430119860485504 0.5086668935500641

0.6826358610062226 0.4308810222107033 0.5045082078711668

0.6221768183045012 0.6709129188656858 0.5045010010413079

0.5577980211296346 0.9241750919565230 0.5050126804468944

0.4962674469986622 0.1734831195322508 0.5056145000755105

0.6207320583293919 0.1745763752378904 0.5047366714714605

0.1245377081531032 0.6713881333336462 0.5086020720503275

0.2445832510751570	0.6715192011095205	0.5077984110502012
0.0598176518502626	0.9302806318138628	0.5088705814968806
0.9964660650550390	0.1718882088285684	0.5086736214356176
0.3089660774704983	0.0930245714505116	0.5062254818667937
0.4331207422597325	0.5907109163434571	0.5065635871293364
0.8084045738772528	0.0940603701784088	0.5050389606042858
0.9358692439968904	0.5903979604871892	0.5062591814632000
0.3089552569113349	0.4216559463732509	0.5062021155226142
0.4331241725795416	0.9239625028986509	0.5065714891210682
0.8083823796403010	0.4207230155504051	0.5050489298828410
0.9358790137045395	0.9245095863444616	0.5062670937252989
0.6819764812338241	0.9258988922750251	0.5042855135277297
0.5585199505731289	0.4243956086263381	0.5050436597971566
0.1845991532762370	0.9230325249044422	0.5081792388633736
0.0584225568877578	0.4220869014784397	0.5108877440641276
0.6819682184773205	0.5887843801328765	0.5043162319692795
0.5585239180521840	0.0902868254718630	0.5050436493975771
0.1845750936820637	0.5918000854975065	0.5081805967340755
0.0584339430083034	0.0928279216703381	0.5109070922968100
0.1300569046638164	0.2575092636616286	0.5291595934924135
0.2331941827350228	0.2573073597635122	0.4947566640571086

Fe-Ru/C₃N-C₂N (n = 0.5)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru

36 16 1 1

Direct

0.3084958998969998	0.9296241331632923	0.5072607180377239
0.3710730871039749	0.1728123734805704	0.5065011218120922
0.4340256158098656	0.4245792213103660	0.5062835340726850
0.4956875059928542	0.6731040626844093	0.5058333399737428
0.3705869972990554	0.6732992330872072	0.5074886081299388
0.8684215626288332	0.1722872946116410	0.5057970391171839
0.7484262246218381	0.1723883338921771	0.5048276214756444
0.9343718345250525	0.4312404398834334	0.5068083675136541
0.9962934713386032	0.6692907692009573	0.5071933014752741
0.3084846131858224	0.5850637907476581	0.5072556756044907
0.3710684607455966	0.3418809469583183	0.5065008610752704
0.4340281252583221	0.0901165770220035	0.5062837957997963

0.4956873259797959 0.8415813126331838 0.5058308587596606
0.3705878805779788 0.8413842612205500 0.5074904247973460
0.8684130216429886 0.3425497146724481 0.5057948371399242
0.7484188818252179 0.3423406563317510 0.5048362882671221
0.9343814195602769 0.0836365666182019 0.5068207708342952
0.9962997914525095 0.8455937808805760 0.5072026129267116
0.6827176787313785 0.0839688545201743 0.5046666103653898
0.6222416834085055 0.8437588745852713 0.5047125248148996
0.5577823090145758 0.5905540051665439 0.5052304916470829
0.4962432042252955 0.3411462796653463 0.5056987244977622
0.6208133370879939 0.3400843874164268 0.5049461274927396
0.1244493245861028 0.8435442066872583 0.5084579155231130
0.2445829749427859 0.8431838797368002 0.5075691520462772
0.0598455520030732 0.5847692053891889 0.5088008220397098
0.9963058821834752 0.3428072115373738 0.5087132057775680
0.6827102599444620 0.4307408349191475 0.5046826558310946
0.6222399363376828 0.6709382032235890 0.5047204797945890
0.5577873438266880 0.9241424342272972 0.5052236481450985
0.4962453666204872 0.1735470174387814 0.5057010525322598
0.6208173040370943 0.1746110205854344 0.5049415212963329
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0.2445833673954296 0.6715696081064111 0.5075712062179698
0.0598519332946105 0.9301298398058906 0.5088116212296748
0.9963114873517395 0.1720728034325708 0.5087212852503069
0.3089495037462383 0.0928169767640272 0.5059180145762593
0.4331119283757998 0.5906943177137755 0.5065274161058027
0.8084216281347587 0.0939785440513408 0.5051865652739393
0.9358074050013995 0.5905204436048592 0.5063733201824590
0.3089341392218794 0.4218689611679056 0.5059049441684357
0.4331120154170033 0.9239922454688321 0.5065291156276935
0.8084040538403259 0.4208073028138437 0.5051935009689202
0.9358151529681553 0.9243635592816348 0.5063901011310770
0.6820373732244124 0.9258202221407449 0.5044655892808508
0.5586055942981386 0.4243162411121565 0.5052514357778598
0.1845743306237150 0.9231626569933240 0.5080669156159986
0.0584951273986173 0.4218667523621092 0.5107801218596804
0.6820305316503866 0.5888750607006047 0.5044945403443745
0.5586089130659033 0.0903816677678187 0.5052486775379500
0.1845505761044190 0.5916677450326852 0.5080731896188626
0.0585056567727082 0.0930285362407101 0.5107991113988049
0.1297995701115605 0.2574960640789413 0.5274828751906430
0.2328810685986885 0.2572749818171701 0.4956152324678262

Fe-Ru/C₃N-C₂N (n = 1.0)

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19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru
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Direct

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0.3710946342336031	0.1727496156332055	0.5060115510353178
0.4340676612406302	0.4244791850764741	0.5059994956806467
0.4958079369878136	0.6730124316075736	0.5059375574670434
0.3706449749103103	0.6734434618301937	0.5070158056525905
0.8684208599313636	0.1722778459994374	0.5065116336844372
0.7483609768315084	0.1723543827549196	0.5057970091813860
0.9342611145603714	0.4312757342454919	0.5071656791039302
0.9962354412981661	0.6694881738080236	0.5072879106198610
0.3084831414917292	0.5852604293277306	0.5067066716720113
0.3710823691930780	0.3418801975658664	0.5060101654923511
0.4340854814391601	0.0901336969242979	0.5059948087869151
0.4958198677279880	0.8415903184339433	0.5059358923756180
0.3706554660588089	0.8411418739976598	0.5070147350049250
0.8684056798911743	0.3426453430497096	0.5065004250422206
0.7483517969271897	0.3423771756444787	0.5057832111296792
0.9342769774478407	0.0837215732939962	0.5071681898928793
0.9962438826327427	0.8455141685022106	0.5072873155789038
0.6828099947382877	0.0840906152568595	0.5056040354097732
0.6223571039385665	0.8436774723279058	0.5055262598431894
0.5578323868946145	0.5905756417174695	0.5056575922413146
0.4962566966440162	0.3410372735146472	0.5057024851124566
0.6208916746980241	0.3400477747998004	0.5055906794942849
0.1243408288151595	0.8436416231609517	0.5077435955257998
0.2445964309157167	0.8431297622753334	0.5068938397873672
0.0598165074724324	0.5850393832926037	0.5082331894898758
0.9961435377205337	0.3427047088676575	0.5083018464104758
0.6827994112746185	0.4305793522323701	0.5055874037139438
0.6223507806912404	0.6709609593739442	0.5055188559424094
0.5578331826139059	0.9240240079524497	0.5056570910526834
0.4962623957116326	0.1735696246527233	0.5057053103068329
0.6208943744230494	0.1745878233078514	0.5055930949909342
0.1243257941729744	0.6713697323794224	0.5077588066531801
0.2445846823351923	0.6716212065170141	0.5069091321087168
0.0598314796532655	0.9299810315728965	0.5082292590804571

0.9961572936572842	0.1723028021144753	0.5082999385304103
0.3089969306443462	0.0925251112640376	0.5054227053010761
0.4331801556812624	0.5906343329529384	0.5062504858253516
0.8084132513708435	0.0938947528635320	0.5060638017338001
0.9356501120831986	0.5907243224614542	0.5069392324676359
0.3089561831939699	0.4220613637638462	0.5054088514448710
0.4331856782601282	0.9239560214150244	0.5062494411838651
0.8083854828277978	0.4209315408481838	0.5060279448887289
0.9356689636471269	0.9242809994522108	0.5069414778157062
0.6821428888884039	0.9256857164933736	0.5055073456132675
0.5587105126327062	0.4242358909248871	0.5055700395266691
0.1845318495267961	0.9233742105660495	0.5073802249348015
0.0584870495813584	0.4218569082660939	0.5097977636430659
0.6821324125901319	0.5889643878056441	0.5054912020073591
0.5587138703814649	0.0903870986766882	0.5055730583775682
0.1844871141529470	0.5915356886103265	0.5074226259211250
0.0585054531501280	0.0931690500800969	0.5097975452523187
0.1295709194115552	0.2575768428193549	0.5250822404942145
0.2327538953323967	0.2571746066359533	0.4956714799031698

Fe-Ru/C₃N-C₂N (n = -0.5)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru
36	16	1	1

Direct

0.3084373630141360	0.9300558129327172	0.5072607003281282
0.3710638770019384	0.1728558023140189	0.5066710572059375
0.4339573200503792	0.4249480047999147	0.5064456090506974
0.4954987356943443	0.6733231718370255	0.5058335894681156
0.3705181566191149	0.6732875712495776	0.5077154070109413
0.8683717218964666	0.1723099372319555	0.5056132103360507
0.7485063145151002	0.1724707412404095	0.5047594647195158
0.9344970602029374	0.4312897348918408	0.5066643512523572
0.9962108153234231	0.6691266172692373	0.5071099113951046
0.3084466955804752	0.5847102599961690	0.5072485857417183
0.3710708140237974	0.3418854141094241	0.5066673365627010
0.4339595282554352	0.0897657624484796	0.5064501478100278
0.4954984228542912	0.8413771591240765	0.5058265816052451
0.3705201777139112	0.8414502678368797	0.5077221542573638
0.8683699648419677	0.3425060830736812	0.5056101703956266

0.7485036325795668	0.3422996400652245	0.5047852260746514
0.9344947769606120	0.0835224969145769	0.5066779394100104
0.9962037891534288	0.8456977531106791	0.5071126727194110
0.6825646324440996	0.0837410367754254	0.5046222037165145
0.6221198973324212	0.8437995411943727	0.5046225969786089
0.5577618845024754	0.5904089299706556	0.5051126267276598
0.4962364495745811	0.3411681926928632	0.5056831231735994
0.6206408132985838	0.3401373700605169	0.5048534078955204
0.1245523078336264	0.8433528177820921	0.5083884548192299
0.2444925271426121	0.8431884382745082	0.5074301109455329
0.0597831400355103	0.5844566631388575	0.5089005732880983
0.9966400478889988	0.3430619535862468	0.5088286328295329
0.6825580079708452	0.4309877279512628	0.5046680864320985
0.6221124892069033	0.6709120508229299	0.5046395520116803
0.5577694088639178	0.9242988327844193	0.5050961688484301
0.4962386061511522	0.1735468282469965	0.5056840529196196
0.6206433581641673	0.1745817427228572	0.5048315180428640
0.1245548408984818	0.6714430645345179	0.5083965084484680
0.2444942568233020	0.6715860816389070	0.5074291435836192
0.0597872889712512	0.9303594168056494	0.5088967137438111
0.9966431647384211	0.1717416637633654	0.5088346787702063
0.3088962132612754	0.0932484622194064	0.5058039294287603
0.4331140791065909	0.5905928500562218	0.5066735136809118
0.8084111440434550	0.0941502186990007	0.5050589424381993
0.9359351285019532	0.5902292295539616	0.5062757895319997
0.3088987387423490	0.4215022749678111	0.5057941421549113
0.4331144464461485	0.9241395851042741	0.5066738053900915
0.8084030072848237	0.4206519775585634	0.5050773972058580
0.9359301592823477	0.9245951526701774	0.5062958603128457
0.6818848041840544	0.9260206585415101	0.5044638590647891
0.5584336484644640	0.4245740238230733	0.5051272614759795
0.1845601361559696	0.9229458037557394	0.5078034146965712
0.0585109641585945	0.4220878311613131	0.5112022293751856
0.6818770732525322	0.5887029907098589	0.5045142041345787
0.5584346038763860	0.0901363704227934	0.5051097316112347
0.1845611782042026	0.5918462488876172	0.5078146516571769
0.0585133534902915	0.0927150750785701	0.5112083620185375
0.1303552538376413	0.2574274502635901	0.5316691913663136
0.2338129405842836	0.2573950563341886	0.4922805179373489

Fe-Ru/C₃N-C₂N (n = -1.0)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru
36 16 1 1

Direct

0.3084194202489742	0.9302196225388323	0.5067742161503593
0.3711061706923722	0.1728210434787082	0.5063186465966216
0.4339713807302742	0.4251261016334979	0.5063282861745739
0.4953751707894624	0.6734624557268127	0.5059776290785778
0.3704446399201765	0.6731911210586081	0.5073976319418541
0.8683598693677521	0.1722761721983208	0.5058113420007413
0.7485427393753600	0.1724806893649225	0.5050656116682057
0.9345383563550702	0.4312792513607331	0.5067760027839278
0.9961862225031762	0.6689591715788130	0.5070284455258713
0.3084216878572416	0.5845392672643064	0.5067788395184250
0.3711076564300849	0.3419229264949901	0.5063216942174092
0.4339739982531974	0.0896095365369446	0.5063224435040214
0.4953726235431488	0.8412603882379873	0.5059762976898071
0.3704439466799206	0.8415549454532545	0.5073954181455095
0.8683591595623281	0.3425100876418979	0.5058070206514865
0.7485409229724104	0.3422622594735883	0.5050758123209341
0.9345366390270350	0.0835321785768528	0.5067925074741265
0.9961823879505881	0.8458583508300928	0.5070341908669121
0.6825148838747999	0.0836808101128932	0.5049907032405991
0.6220866600072757	0.8438196541049046	0.5050627903340312
0.5577537726946369	0.5902972340861093	0.5054610629829196
0.4962195757069628	0.3412197672606648	0.5058175920609307
0.6205099063354453	0.3402103171167325	0.5052139081370178
0.1245484185519597	0.8433347548964637	0.5079899690232089
0.2444157133772117	0.8431538200699530	0.5068486203370182
0.0597957210026134	0.5844027961916940	0.5087843471083999
0.9967345746746925	0.3433164019461442	0.5090236215965217
0.6825133284609437	0.4310522290041980	0.5050052317084019
0.6220888237986145	0.6709034949593906	0.5050685675393837
0.5577562442704115	0.9244265286824016	0.5054535659262996
0.4962196055672353	0.1735063684009920	0.5058170093617517
0.6205127179996990	0.1745200674052951	0.5052064389839589
0.1245509730704435	0.6714836230089283	0.5079863155862882
0.2444190448404517	0.6716258693306754	0.5068478002343865
0.0597942749147664	0.9304120627519993	0.5087984156599417
0.9967327066676032	0.1714866793735771	0.5090366846111228
0.3089263358536250	0.0934971805863944	0.5053186796004745
0.4330784779956448	0.5906517830663551	0.5065427040835329
0.8084282258728096	0.0941669402803029	0.5053227012478217
0.9360175655702601	0.5902565412396781	0.5063266391166110
0.3089245011889563	0.4212500367007129	0.5053175989707815

0.4330763304180252	0.9240855840456585	0.5065401038132045
0.8084205142697316	0.4206000999752931	0.5053272826602546
0.9360144755726301	0.9245531420630123	0.5063427643966535
0.6817942240206412	0.9261313213411894	0.5048601679747345
0.5584079612475072	0.4248561293140832	0.5054438878191034
0.1845509875322149	0.9228843967895710	0.5071762572511445
0.0584798912803579	0.4220758247634643	0.5114273369000022
0.6817966683975216	0.5885980379408648	0.5048853587504812
0.5584077425878968	0.0898726812719935	0.5054396438498024
0.1845478327676393	0.5919246162923993	0.5071719706691279
0.0584796870989868	0.0927266438940114	0.5114527729924140
0.1306117920932340	0.2574059835310309	0.5334276463099700
0.2343560091580309	0.2573608517517928	0.4902208748523249

2. NRR vis Associative pathway

2.1: Step ab ($\text{N}_2 \rightarrow \text{N}_2\text{H}$)

Initial state ab (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 7 3

Direct

0.3094860477250036	0.9286370258790168	0.3036224340782006
0.3724147340272937	0.1718311423828940	0.3041619247605437
0.4350614387144395	0.4238668949533363	0.3047592667514132
0.4965261339063980	0.6724620958754820	0.3048603558285564
0.3712580289491180	0.6724318625372511	0.3043594555683806
0.8686421895952572	0.1725189001048598	0.3056742494092443
0.7488127160471943	0.1721008099346600	0.3052126723570112
0.9341798095012844	0.4322291188429592	0.3064540951558578
0.9964359809172160	0.6702387932827661	0.3065176681436013
0.3091022070909893	0.5839367660527098	0.3040488409813895
0.3721675572000905	0.3411062143846370	0.3043443909203488
0.4352316131401237	0.0891326830879468	0.3046023524341814
0.4966084948406820	0.8407090665343400	0.3048108544643410
0.3714297385940875	0.8400841463977242	0.3041708931474100
0.8685327392326346	0.3431794811287101	0.3056712114748297
0.7487151982685818	0.3421318321464912	0.3052092346703131
0.9343486862652478	0.0840705918286292	0.3064782639143213
0.9965940243790368	0.8462834742445429	0.3065610597976924
0.6834049929051607	0.0834943268340534	0.3051739488591265

0.6231082606191244 0.8431249932676959 0.3051699027213858
0.5585869102913490 0.5900158742245659 0.3050677435614930
0.4970412296047916 0.3405359412415357 0.3049328551975044
0.6214217031132981 0.3396667406797305 0.3051330306440003
0.1250155606335575 0.8444624359447570 0.3071926144677984
0.2454320107566288 0.8429206577445633 0.3045508162898978
0.0600981799094904 0.5856034823904720 0.3079270873700540
0.9960481485915456 0.3436034214198737 0.3082705821898574
0.6832844074001465 0.4302711634545908 0.3051642744722748
0.6230458103838148 0.6704973417963827 0.3051638575837373
0.5586515138540999 0.9233898947571542 0.3050483187826229
0.4971341385880857 0.1726632047464580 0.3048967979660939
0.6214822938612323 0.1739118992803462 0.3051339725962854
0.1248376433603639 0.6721703520258436 0.3071543191440190
0.2451828221404483 0.6708979143069691 0.3047285340145242
0.0603518605691372 0.9312070880694688 0.3081050647307924
0.9961739715504496 0.1728553054603433 0.3083779614768576
0.3105628637568699 0.0920877821272363 0.3033216352983160
0.4339458613816259 0.5901224121605054 0.3046826087547120
0.8087862156710264 0.0939313944925986 0.3053148233715876
0.9359168979310630 0.5915035713691114 0.3059378287854370
0.3100140302031266 0.4201036529555301 0.3037552017721878
0.4340330809205526 0.9228015205203006 0.3044842071946985
0.8085307487815905 0.4210179797794908 0.3053049645793405
0.9361211624389298 0.9248715035984810 0.3059916398236234
0.6828713040987697 0.9252739603621468 0.3052398498830334
0.5594561997255938 0.4237483493651461 0.3051382161217726
0.1854469196879983 0.9225762383778056 0.3049467870881213
0.0581396265975267 0.4227852051268992 0.3105149749741514
0.6827762575684841 0.5884422491999360 0.3052234070714002
0.5595540626193249 0.0896681522454182 0.3051200562370904
0.1848557106900203 0.5929435622269030 0.3050882133614192
0.0583414929983440 0.0940774517199163 0.3109237011254766
0.1952252482468314 0.2586288953024392 0.4089837302929616
0.2071567239563663 0.2592050617002323 0.4665302288620555
0.1250228291142650 0.2599478648056064 0.3367271655786705
0.2334415121179922 0.2535964525614601 0.3175147333015690
0.1457547156133323 0.2787401726361274 0.5279866045577594
0.0697106938125468 0.2284711261144694 0.5434848546781668
0.1168220053665242 0.2818518605790789 0.6271542318853162
0.0837896197929305 0.3359580545124526 0.7013805626735355
0.1671518276563976 0.3028909300763228 0.7023737693053989
0.2547710892870128 0.4238101075748191 0.7171226351242096

0.2238525859898755 0.3534243459264155 0.7827679854619969
0.1063087313278821 0.2968080694291796 0.5589225771945623
0.1194557601893511 0.2711640046590389 0.6812289878502603
0.2306841709304363 0.3330329902511523 0.7351844908652206

Initial state ab (n = -0.25)

1.0000000000000000
19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 18 1 1 7 3

Direct

0.3095144706699936 0.9286518524263003 0.3036262169990698
0.3724125930325655 0.1718157845878043 0.3041613460124086
0.4350757325237257 0.4238703706959920 0.3047599676159488
0.4965030343894626 0.6724975930099526 0.3048638105832549
0.3712531980930076 0.6723649219726281 0.3043618587733813
0.8686108527287979 0.1726077331984473 0.3056763605805915
0.7488673172069573 0.1721784140574794 0.3052167820644593
0.9342104342564118 0.4322845618670990 0.3064653833353774
0.9964458203708432 0.6702291692070625 0.3065247120503693
0.3091231842992944 0.5838695767061770 0.3040609823643360
0.3721589707915835 0.3410778763943207 0.3043492937035184
0.4352496513706454 0.0890836297853255 0.3045968524609913
0.4965865103696114 0.8406436452621797 0.3048109772458973
0.3714299812751414 0.8400944218673042 0.3041703686644119
0.8685011561426962 0.3431231002466952 0.3056718158296212
0.7487675882843474 0.3420501706929176 0.3052123352350950
0.9343856385797977 0.0840620927611637 0.3064879849059833
0.9966100790266432 0.8463516959997930 0.3065689433322411
0.6833709106574321 0.0834082424008259 0.3051756494841002
0.6230832019609063 0.8430953037589053 0.3051716342943926
0.5586190934499291 0.5899484783226151 0.3050717338607065
0.4970481322183510 0.3405519125476905 0.3049388960247826
0.6213941857114180 0.3396399478380434 0.3051325549082630
0.1250565313469015 0.8444210717485494 0.3071946475184285
0.2454307239659525 0.8428951925023330 0.3045487141118553
0.0600635425682781 0.5855930091596468 0.3079356068993437
0.9960637364163324 0.3436684697669256 0.3082795025430872
0.6832465011091425 0.4303347470841123 0.3051655172347855
0.6230187568945936 0.6705027620132460 0.3051655969113929
0.5586853368200847 0.9234331395493360 0.3050508734818113

0.4971437768523328	0.1726114139925738	0.3049005035743900
0.6214574375304098	0.1739133843809789	0.3051349351197822
0.1248694124631492	0.6722733137844125	0.3071543421977642
0.2451725768280801	0.6709043960076159	0.3047304759390746
0.0603213513632981	0.9313045264427918	0.3081194942080923
0.9961911344117064	0.1728497936720163	0.3083877542415095
0.3105889605624472	0.0920730129430577	0.3033534319310960
0.4339558086306602	0.5900429906912861	0.3046846091379859
0.8087974321140964	0.0939854444083396	0.3053196180443293
0.9359319131496039	0.5914439311016704	0.3059413472875735
0.3100326821424514	0.4200667105202232	0.3038023315673951
0.4340465748310704	0.9228379856749960	0.3044825512374999
0.8085332742770922	0.4209806505957179	0.3053096694824794
0.9361420413526897	0.9249893122735257	0.3059955246700433
0.6828847785155939	0.9253714718569924	0.3052408571468793
0.5594438993277360	0.4238297759615385	0.3051392371527278
0.1854660149174952	0.9225346525053099	0.3049761917974246
0.0580998632547376	0.4229192546100462	0.3104491123753644
0.6827866715504668	0.5883233603948697	0.3052247010432419
0.5595421021096244	0.0895609577090749	0.3051211476826214
0.1848627504963875	0.5930080223488261	0.3051158580751626
0.0583059102597931	0.0940077355515208	0.3108648318800204
0.1953307718573518	0.2586689096492277	0.4090202031309078
0.2071209995382347	0.2592328137439850	0.4665199268466301
0.1250169933462140	0.2600140219142979	0.3368053908365818
0.2334372942439469	0.2535305141649878	0.3174292631354393
0.1456572479803528	0.2788444115199521	0.5279885497353872
0.0696811636570003	0.2284138842107774	0.5435114020929356
0.1168211879433820	0.2818475869257810	0.6271739018511190
0.0837828222423301	0.3359052949933516	0.7013619405698790
0.1671426677555685	0.3028408760953856	0.7023558432518242
0.2547351567322920	0.4238258133952580	0.7170740103854578
0.2238920853834582	0.3534010443387460	0.7827149575753213
0.1062381041848480	0.2968686148565992	0.5589009718045794
0.1194451528494042	0.2711197527590870	0.6812023051693291
0.2306838638138685	0.3330333355743121	0.7351374677922768

Initial state ab (n = +0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O

36 18 1 1 7 3

Direct

0.3094828305390647	0.9285378335890674	0.3036080898786381
0.3724320242958331	0.1717907244709093	0.3041680395982990
0.4350613142376412	0.4238006359250970	0.3047742910334587
0.4965594081381460	0.6723991550721055	0.3048642426555940
0.3712678872064689	0.6724289963773457	0.3043661899006175
0.8686787119766435	0.1724853359037626	0.3056832696104256
0.7487820198560070	0.1720317639467674	0.3052161890685151
0.9341541863227922	0.4322535606295124	0.3064571424165051
0.9964330898892045	0.6703841385013314	0.3065201374460243
0.3090779578258835	0.5839448115543960	0.3040537993454238
0.3721727705206548	0.3410681240953498	0.3043596808036691
0.4352423602111987	0.0891215630956650	0.3046070412374443
0.4966467367023605	0.8407028550428063	0.3048108300442110
0.3714474179669709	0.8399899564271637	0.3041686582129414
0.8685607725813671	0.3432842202232502	0.3056821097473022
0.7486759970598829	0.3421971110419007	0.3052119467317194
0.9343339112646739	0.0841429024119340	0.3064801725929018
0.9965998825529354	0.8462494918333672	0.3065670130554198
0.6834572216405835	0.0835328241053524	0.3051769279071353
0.6231264785083904	0.8430760589659446	0.3051740665682610
0.5585817853566475	0.5900243648365185	0.3050712816681356
0.4970435983568000	0.3404797289768088	0.3049322692479512
0.6214635225289236	0.3396270047431815	0.3051370348175286
0.1249949277366458	0.8445872181494930	0.3072052205984974
0.2454602688247360	0.8428980100362796	0.3045649036343544
0.0601331674726062	0.5857279620055216	0.3079298798768170
0.9960450163427302	0.3435930053797417	0.3082733607166604
0.6833324272183245	0.4301975737281970	0.3051670975625089
0.6230617914774174	0.6704963181193319	0.3051673457721694
0.5586518584119110	0.9233167479488892	0.3050506733709463
0.4971425954412704	0.1726475540060552	0.3048926431771468
0.6215298845291409	0.1739027872922233	0.3051407778461548
0.1248118387552004	0.6721652079140343	0.3071658968714104
0.2452018944270234	0.6708811082713594	0.3047507217025908
0.0604041421780713	0.9312113882370646	0.3081184708044957
0.9961826048791779	0.1729697670732154	0.3083908775351276
0.3105687982343309	0.0920195533317972	0.3033024649256070
0.4339477325002992	0.5901010055556468	0.3046956035816563
0.8088013837150553	0.0939157338713178	0.3053199551532046
0.9358969572219513	0.5916122912716431	0.3059567447838359
0.3099903567575072	0.4200638066580342	0.3037525034114756

0.4340401416297082	0.9227440990938668	0.3044853360204061
0.8085357029779779	0.4210699667656804	0.3053087262108823
0.9361106875874213	0.9248585962390213	0.3060084634667656
0.6828992920545340	0.9251439476554467	0.3052405928869843
0.5594780385219399	0.4236793197789323	0.3051392499532564
0.1854637805287934	0.9226688457844232	0.3049082747675663
0.0581624875742219	0.4228164584082919	0.3105886745885579
0.6827982700199001	0.5885366393360331	0.3052256445752767
0.5595820293880098	0.0896746136561363	0.3051211417848920
0.1848373488329959	0.5929061342029329	0.3050629997966173
0.0583873580627066	0.0942012594763224	0.3110310645345399
0.1950587994092444	0.2586548670735992	0.4089966803532558
0.2070416088600380	0.2592987435710039	0.4666103736849693
0.1250386666888507	0.2601347138458450	0.3366090900115905
0.2334765976845153	0.2534517418937631	0.3177217540084086
0.1456540271749188	0.2789451933388689	0.5278198292294008
0.0696498928503959	0.2283723269536815	0.5435428711715242
0.1167984113479826	0.2818362598275530	0.6271014786897600
0.0837767047687193	0.3358673041517973	0.7013525806732253
0.1671267959366762	0.3027993054573457	0.7023394960014125
0.2547077199341379	0.4238431072392412	0.7170226362399219
0.2239248366373364	0.3533768165931654	0.7826773871648833
0.1062304670276996	0.2968640364482906	0.5589120365091552
0.1194349807868916	0.2710791738653784	0.6811953590426335
0.2306945670519335	0.3330441877240016	0.7351042727213656

Transition state ab (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 7 3

Direct

0.3110230441497361 0.9235945163584021 0.3049425683291616

0.3737994823979536 0.1673547730351355 0.3055946539208886

0.4354764784645646 0.4195012614522780 0.3060148804959715

0.4969685974029905 0.6684140509237694 0.3054180931734916

0.3714910497764395 0.6670101314512851 0.3058995259050217

0.8695108514657778 0.1758010568783503 0.3066096409987682

0.7497590193142638 0.1709094618648331 0.3057583686568950

0.9341506660106346 0.4373256155004012 0.3072289950208187

0.9964831989752952 0.6757232572605583 0.3073399412871414
0.3089232870105423 0.5788052614786391 0.3070209674701787
0.3725810934088798 0.3366496893445164 0.3066294063863615
0.4363600817310117 0.0846523263505949 0.3051331035055820
0.4974311636376114 0.8364882977929872 0.3051403287120964
0.3724137252427629 0.8348504024653622 0.3049245319354405
0.8687336237899567 0.3465276797740480 0.3065458217399140
0.7490780985181255 0.3409258026965981 0.3057535305571257
0.9353233663705477 0.0891251671823418 0.3076230852879392
0.9974993657345670 0.8520789837111097 0.3077878601821764
0.6843660935721954 0.0807246286823629 0.3055011446758600
0.6239609928104618 0.8400782801169935 0.3053892522380677
0.5591154425681075 0.5863175918093392 0.3053739958930737
0.4976351236253086 0.3365194720271192 0.3054717375794751
0.6219041314717560 0.3364384233185634 0.3053590498717917
0.1260378982032834 0.8497187323534712 0.3090896491571964
0.2465979938721945 0.8405614654006220 0.3066173965776419
0.0598723768877955 0.5917625130246302 0.3082602979691627
0.9960381978132729 0.3492478320395408 0.3087267551352922
0.6835529932840733 0.4276689480965601 0.3055124464149160
0.6235467069028694 0.6674314473560955 0.3053956619852762
0.5595396665506881 0.9197644121164361 0.3052206443541587
0.4981435779194914 0.1685664552663813 0.3052320844257437
0.6223077220639549 0.1706228388516223 0.3053283482937835
0.1249053741732123 0.6772736212946149 0.3084038607671362
0.2451688118814594 0.6686609156898201 0.3072045195656851
0.0615423547787722 0.9373166078859944 0.3098080469228293
0.9968686701477940 0.1782637572631590 0.3096147394624357
0.3125796472751748 0.0863998651921933 0.3056063541147179
0.4344291383373370 0.5855424565436887 0.3058699549040155
0.8101294458054841 0.0950302793461087 0.3060682235933883
0.9358670177963998 0.5970285596072885 0.3067261736294851
0.3098363558048730 0.4141417794841880 0.3079911852256019
0.4349942093266352 0.9182165312020250 0.3048647202768979
0.8083180360618253 0.4219958624737168 0.3060019867054871
0.9372321105312390 0.9299131369651110 0.3071910999859506
0.6838023820631260 0.9224704155974596 0.3055329227683705
0.5599035343339199 0.4202753674608298 0.3053583238789327
0.1874920227000902 0.9246348436396917 0.3074164552016578
0.0579229908052203 0.4290148503730122 0.3099239304766301
0.6831042578154840 0.5855803519805953 0.3055206962386834
0.5604311972343659 0.0858773882174957 0.3052016861405737
0.1839214693020035 0.5947772970385501 0.3072223972110317

0.0593010812001668	0.1006191210703256	0.3128573555788426
0.1902383073180231	0.2661909477655391	0.4094740403729547
0.1988861015727549	0.2698208151909428	0.4685669738364772
0.1260781370873519	0.2723245495255280	0.3339578182641774
0.2351581627167801	0.2391275939594623	0.3234544404922714
0.1486998885559961	0.2851932165441438	0.5108252703586248
0.0665200291304933	0.2281219450386013	0.5375823406185883
0.1139310694336320	0.2878252263497607	0.5997762023364681
0.0845642184397998	0.3265236618174581	0.6963894724851462
0.1638540710071806	0.2946241655573006	0.6963717748155849
0.2581230929994296	0.4274187479305774	0.7169800289521501
0.2298663781935826	0.3535120690880554	0.7822681626907984
0.1025682993338449	0.3025611151511454	0.5489382937119979
0.1198037541571578	0.2657923802737404	0.6738990151720424
0.2370965171420477	0.3327105334553750	0.7348524743252249

Transition state ab (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
---------------------	--------------------	--------------------

0.0000000000000000	8.5216999054000002	0.0000000000000000
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0.0000000000000000	0.0000000000000000	20.0000000000000000
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C N Fe Ru H O

36 18 1 1 7 3

Direct

0.3110631967181557	0.9234142195890804	0.3051952542326912
0.3738341429616941	0.1671571863499163	0.3057799225629310
0.4354773825719601	0.4193260464490373	0.3061502125848627
0.4969116612737884	0.6682557030300038	0.3054832602729537
0.3714643828623150	0.6667019117581128	0.3061044609117045
0.8694486421855628	0.1760297083260201	0.3066565474436511
0.7497754466858393	0.1709112305433567	0.3057376408405038
0.9341238389744621	0.4376057787275088	0.3073432149111128
0.9964322389405966	0.6760018615474181	0.3075680165461481
0.3088982680714666	0.5784761615094813	0.3073514057131952
0.3725781003676039	0.3363861372079466	0.3068707971714252
0.4363800842367702	0.0843743760412902	0.3052632118793305
0.4973857785297739	0.8362283316045303	0.3052283381523482
0.3724155311389291	0.8346385210751742	0.3051196611618363
0.8686465969620549	0.3466321093156853	0.3065819742384089
0.7490690655798939	0.3407875006681658	0.3057289451256031
0.9353394447357567	0.0893110996958576	0.3077187443018793
0.9974871461085614	0.8523067682700637	0.3079849409216474

0.6843245664462891 0.0805344350610506 0.3054788063742314
0.6239396934756993 0.8399422848544310 0.3053894177253167
0.5591030192913731 0.5860787516955854 0.3054014827684156
0.4976308832461249 0.3363405930228834 0.3055455731388712
0.6218302612259877 0.3362841994892030 0.3053641592125119
0.1260866247901754 0.8498712104333366 0.3093388138911366
0.2466133525832331 0.8404682813909162 0.3069331635368652
0.0597997932024876 0.5920111711270460 0.3084577877675478
0.9960425866005995 0.3495215384905744 0.3087845160531788
0.6834769429439457 0.4275620422182445 0.3054854304131476
0.6235087828504464 0.6672499171793561 0.3053846864301654
0.5595432498552172 0.9196429161931472 0.3052807078018510
0.4981559920174070 0.1683405989619178 0.3053287911850318
0.6222472759691128 0.1704384020950359 0.3053463386689655
0.1249059456781555 0.6775360314118486 0.3086823014986526
0.2451302077607432 0.6684840751729141 0.3075453427255752
0.0615206657528996 0.9376089087512779 0.3099104500671219
0.9969044681719428 0.1784987286966246 0.3096048167690907
0.3126545056512470 0.0861877525068919 0.3057926581922040
0.4344016165903518 0.5852887612775618 0.3059620158414872
0.8101441763425189 0.0951183830561712 0.3060734319990184
0.9358362825844072 0.5971097598374884 0.3068822044477258
0.3098480094172420 0.4138045664619746 0.3083324450666912
0.4349929046415082 0.9180101448064181 0.3049975545033581
0.8082451409202640 0.4220140044045803 0.3059890842761923
0.9372466965013208 0.9303440837783373 0.3073370749573296
0.6837740972330989 0.9224274365783219 0.3054911521887573
0.5598678120858721 0.4201583539882888 0.3053790153041820
0.1875696404447547 0.9246534434819599 0.3077560671114026
0.0578183118253931 0.4294672636077156 0.3099127522945573
0.6830457447262188 0.5853190719420107 0.3054734467765821
0.5604059445983930 0.0856277240250081 0.3052727150186350
0.1838699227602909 0.5948735840398705 0.3075717392164620
0.0592479452922053 0.1007064487359082 0.3126385291771571
0.1906488332592355 0.2665068019770985 0.4095042340785051
0.1991425380001473 0.2701777938527766 0.4686542375377379
0.1261055398904201 0.2728676293731840 0.3342193459758995
0.2351531915555841 0.2384822111801475 0.3235399909312042
0.1493948337122485 0.2856289794619288 0.5091771934600304
0.0660299707224399 0.2283425938827073 0.5366933199389512
0.1133507621204667 0.2885388406836136 0.5983303514596591
0.0847767128649267 0.3255106579986166 0.6962286111647757
0.1639986069866781 0.2944964902737316 0.6959214393926765

0.2585262722257671	0.4277572433799704	0.7169376369522213
0.2303146296544919	0.3532954370383878	0.7821258752590765
0.1018412002688041	0.3035069956475114	0.5478715051352493
0.1200306071644715	0.2655134765337027	0.6734243865627603
0.2373814952858821	0.3330260842845753	0.7346459976206925

Transition state ab (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
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0.0000000000000000	8.5216999054000002	0.0000000000000000
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0.0000000000000000	0.0000000000000000	20.0000000000000000
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C N Fe Ru H O

36 18 1 1 7 3

Direct

0.3110186720057516	0.9234975957162136	0.3049352893651835
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0.3738041755485229	0.1673149426057038	0.3055983817120385
--------------------	--------------------	--------------------

0.4354803727110202	0.4194262636997438	0.3060228871781501
--------------------	--------------------	--------------------

0.4969887359903332	0.6683574444935442	0.3054269516248957
--------------------	--------------------	--------------------

0.3714880507931972	0.6669925669372861	0.3059105904665413
--------------------	--------------------	--------------------

0.8695623633839051	0.1757810681868048	0.3066078172844258
--------------------	--------------------	--------------------

0.7497424405554017	0.1708431938202199	0.3057527436755318
--------------------	--------------------	--------------------

0.9341349849961110	0.4373105250299922	0.3072303342848251
--------------------	--------------------	--------------------

0.9964782436933549	0.6757662373610677	0.3073667395116800
--------------------	--------------------	--------------------

0.3089057519701309	0.5788164578158033	0.3070421681625685
--------------------	--------------------	--------------------

0.3725842050990801	0.3366156269671923	0.3066492414035393
--------------------	--------------------	--------------------

0.4363697268492680	0.0846543141662457	0.3051495375821924
--------------------	--------------------	--------------------

0.4974578989139574	0.8364599947175495	0.3051551520408240
--------------------	--------------------	--------------------

0.3724155713788456	0.8347757844014010	0.3049336851725974
--------------------	--------------------	--------------------

0.8687730845580556	0.3466049103215734	0.3065417963763477
--------------------	--------------------	--------------------

0.7490548330768597	0.3409620849784955	0.3057484307577795
--------------------	--------------------	--------------------

0.9353105706908034	0.0892243159541644	0.3076209943012794
--------------------	--------------------	--------------------

0.9974896432756845	0.8521067082105178	0.3078003280324308
--------------------	--------------------	--------------------

0.6843995038774888	0.0807098492209328	0.3054973039543084
--------------------	--------------------	--------------------

0.6239592788096305	0.8399904449608683	0.3053912275769983
--------------------	--------------------	--------------------

0.5591204246204163	0.5863213888665115	0.3053800079780689
--------------------	--------------------	--------------------

0.4976320956834593	0.3364776094596190	0.3054759110026253
--------------------	--------------------	--------------------

0.6219459686199191	0.3363695193551652	0.3053626933008864
--------------------	--------------------	--------------------

0.1260009881534869	0.8498048893656074	0.3091168362141818
--------------------	--------------------	--------------------

0.2466114293851121	0.8405133460687584	0.3066434269757107
--------------------	--------------------	--------------------

0.0598937715270470	0.5918625556591151	0.3083119407777784
--------------------	--------------------	--------------------

0.9960156452187038	0.3492657395548548	0.3087417081197581
--------------------	--------------------	--------------------

0.6835835112504357	0.4276293121972704	0.3055093591443487
--------------------	--------------------	--------------------

0.6235451445165923	0.6674431852848952	0.3053931943497923
0.5595420717995315	0.9196703496705452	0.3052357602193967
0.4981387969047891	0.1685287175946797	0.3052462370499762
0.6223512608985702	0.1706184218361813	0.3053363275528216
0.1248749883274733	0.6772571923401299	0.3084548815752755
0.2451814426768639	0.6686528519571623	0.3072419280674707
0.0615735850044565	0.9372913862274271	0.3098108250600660
0.9968515209280319	0.1783244537255121	0.3096158666514655
0.3125790684011589	0.0863507293839771	0.3055659646378210
0.4344342866445466	0.5855176929958876	0.3058636972150933
0.8101401672101826	0.0950123875759716	0.3060555357467395
0.9358420646737210	0.5971797822288470	0.3067494926007818
0.3098212729242782	0.4140842397190547	0.3079974787665227
0.4349940184041060	0.9181562216986378	0.3048758779389513
0.8083214926819953	0.4220261777095262	0.3059838268598014
0.9372148218713001	0.9298210605009520	0.3072146957890413
0.6838393739597007	0.9223686285569058	0.3055207021891754
0.5599128258807361	0.4202309785699212	0.3053594383461009
0.1874916699441039	0.9247069946867139	0.3074123280548751
0.0579761716688094	0.4289383690009485	0.3100444784242215
0.6831403156930680	0.5856137757634180	0.3055073128663998
0.5604468849226191	0.0858446480903828	0.3052199045658440
0.1838965461936567	0.5947174337311090	0.3072567781772031
0.0593576657554740	0.1008067317391039	0.3129551156878854
0.1901594656202988	0.2662520905736673	0.4093921574066841
0.1988879984323975	0.2699726698077426	0.4685819384908517
0.1260582785789415	0.2723772935434715	0.3338588562609703
0.2351998442593567	0.2390847808218711	0.3235040307302932
0.1486470997371351	0.2853675652801608	0.5108616606353387
0.0664929381917145	0.2281967046550346	0.5375306702382062
0.1138852419929714	0.2878273830323329	0.5999718873637445
0.0845781336296958	0.3263930759288437	0.6962799722335824
0.1639341782757243	0.2948239657045840	0.6962219970196865
0.2581098403858044	0.4273556277082947	0.7169096617902435
0.2297880763733991	0.3533138149350174	0.7821582092809369
0.1024467404432588	0.3027277359545519	0.5490510575148446
0.1198701392828211	0.2659207172113769	0.6737478956842845
0.2369375268750744	0.3327537534115839	0.7347128521176252

Final state ab (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 7 3

Direct

0.3118012191139283	0.9216946049098828	0.3039292092461267
0.3746355786504423	0.1655542681433314	0.3048084204886053
0.4360330464507585	0.4178074118854719	0.3057935647186965
0.4974179068947301	0.6667489216984557	0.3053135168006979
0.3719286753207088	0.6649432794876325	0.3053874178508618
0.8699766609237612	0.1762244896136284	0.3069475180655057
0.7503468414953121	0.1700265481367687	0.3059172210321737
0.9344320822479020	0.4382479476554704	0.3075485856542041
0.9967597106539694	0.6765524166931841	0.3075579502758000
0.3093229924763632	0.5770310247083696	0.3061168911962976
0.3732312978632131	0.3348548688356949	0.3058931976198292
0.4370527621252391	0.0827556357167533	0.3048850184453171
0.4979562678567721	0.8345915899705769	0.3050395317986721
0.3730010821621780	0.8329984366425219	0.3043615825620074
0.8690365378416639	0.3468706215467167	0.3069058255634985
0.7495158003748159	0.3398404679903071	0.3059246234940677
0.9358659463793716	0.0898982615089911	0.3078862614049656
0.9979735725621988	0.8531703830758151	0.3079389524007290
0.6849274247461360	0.0792033181379254	0.3055717781908595
0.6245466722156363	0.8385334159511648	0.3053932343999571
0.5596553815538708	0.5845611414186055	0.3053779645954722
0.4982433450723071	0.3347842172091273	0.3055024433364698
0.6223478213776322	0.3348654138398739	0.3054416910625433
0.1266289177602577	0.8504778242196137	0.3085318761016593
0.2472098984228608	0.8393068130859574	0.3057363051302147
0.0600971754705694	0.5927745145821439	0.3079917812605644
0.9962233232463448	0.3503566752811477	0.3086107613069154
0.6839165218355269	0.4263162631417928	0.3055832798050998
0.6240321066873796	0.6659183567012289	0.3053922840908616
0.5601747985269323	0.9181764229547910	0.3052483388495879
0.4988424503701290	0.1668258690189107	0.3052731360119550
0.6228435026670461	0.1690277817160090	0.3054227334032505
0.1252482366851008	0.6779502084165354	0.3079275506640017
0.2454971112889650	0.6676095897615404	0.3064186717648102
0.0620585772501325	0.9384205251661418	0.3094535141368491
0.9972060547132796	0.1790826589462055	0.3094796276262921
0.3135393715170551	0.0844472322324342	0.3040398503687003
0.4349525600394448	0.5836418317136343	0.3055640519091638

0.8108139218987588	0.0947977430390607	0.3063051891580116
0.9361218926513416	0.5981095450468152	0.3071710111774648
0.3103736238858737	0.4121243303146028	0.3064461436674484
0.4356632181929321	0.9164231490536906	0.3045420438382771
0.8085300893774695	0.4216317444315477	0.3062691963596704
0.9377590045473936	0.9306685561212216	0.3076527395623580
0.6844038514587858	0.9211025503372048	0.3055283220961578
0.5603879114044664	0.4188657639228508	0.3054198531895405
0.1882836622977916	0.9244122952254256	0.3065170711796590
0.0581208545112860	0.4299774986533182	0.3092436602274146
0.6835230924681527	0.5839700469275145	0.3055160580920150
0.5609887097679062	0.0839666719025361	0.3053037782680456
0.1840488769194897	0.5947201807800299	0.3065719603385762
0.0597539397318649	0.1017980652653148	0.3124102318773899
0.1905483653280356	0.2690295515905528	0.4030057146648515
0.2031520362166860	0.2755375200366477	0.4628910707948470
0.1266471190931620	0.2738776890125694	0.3305323123872974
0.2360964432203738	0.2366781749691885	0.3195798667479077
0.1598443785685156	0.2909754734843385	0.4948971841913827
0.0635088005999972	0.2240098080279785	0.5403577100894282
0.1081520678424576	0.2899986724528023	0.5992995215933068
0.0838071804000226	0.3332266869260039	0.7028747845996333
0.1617713873632339	0.2936346358214629	0.7017838539551527
0.2571251614676394	0.4293437437285517	0.7182494273366695
0.2299907011810343	0.3583941790129181	0.7845549175247727
0.0967670523912876	0.3051735508835376	0.5506219078734492
0.1169190060716120	0.2644822995373308	0.6815897409552147
0.2374683873024862	0.3345368617806338	0.7374523486208002

Final state ab (n = -0.25)

1.0000000000000000		
19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	18	1	1	7	3

Direct

0.3118225091247851	0.9217579515190206	0.3039789350075860
0.3746412490704049	0.1655547561363784	0.3048470013920523
0.4360207326839975	0.4178840146472141	0.3057990869296788
0.4973899831955154	0.6667775746591905	0.3053175404649762
0.3719359826041234	0.6649464082415067	0.3053920242013689
0.8699550334461078	0.1762230416309447	0.3069511939543192

0.7503747116808436 0.1700434261632737 0.3059144646601411
0.9344443383840191 0.4381907325224176 0.3075764037533857
0.9967474853247993 0.6763543733023875 0.3075805497441667
0.3093489573674896 0.5769953506826696 0.3061478960027751
0.3732378191433294 0.3348868259744520 0.3059113708398104
0.4370382387372026 0.0827136592219968 0.3048937164845477
0.4979285050144203 0.8345971857034823 0.3050464390017409
0.3730056690003381 0.8330331286960981 0.3043706898243226
0.8690165324948046 0.3468418762108173 0.3069150425991127
0.7495437823751279 0.3398332442707985 0.3059202275503619
0.9358752617156075 0.0899077163879730 0.3078994434494619
0.9979684588164914 0.8533128119299773 0.3079529410286438
0.6849069080413286 0.0792121482927471 0.3055700189023831
0.6245596917712609 0.8385959384011014 0.3053950872320528
0.5596544601617877 0.5845158152208366 0.3053808618084152
0.4982598123601712 0.3347771753015175 0.3055099263062487
0.6223116786912387 0.3349180659270971 0.3054412947238000
0.1266550397756089 0.8504293685468954 0.3085747511393542
0.2471907098012402 0.8393003810101983 0.3057773263344142
0.0600842855503689 0.5927206110557680 0.3080248077997492
0.9962505700446527 0.3504806094554091 0.3086616635961899
0.6838983752085449 0.4263229483424203 0.3055808560966639
0.6240435196384980 0.6658834932639626 0.3053944487668829
0.5601748297267822 0.9182576075458562 0.3052541178810793
0.4988575920156249 0.1668715778298639 0.3052803462949010
0.6228069777389298 0.1690038847344769 0.3054214009062286
0.1252743819615903 0.6779601314223471 0.3079760786392687
0.2454796580437447 0.6676402588547392 0.3064561699088332
0.0620446674202009 0.9384222649019917 0.3094724948965631
0.9972383928970294 0.1789070087177059 0.3095120516300444
0.3135411661920818 0.0844411072715606 0.3041577488968877
0.4349698777487988 0.5836197978394325 0.3055634972161535
0.8108148725338226 0.0948004112391288 0.3063066005876061
0.9361765118925320 0.5980919159120539 0.3071667850465630
0.3103799685624508 0.4121778312211218 0.3064951608699213
0.4356819108530617 0.9164865336368457 0.3045559984186484
0.8085345653005477 0.4216205402307817 0.3062725343382769
0.9378133836712998 0.9306468254300723 0.3076510196833289
0.6843610773331937 0.9211540768025621 0.3055289087280925
0.5603774948285791 0.4189368483206388 0.3054218042094328
0.1882870912037296 0.9243819673404597 0.3065742272791955
0.0580704277955285 0.4299416515057222 0.3092378995624965
0.6834830235676743 0.5839387917675726 0.3055169429299304

0.5609770947074174	0.0839271997843902	0.3053074024923859
0.1840583213915488	0.5947423926398723	0.3066275617797170
0.0596997510810600	0.1017805042979719	0.3123815246061580
0.1907995396636907	0.2689361873653684	0.4032017523903475
0.2031785151265116	0.2753812724671414	0.4630129537586488
0.1267330230664940	0.2739975000899855	0.3306337567115280
0.2360735793303982	0.2367057461862231	0.3195311728213552
0.1598027991007329	0.2908360783243325	0.4951424272704930
0.0633727433934356	0.2241363469352924	0.5400098431907618
0.1079500442516342	0.2901431996113453	0.5990285742495143
0.0837222893664150	0.3327140446249515	0.7028828347215260
0.1617274016500511	0.2937003488732532	0.7016216835481136
0.2571900465084019	0.4294442597921007	0.7182030920137480
0.2302062658801302	0.358366665813688	0.7845392659347454
0.0967041081405730	0.3051579082431731	0.5502923748285562
0.1169086798846450	0.2645935109186043	0.6813479617612795
0.2374675939455390	0.3346834080211265	0.7373918034031119

Final state ab (n = +0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	18	1	1	7	3

Direct

0.3117838690467402	0.9216991505633215	0.3039384904408493
0.3746339570559652	0.1656165629024011	0.3047989090818297
0.4360645983626307	0.4177922058954880	0.3058130997514962
0.4974583665588332	0.6667834817692148	0.3053273650291031
0.3719372854391264	0.6650100686493965	0.3054331673909127
0.8700297905295680	0.1761763807943344	0.3069481518294551
0.7503472554295398	0.1700156169088513	0.3059164972958660
0.9344541807974948	0.4382047407038220	0.3075620049813294
0.9968018604217196	0.6765974088082787	0.3076098179778482
0.3093219174705402	0.5771325525746628	0.3061479978086349
0.3732398240112854	0.3348882881379301	0.3059098636219580
0.4370793824201781	0.0828645079647407	0.3049065877676423
0.4979922212700931	0.8346445909882233	0.3050520074386314
0.3730044144174710	0.8330433189694066	0.3044066024853025
0.8690973734364674	0.3468615365865740	0.3068946477936570
0.7495238564632098	0.3398700237451487	0.3059225963674360
0.9358802133904887	0.0898549560535226	0.3079170521460189

0.9980009114741504 0.8530379046939788 0.3079937029191830
0.6849717605276745 0.0792156550178994 0.3055759422825887
0.6245492375375470 0.8385046676425477 0.3053986450295868
0.5596807589244133 0.5846531336890967 0.3053860362245048
0.4982501611466607 0.3348547193116463 0.3055108733236652
0.6224123053801986 0.3348590332153378 0.3054482880603961
0.1266139697902371 0.8504718564669167 0.3086285982040019
0.2472353703077584 0.8393476252634204 0.3057892040255748
0.0601501062117044 0.5927490736846188 0.3081157900020788
0.9962260406013173 0.3502184160178395 0.3087053073798663
0.6839657910100502 0.4263591341532569 0.3055870040833407
0.6240391046631263 0.6660002183222999 0.3053968039675874
0.5601939802782350 0.9181519899247442 0.3052553523771014
0.4988456544256429 0.1668312938661382 0.3052860980929375
0.6229043147706581 0.1690979259900207 0.3054301874093540
0.1252428980207313 0.6778644449632660 0.3080282370920359
0.2455336780923328 0.6676048408750827 0.3064827947465025
0.0620971970535135 0.9383548988473367 0.3095746837334769
0.9971991955292507 0.1791333365091279 0.3095805257651844
0.3135378196386045 0.0845305013531417 0.3039345592179898
0.4349541601174035 0.5837268532967586 0.3055900190550931
0.8108368134186278 0.0947770359793231 0.3062995831127243
0.9361191636693255 0.5981033043428546 0.3071834195563887
0.3103907987763940 0.4121469155123959 0.3064394737308995
0.4356557107775047 0.9164284214175905 0.3045568296664221
0.8085692125355827 0.4216314825460978 0.3062521321312383
0.9377447101391528 0.9305835079373054 0.3076773627443284
0.6844674069840440 0.9210801592291651 0.3055311103474709
0.5604188608013770 0.4188589295680336 0.3054258095502019
0.1882797165898812 0.9244188210903477 0.3065826827290781
0.0581991608042294 0.4298640449303167 0.3094702788655850
0.6835925886787491 0.5840440456079677 0.3055185772795740
0.5610187928677395 0.0840432406757495 0.3053108899900476
0.1840761637358131 0.5946701399753617 0.3066561090008847
0.0598233405821875 0.1018126637141449 0.3126315597335994
0.1904865228698638 0.2687869836123232 0.4030101635711407
0.2034154903834683 0.2752631532453650 0.4629828993482710
0.1265766320033636 0.2737058410177576 0.3307775846142866
0.2361452688117307 0.2367834169357850 0.3197349683377966
0.1601197604648571 0.2908559545072226 0.4947303614969257
0.0630689312878746 0.2239570088728974 0.5397856476727609
0.1074278738019786 0.2901489225033101 0.5988904894538600
0.0836414585946694 0.3322107081614927 0.7029258307607701

0.1616996514767056	0.2938055819597092	0.7015236203427161
0.2572651582945594	0.4295518590716512	0.7181494777094233
0.2304124665747712	0.3583512103464477	0.7845230465390338
0.0959547033337449	0.3057298913882625	0.5503017531763080
0.1169034307389618	0.2644616840890033	0.6812995239021596
0.2374853979802681	0.3348603966423133	0.7373290854361298

2.2: Step cd ($\text{N}_2\text{H}_2 \rightarrow \text{N}_2\text{H}_3$)

Initial state cd ($n = 0$)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3112636058615078	0.9303763588487224	0.3064444473447220
0.3750742579138282	0.1732337772249134	0.3058699975224977
0.4375730483191086	0.4250235506379569	0.3053578987834890
0.4987698205376620	0.6734704538476581	0.3050569592987647
0.3731872515466793	0.6731199574420643	0.3057180387282240
0.8705496438037980	0.1724539643281914	0.3064290756103883
0.7507405679265505	0.1725198658361050	0.3054122769656792
0.9360100010582338	0.4324722832345964	0.3073046422835927
0.9985554972300212	0.6699024118151088	0.3080277773410123
0.3111989252620026	0.5848655931573039	0.3065012764858068
0.3750240426306080	0.3420690381964299	0.3059246438240386
0.4375950365372921	0.0902279035966929	0.3053085336979653
0.4987793583191475	0.8417784032660240	0.3050369395350191
0.3732198640175314	0.8421052604738180	0.3056837282891051
0.8705185371321714	0.3433897172379616	0.3064327259280649
0.7507133778694048	0.3428827994338550	0.3054226014408852
0.9360599774810844	0.0835450307827569	0.3073208240402227
0.9985915243977496	0.8461763363110437	0.3080633795313080
0.6855868834443675	0.0842527834171520	0.3050622538671471
0.6252557542814894	0.8438942022624880	0.3049551245853367
0.5607316084281080	0.5910344599106780	0.3049199890210695
0.4994532641831346	0.3415909328700067	0.3049710769045687
0.6237897762422699	0.3404560410963405	0.3048869484676858
0.1267973417948325	0.8443847369581576	0.3089484955432069
0.2473669202264985	0.8438169400205797	0.3073277972028399
0.0622532382519881	0.5847614266885740	0.3089937194009131

0.9975251156723660 0.3431131728973463 0.3083459653770428
0.6855574708261134 0.4310345670419351 0.3050817873669747
0.6252422297913035 0.6713870323932752 0.3049689905811621
0.5607458828224243 0.9242204360036969 0.3048986417559733
0.4994760964183086 0.1736462309001654 0.3049578213059421
0.6238059309313820 0.1747992105572274 0.3048762206397513
0.1267635059528810 0.6717025888292214 0.3088244573604015
0.2473032674575086 0.6717030550760131 0.3072762607962524
0.0623070803952128 0.9314001637193892 0.3091571508594927
0.9975497806972774 0.1729663511804103 0.3084246072791150
0.3125967565314976 0.0953961305900550 0.3072301314025469
0.4359929721987579 0.5916317071581126 0.3053652482699477
0.8106734998057580 0.0942393162177356 0.3058254962192183
0.9378458607397796 0.5918151460432612 0.3075232819618005
0.3125431786588755 0.4198662587059750 0.3073446188847170
0.4360149078677706 0.9236073798815934 0.3053177754966938
0.8105977418808611 0.4213763232982463 0.3058344766179037
0.9378930360262744 0.9242119944257776 0.3075292616627662
0.6850206353272200 0.9257635807451288 0.3051109675228296
0.5618149223353841 0.4245647210031002 0.3048693240443268
0.1870892393353636 0.9221757696425756 0.3076519026603234
0.0601513789383934 0.4209852911446061 0.3109702929930589
0.6849963729812167 0.5895116577368791 0.3051388098473003
0.5618233914972002 0.0906864486461801 0.3048557775095373
0.1869756576499534 0.5937167380194833 0.3074230183856039
0.0602100902145979 0.0952290706708676 0.3112455863844086
0.1827225146994542 0.2613256684491972 0.4078555013156759
0.1838656715590338 0.2731798163056071 0.4760158100452878
0.1253900945296327 0.2584954706148735 0.3354085969337071
0.2407108372021536 0.2571247419641745 0.3344934457796291
0.1422018243049008 0.2219016654496542 0.4975783192228840
0.2282497945144486 0.2305369808875178 0.4956850607566045
0.1802778794401654 0.4648248630687415 0.5019946795324206
0.2095361133603503 0.6385225229069502 0.4929087120349006
0.1897653298341471 0.5887802798826427 0.5857677259115855
0.2045905295090227 0.7157793020669305 0.6557021457276678
0.1616789812733314 0.5496169715232646 0.6644989942822511
0.1763816030039257 0.9423221864390674 0.6652092727790857
0.2189604490632297 0.8820460370322764 0.7260233497401198
0.1769794360526807 0.5771236881773415 0.5188440592796397
0.1993665720876547 0.5975769245186374 0.6398896817822738
0.2149332529151003 0.8762375492896870 0.6774111750476329

Initial state cd (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3112933302933183 0.9303541852607596 0.3064629529408845

0.3750700776980458 0.1732155669748890 0.3058871945399175

0.4375595753664172 0.4250590492824732 0.3053839654873754

0.4987319620412309 0.6735333858262265 0.3050972432156011

0.3731792363274783 0.6730645180375782 0.3057590923735621

0.8705332394121668 0.1725349908148670 0.3064116895927453

0.7507874428664532 0.1726148168684837 0.3054107433902212

0.9360425571427489 0.4325136026473161 0.3072979599334180

0.9985276488781158 0.6699182877949992 0.3080112905004372

0.3112232026092809 0.5848709875985137 0.3065361536064219

0.3750178460140965 0.3420792841919831 0.3059493776607823

0.4375812511433072 0.0901904036324139 0.3053299143232204

0.4987449988257900 0.8417244209751938 0.3050742509629663

0.3732133252722932 0.8421495343952954 0.3057172552588336

0.8705008343393579 0.3433546056635421 0.3064138774020022

0.7507602491557523 0.3428051252198263 0.3054220705394277

0.9360953788376484 0.0835587960251266 0.3073156358950461

0.9985666417526047 0.8462179517092550 0.3080484750476901

0.6855469911138896 0.0842060128718527 0.3050733367622465

0.6252420337023314 0.8439015298746142 0.3049816135575033

0.5607508640155027 0.5909852844212046 0.3049604988137244

0.4994614045239006 0.3415907301373117 0.3050088245398977

0.6237441858193957 0.3404639372516872 0.3049154614457252

0.1268290151466385 0.8443636078607146 0.3089313774185991

0.2473554444666818 0.8437712525286458 0.3073305360772531

0.0622195836335208 0.5847541701065967 0.3089854138250773

0.9975656598224752 0.3431847345691861 0.3083666635556405

0.6855149092834417 0.4310919617840719 0.3050926876516423

0.6252259139236027 0.6713897029922135 0.3049943706407564

0.5607644380523223 0.9242787421647871 0.3049391268760095

0.4994839977723457 0.1736495069862328 0.3049949722131337

0.6237597339078518 0.1747994886283074 0.3049043796251987

0.1267906999738217 0.6717666068627138 0.3088099137023501

0.2472902235627960 0.6717382997537353 0.3072863730438918

0.0622799746910743	0.9314608609010337	0.3091472682211590
0.9975923420407077	0.1729490771451719	0.3084423180965095
0.3126115922930785	0.0953505887489525	0.3072617366804864
0.4360152626286124	0.5915930579676231	0.3053903572159428
0.8106788160668219	0.0942949907436126	0.3058107406476470
0.9378534195690962	0.5917723475197348	0.3075216444594441
0.3125539504346691	0.4198877829862029	0.3073919346121416
0.4360358271015785	0.9236444408721790	0.3053379299701623
0.8105991881451055	0.4213524269582068	0.3058194311436365
0.9379047753801317	0.9243089377451965	0.3075298602146398
0.6850057374897466	0.9258832228607172	0.3051222103238602
0.5617894121710544	0.4246659613516348	0.3049188016546009
0.1871031412452988	0.9221260371187461	0.3076792688412187
0.0601282906419927	0.4211782794942253	0.3109589689960370
0.6849800953413162	0.5894013435725146	0.3051472357988941
0.5618002513896996	0.0905916624750785	0.3049042015436527
0.1869774682384764	0.5937785603450062	0.3074615611691873
0.0601917102235684	0.0950922846899152	0.3112242243082199
0.1828588270332492	0.2611077127329832	0.4079960349312438
0.1838695394238720	0.2723815358667219	0.4759752985743312
0.1255813920257301	0.2585342310505518	0.3353572917182385
0.2406445162135901	0.2570806118819090	0.3344118440717831
0.1420761986647757	0.2216616548473590	0.4975475062715199
0.2282467033420058	0.2303750341021064	0.4958937703030328
0.1802665476653057	0.4653499683396589	0.5019668407071507
0.2095683362535862	0.6388402215514820	0.4928705209480435
0.1897058809009021	0.5888764965085319	0.5856935748621390
0.2045085583176426	0.7156661446131538	0.6556220656388683
0.1617173982579469	0.5492629235296154	0.6643775515664734
0.1763832933801259	0.9424565572088539	0.6651799801023451
0.2191105327218510	0.8821793885833598	0.7258902276165442
0.1769204754511335	0.5774359433615580	0.5187048671409730
0.1993369599707023	0.5975023683569358	0.6397591850648521
0.2149156995889177	0.8762115022568435	0.6772946291658295

Initial state cd (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3113330890882196	0.9303577912858604	0.3065001446151738
0.3750530669586892	0.1731553827755977	0.3059503034026854
0.4375446597768027	0.4250876221065596	0.3054316178204292
0.4986788233426219	0.6735855805706953	0.3051372034807851
0.3731743382571920	0.6730655946091066	0.3058048058675463
0.8705269793208025	0.1726014816715518	0.3063979169723934
0.7508328541623212	0.1726913101980601	0.3054113968158066
0.9360877996572647	0.4325546119363062	0.3072942856965696
0.9985082159718133	0.6699438541897516	0.3079799314385216
0.3112619557606962	0.5848581979564283	0.3065904280792309
0.3750013709645921	0.3421310757778541	0.3060183438397320
0.4375685348483119	0.0901619112554449	0.3053731436180300
0.4986934235349839	0.8416735197492130	0.3051151625378284
0.3732095461565607	0.8421458799141145	0.3057538302880349
0.8704927838753118	0.3433359620384375	0.3063988033308058
0.7508034722645061	0.3427512688922998	0.3054217372648404
0.9361442304120178	0.0835775398095549	0.3073133521684582
0.9985504456929193	0.8462649624601934	0.3080166131644870
0.6854896810706443	0.0841455679378052	0.3050899745453891
0.6252297122284681	0.8439311410527064	0.3050139469218628
0.5607617491335755	0.5909368470977713	0.3050040769619101
0.4994572429371203	0.3415783396301660	0.3050574940711139
0.6236877926800469	0.3404686627931136	0.3049504112392971
0.1268720258457303	0.8443335026726385	0.3089426924082431
0.2473463035255335	0.8437216753031375	0.3073627950741181
0.0622072715896081	0.5847561587057961	0.3089946167104934
0.9976116364324824	0.3432619561535819	0.3084157816127471
0.6854545280411523	0.4311692918202739	0.3051087866875474
0.6252116948778220	0.6713713087701868	0.3050252543915020
0.5607752448977139	0.9243333492442319	0.3049840142255789
0.4994802497690692	0.1736640254840620	0.3050434618020822
0.6237040448579283	0.1748051430815984	0.3049405495079661
0.1268298159116029	0.6718382627411609	0.3088286358177366
0.2472801425514175	0.6717758470286435	0.3073271821860822
0.0622743594521968	0.9315204626305326	0.3091510020659821
0.9976416035269693	0.1729305831797591	0.3084887781672792
0.3126240341153589	0.0953073837094686	0.3073154815927472
0.4360333723450240	0.5915593771937531	0.3054182016568556
0.8106875950795881	0.0943612594069507	0.3057936069321172
0.9378771652947049	0.5917220103706163	0.3074900417657405
0.3125650742394138	0.4199198057313059	0.3074580342424084
0.4360536429982263	0.9236783630487921	0.3053611868473252

0.8106024154769723	0.4213212365213356	0.3058019373603512
0.9379344296313269	0.9244271943842071	0.3075008201454352
0.6849767828685633	0.9260291777415092	0.3051384794015284
0.5617479904356901	0.4247914597329045	0.3049706077919507
0.1871259903545128	0.9220815427375120	0.3077151533738670
0.0601303733909607	0.4213347625120261	0.3109896674161818
0.6849504794541224	0.5892676106331024	0.3051608329900143
0.5617623888782510	0.0904715848414704	0.3049558272042445
0.1869906555265462	0.5938318481353403	0.3075193596581235
0.0601979956727620	0.0949967064310818	0.3112408269621406
0.1829790730739134	0.2606864364689101	0.4080451161608450
0.1839016223664346	0.2712630529078320	0.4758458638631995
0.1257394088269088	0.2585666732862285	0.3353225191781420
0.2405403937869305	0.2570796918273940	0.3342084896820494
0.1419213366232835	0.2215286273206384	0.4974693259075286
0.2282920483461780	0.2301819678122052	0.4960696479704251
0.1802448161452134	0.4660319212957212	0.5018958935614873
0.2096191575491381	0.6391651412924020	0.4927824937823016
0.1896372644283282	0.5890379815416638	0.5856951029861878
0.2044160262133819	0.7156266446255702	0.6555391328764566
0.1617619174125531	0.5488620882740831	0.6642432170242690
0.1763756224701289	0.9425832936009509	0.6651402188214949
0.2193005837640073	0.8823026117763503	0.7257152949161148
0.1768245253541438	0.5778889767593340	0.5184920237536201
0.1993031368007371	0.5974420722620999	0.6396265918485263
0.2148880027019914	0.8761150632930328	0.6771561025280397

Initial state cd (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3112408194155534 0.9303934439698845 0.3064481060691781

0.3751062707106498 0.1732319194609125 0.3058231505502866

0.4375975800950926 0.4249884304336732 0.3053567397115624

0.4988059431459396 0.6734211986439141 0.3050975117553488

0.3731884389964014 0.6731827548600250 0.3057353196458353

0.8705719167962159 0.1724286062758473 0.3064241712122192

0.7507040693256808 0.1724613269396202 0.3054076274271117

0.9359824815362630 0.4324711984991606 0.3072915425332010
0.9985608289700738 0.6699449914466766 0.3080415635506936
0.3111720351358985 0.5848282517728877 0.3065126496750114
0.3750525815350952 0.3420539081721549 0.3058836307075575
0.4376220613746701 0.0902520101724017 0.3053048803699648
0.4988177824456504 0.8418195967313666 0.3050766159954902
0.3732208791677504 0.8420216084514086 0.3056981906193910
0.8705405657769898 0.3434638888304265 0.3064263233366048
0.7506755281164234 0.3429687501099972 0.3054180001962732
0.9360319039459412 0.0835975967926282 0.3073100845467442
0.9985979685374349 0.8461837674471568 0.3080780426727349
0.6856370536409591 0.0842938642122568 0.3050722174899744
0.6252779971265010 0.8438975284543060 0.3049806726375619
0.5607223735722795 0.5910913779000306 0.3049595834953381
0.4994617955840008 0.3415909194924868 0.3050019108848006
0.6238386311123703 0.3404378493433644 0.3049186319353755
0.1267529424666262 0.8444362457878312 0.3089294119400237
0.2473679222402159 0.8438554232458293 0.3073296780012907
0.0622711756448057 0.5848170825108224 0.3089719588037960
0.9975010341955439 0.3430930686770919 0.3082871734473828
0.6856065216114491 0.4310070325283351 0.3050929777342203
0.6252637714536365 0.6713936424490016 0.3049941004612856
0.5607379154425046 0.9241628120708825 0.3049379922957014
0.4994869439518174 0.1736414195643064 0.3049881151920577
0.6238563427898003 0.1748269990476038 0.3049070525168862
0.1267165529580452 0.6716820899837697 0.3088048445034074
0.2473014671676272 0.6716600775512819 0.3072792780163019
0.0623237331873641 0.9313883895231116 0.3091343559890907
0.9975239131557645 0.1730363422522033 0.3083654735133174
0.3126064530474559 0.0954118035088962 0.3071949805968011
0.4359869362227325 0.5916496109005096 0.3053980172310325
0.8106773662891263 0.0942173102301297 0.3058213280136844
0.9378225919680339 0.5919012624040167 0.3075468490340880
0.3125452204965666 0.4198311820359691 0.3073384970865941
0.4360126581505520 0.9235731903728687 0.3053452160914564
0.8106008103635417 0.4214395387832126 0.3058288749155321
0.9378701836348979 0.9241817923104245 0.3075534398126671
0.6850459958460408 0.9256601027352090 0.3051174274698765
0.5618501686182187 0.4244921741564743 0.3049175973909063
0.1870648007325310 0.9222373547321396 0.3076012651850378
0.0601878699858230 0.4208391191258926 0.3109688912390534
0.6850193360184031 0.5896309303833506 0.3051474408977681
0.5618594046476988 0.0907597950943171 0.3048992964845297

0.1869500450086223	0.5936680496291036	0.3073708874443398
0.0602418996294273	0.0954178998546963	0.3112342325771238
0.1826771049199273	0.2612068158917121	0.4078722356242651
0.1837563369107282	0.2735105785205932	0.4762588897398232
0.1252761143312693	0.2584900568116718	0.3354812131434058
0.2408996289234930	0.2570945843155986	0.3348076091795316
0.1421871340559288	0.2213625416574241	0.4976183993969562
0.2280664016669304	0.2301637707160769	0.4958355224746290
0.1802628774287888	0.4648310943781023	0.5019232058798625
0.2095411844917787	0.6388494157375481	0.4928943369970263
0.1896988565397836	0.5888585112106437	0.5855244393263460
0.2045020253348040	0.7155783649286208	0.6556209895815788
0.1617171477723463	0.5492804086004969	0.6643795763516647
0.1763839863195619	0.9424682792693424	0.6651748015630849
0.2191082040115771	0.8821946936286263	0.7258962750579485
0.1769722083942934	0.5773654484382799	0.5187863092989333
0.1993383633414647	0.5974986299471403	0.6397659690910963
0.2149189535686069	0.8762595160862492	0.6773019813903455

Initial state cd (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3112304188874005	0.9304585516912307	0.3064652245567326
0.3751784287056902	0.1732485013359827	0.3057037719826174
0.4376496481771237	0.4249616380122975	0.3052931250793710
0.4988533013988302	0.6733953979407399	0.3051654243890656
0.3731891694011322	0.6732350047463856	0.3057307126052159
0.8706080750349782	0.1724097203079711	0.3064149625278308
0.7506997608056820	0.1724349145284244	0.3054129187965375
0.9359574007518453	0.4324876071963776	0.3072530158487056
0.9985982375718020	0.6699288395044274	0.3080676653568970
0.3111609328489880	0.5847577975182678	0.3065350908114165
0.3751273822361900	0.3420337311241835	0.3057679568158603
0.4376730073580337	0.0902713995535497	0.3052407517835119
0.4988671196693320	0.8418391059433814	0.3051410019974941
0.3732231958114917	0.8419544884683912	0.3056903094826275
0.8705789902584596	0.3435643367408103	0.3064153053179415

0.7506713607019417	0.3430382460559586	0.3054220200299639
0.9360014058156394	0.0836577823630186	0.3072713360314802
0.9986325012404265	0.8462668652076951	0.3080997924239172
0.6857191389412993	0.0843328389862535	0.3050981709109356
0.6253310685710820	0.8438754573645900	0.3050283016525857
0.5607650559645472	0.5911364190928061	0.3050356207994804
0.4995206700479566	0.3415833551586305	0.3050209415510093
0.6239106311269202	0.3404388054562587	0.3049827891945557
0.1267143245724938	0.8445469277312063	0.3089134731213261
0.2473836677508307	0.8439075428689963	0.3073295253307114
0.0623191917521159	0.5847713537992230	0.3089745016923736
0.9974602893344084	0.3430797908916304	0.3081691039208035
0.6856865493382214	0.4309821093575177	0.3051189237547003
0.6253135085171804	0.6714219446300520	0.3050431141052387
0.5607815124917066	0.9241187659197111	0.3050120868012365
0.4995442378955376	0.1736448045592552	0.3050069780842942
0.6239280540293350	0.1748273046422181	0.3049731894985386
0.1266794743031632	0.6716181252355785	0.3087868777425629
0.2473153257247107	0.6716208070225516	0.3072754795350128
0.0623654370138928	0.9314843857044203	0.3091247822900723
0.9974761709689886	0.1731240800706523	0.3082448617262576
0.3126350980192849	0.0955106691764032	0.3072380348558784
0.4360271913296731	0.5916604057085406	0.3054264964516656
0.8107008256320083	0.0942045946483985	0.3058280906365784
0.9378240467560117	0.5920532613752045	0.3075909786156822
0.3125783943061854	0.4197321624663262	0.3073998868677655
0.4360518840745501	0.9235545638719341	0.3053692351468014
0.8106209144096730	0.4215177592344431	0.3058306255316061
0.9378683841837859	0.9241070341158298	0.3075941875586621
0.6851167374530019	0.9255623221591794	0.3051349356209968
0.5619212441209404	0.4244658919669455	0.3050156541582629
0.1870503805859926	0.9223077726663419	0.3075363258158091
0.0602392191966993	0.4204955373132462	0.3110162064515932
0.6850851090515626	0.5897403480234585	0.3051675531299028
0.5619301415305471	0.0907868054926218	0.3049979105331622
0.1869351371864196	0.5936332945281155	0.3072934471529374
0.0602769165679802	0.0958083741507856	0.3112670790211552
0.1823568147984005	0.2614315307366287	0.4079821843630609
0.1833559662855380	0.2742126258728628	0.4766670992896827
0.1249688514013233	0.2584358065961796	0.3358299389610864
0.2411899282272945	0.2571340607704842	0.3354784214232425
0.1420156438157876	0.2205431801409908	0.4977950258933026
0.2275917173877108	0.2297503703726683	0.4959920136665918

0.1802180902421852	0.4645183087377707	0.5018294042619461
0.2095021514261769	0.6392155808091768	0.4928576141754754
0.1895501076669331	0.5888596180968036	0.5848663755634796
0.2043341754995845	0.7150562052503221	0.6553987983393024
0.1617908284907026	0.5486662581578753	0.6640975837070187
0.1763721756222210	0.9427752563903813	0.6651186864343898
0.2194026762071402	0.8825557838078923	0.7256359819636412
0.1769800354354470	0.5774798791129143	0.5187012253065212
0.1992707078112410	0.5973142028512651	0.6394449477996456
0.2149098712586029	0.8764010286673543	0.6770845187542607

Transition state cd (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3112615905281170	0.9308161389430710	0.3069797744115735
0.3748343218616293	0.1734149572668359	0.3063847626155772
0.4374357967132950	0.4251549653596321	0.3055058813804174
0.4986792617000996	0.6736155590939130	0.3052129748746893
0.3731520183612592	0.6734403451541435	0.3059337040201023
0.8706362497667748	0.1730323381223320	0.3063685644899922
0.7508028216334778	0.1729967595207067	0.3052614133333581
0.9362598519279816	0.4331662537554661	0.3071430197703711
0.9989835423397651	0.6701828552957542	0.3078024133648695
0.3111688441867219	0.5847570148315452	0.3070812492539628
0.3747890153154669	0.3421367720392288	0.3064590037144865
0.4374638147448420	0.0903390240293726	0.3054470705187759
0.4986980736486616	0.8418692931296775	0.3051831160931058
0.3731885454478741	0.8420350233799498	0.3058824542412026
0.8705862574528608	0.3438156564348818	0.3063706565084829
0.7507552877122743	0.3429624852863481	0.3052660970994188
0.9363328599468179	0.0839533828507321	0.3071502826669580
0.9990378936728966	0.8469619069020222	0.3078279522502613
0.6855090698704450	0.0844180089591074	0.3049409761552928
0.6251966589433080	0.8439980111007906	0.3049230642559044
0.5606972858409128	0.5911426988398367	0.3049912280763062
0.4993063511591699	0.3417244311285444	0.3050877677666688
0.6236548326257101	0.3406056346080092	0.3048351570395604

0.1269696128912512	0.8449290258602583	0.3094511067350049
0.2474383476728455	0.8439789586568563	0.3078937513765442
0.0626545671972070	0.5844477493125779	0.3092955121173434
0.9977133975408439	0.3433933956709420	0.3083132398581117
0.6854504954195381	0.4312372186872680	0.3049528896357045
0.6251699471466998	0.6716006056704243	0.3049330882685482
0.5607258846123335	0.9243642291606712	0.3049699064649731
0.4993314454265422	0.1737568941167149	0.3050684270124009
0.6236814033368071	0.1749432490395956	0.3048297221011620
0.1269190345847571	0.6720342339463081	0.3093594995902727
0.2473571317488978	0.6719907171064541	0.3078724851196808
0.0627162259702081	0.9326866908116506	0.3094078423522304
0.9977378972257155	0.1737626383352431	0.3083614913713957
0.3124173417739339	0.0954531617066213	0.3083694411731575
0.4359697085683539	0.5916025435758026	0.3055499287949779
0.8107793231830160	0.0947139945966795	0.3057076035771785
0.9381457826169237	0.5923015796755762	0.3071590240862035
0.3123528227289986	0.4201083722759580	0.3086039374797980
0.4360066773987943	0.9238730865061219	0.3054635522972645
0.8106347909140144	0.4216968572604478	0.3057115213172276
0.9382128050154603	0.9248428725403492	0.3071445046309847
0.6850242211800525	0.9261556683965169	0.3049902240330724
0.5617267153148247	0.4247902967315489	0.3049262734289637
0.1872673465975104	0.9225671923566550	0.3076528273475718
0.0606889847309170	0.4200263607272017	0.3115151549739499
0.6849683343433612	0.5894729335560590	0.3050069085297155
0.5617464685527769	0.0907173551387301	0.3049107860385765
0.1870974004302148	0.5939929410402036	0.3074814652333257
0.0607254201827605	0.0971678796740819	0.3116314200052671
0.1795663773775299	0.2612246057478770	0.4077955698588035
0.1810781556784185	0.2730701601434520	0.4763575034007058
0.1237612481620746	0.2587890794650977	0.3379626266579223
0.2394048762973015	0.2574762454255031	0.3342163641014113
0.1391171988684776	0.2224635425585802	0.4976817385199876
0.2249096790504963	0.2272424376742037	0.4959700724913272
0.1794928313691010	0.4619994577039893	0.5011440460816616
0.2098005816114581	0.6363729441494600	0.4918474227761853
0.1885917447969749	0.5873920181011745	0.5812957919532947
0.2035779915779041	0.7122665704092419	0.6535468831572044
0.1619201587219480	0.5463059541558366	0.6622895203156537
0.1760941025125798	0.9449077700114359	0.6652951497096815
0.2201378716630556	0.8842862710815453	0.7248537790611884
0.1766641188149658	0.5757225956331993	0.5174372332026529

0.1987815720903838 0.5962265146795780 0.6372424080661642
0.2145406146977352 0.8775210373798696 0.6764427858876194

Transition state cd (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3112520087584263 0.9311623569799958 0.3075315752998582
0.3747559605994897 0.1737046611093378 0.3068721354008576
0.4373451080851171 0.4254858398648328 0.3057895417717783
0.4985751915016531 0.6739892039122936 0.3053729148369834
0.3730873061920709 0.6736678775833469 0.3063166563498097
0.8706113051737652 0.1734717905215808 0.3062884242777518
0.7508336581928994 0.1734302064295459 0.3051922499977716
0.9362978924099495 0.4336228102066825 0.3070981511558794
0.9990157906441653 0.6705333192828812 0.3077826117861218
0.3111477521753561 0.5849810460044542 0.3076050489175797
0.3746982599932113 0.3424079328980533 0.3069379870401075
0.4373787832471601 0.0905780820790862 0.3057189608905261
0.4985969538269133 0.8420735800764694 0.3053351008935385
0.3731283745545132 0.8423655337803274 0.3062634401890101
0.8705576733122480 0.3441508057244844 0.3062918633427312
0.7507798440845520 0.3432086465250949 0.3051975052169686
0.9363770994229235 0.0842912347949767 0.3071125576518071
0.9990783693448122 0.8474135246854383 0.3078226721694445
0.6854147069062724 0.0846681396600973 0.3049125201497188
0.6251244816435338 0.8443080550729595 0.3049588641542742
0.5606645544001925 0.5913803946927482 0.3051027992076432
0.4992386507386631 0.3420395301174713 0.3052683371113611
0.6235403421374234 0.3409227599434064 0.3048719655385006
0.1270363292145313 0.8452687521031941 0.3098349870146100
0.2474371875727499 0.8442566983845080 0.3084212384822567
0.0626628631337084 0.5847914446476056 0.3094458546530422
0.9977241958227079 0.3438372731313758 0.3083780894065242
0.6853440726997533 0.4316202673851270 0.3049266508120222
0.6250914981749707 0.6719208518670633 0.3049710380288915
0.5606992187917321 0.9247340392437304 0.3050726828573708
0.4992722733261110 0.1740362145740842 0.3052422810889385

0.6235718456791945	0.1752440524883482	0.3048619989488405
0.1269767563043419	0.6724675520698267	0.3096890510989020
0.2473453775044854	0.6723394197323699	0.3083636929956705
0.0627307200324755	0.9331471635717983	0.3096187235556784
0.9977519049473368	0.1741077230196022	0.3084487539695233
0.3123513441480998	0.0958327137086578	0.3090351532045810
0.4359309887871850	0.5918334523376492	0.3057959842575280
0.8107753871801080	0.0951442758013351	0.3056207274769886
0.9382146452947934	0.5926661590402357	0.3070190604359135
0.3122718316146290	0.4202982275565460	0.3092353070082505
0.4359778831996903	0.9242104262452753	0.3056797348536129
0.8106136926252262	0.4219965490883196	0.3056274172637915
0.9382866908737250	0.9252848270879094	0.3070104319211220
0.6849623956739819	0.9266341772053409	0.3049600155340665
0.5616187298317523	0.4252071056500240	0.3050466286552962
0.1873014652568678	0.9228883828789404	0.3081988253721060
0.0606555117693739	0.4205198175254479	0.3116017939698785
0.6848941702766085	0.5896225352457605	0.3049804689337854
0.5616415087639433	0.0909098788356069	0.3050139502088501
0.1871089949697164	0.5943841537971056	0.3079271525920824
0.0606979391810199	0.0974821966344931	0.3117964333477307
0.1789542739842363	0.2624426661222239	0.4081094169744438
0.1797998392046482	0.2754104996090421	0.4769199353954659
0.1235750285588655	0.2593014731591051	0.3381046719394886
0.2392467301548940	0.2577247778653835	0.3348476654196568
0.1374347168118751	0.2251839294161391	0.4977311743703762
0.2230991326035954	0.2274899631973733	0.4968222091102312
0.1789740118578271	0.4539473468575305	0.5000624338942401
0.2099869835821035	0.6319383991744691	0.4909712457267908
0.1869155610711925	0.5824697079762237	0.5735130984235142
0.2030108670656831	0.7067013678782440	0.6519621176528914
0.1619049951398923	0.5442600162362914	0.6613997344399379
0.1758437402401917	0.9477284172132140	0.6656617339154767
0.2209281464964017	0.8877111571418058	0.7242829900945128
0.1764836059967952	0.5710026507276543	0.5161383760412761
0.1982760465783179	0.5933620023730266	0.6355621980208789
0.2146502750114344	0.8808053783411330	0.6759833907459404

Transition state cd (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 18 1 1 9 3

Direct

0.3112371956227833	0.9312252903618381	0.3077331636288964
0.3747334917142861	0.1736878607135348	0.3069165518649915
0.4372662761115619	0.4255505570751847	0.3057901830724061
0.4984306739459353	0.6740825392950026	0.3054024823581143
0.3729808283142227	0.6735836274647805	0.3063779795600510
0.8705704369747643	0.1738007983412485	0.3061859755727876
0.7508569468479097	0.1735977566422676	0.3051528821046783
0.9362949494894011	0.4340499244224940	0.3069966245798130
0.9990309420848339	0.6707701172752821	0.3076293612807705
0.3110815981927811	0.5849324925271296	0.3077844967191282
0.3746478800691151	0.3424109867656815	0.3069915242007144
0.4373159502085090	0.0904785376279413	0.3057103722204082
0.4984594760846028	0.8419421105319201	0.3053550005908740
0.3730385037167879	0.8423954238030786	0.3063285456235147
0.8704940230689301	0.3444389820837930	0.3061793050681334
0.7507783141465195	0.3432162401981752	0.3051510692501558
0.9364095811812888	0.0846372576131428	0.3070302080886251
0.9991226407066303	0.8479778176024729	0.3077046113556433
0.6853193623895356	0.0845843069949438	0.3049290213025509
0.6250375140089202	0.8443351713795023	0.3050276460276942
0.5606223158404158	0.5912980414144786	0.3051625471164925
0.4991915182544671	0.3420434012280886	0.3052994015052198
0.6234020002688714	0.3409158168513573	0.3049029951223172
0.1270753127896768	0.8456542543169919	0.3100296358254402
0.2474103933266740	0.8443699566767735	0.3086662356841645
0.0626636010768088	0.5850418449545460	0.3094369187630701
0.9976995752176703	0.3443082102658702	0.3084072344116056
0.6852145731893567	0.4317386046129873	0.3049371935948100
0.6249884804792141	0.6719121807838189	0.3050360463598216
0.5606698806494471	0.9248010909861182	0.3051267820861965
0.4992400821047309	0.1739968645193180	0.3052665839843997
0.6234514256887217	0.1752447791841086	0.3048916687173874
0.1269883939339613	0.6728575631770124	0.3097758658759616
0.2472736819808807	0.6724841661212644	0.3085467379427870
0.0627574626741387	0.9337325538740232	0.3097423460543087
0.9977388507505730	0.1744326635689388	0.3085275365135018
0.3123368769995797	0.0959754685975372	0.3092663311213754
0.4358774553678758	0.5917571986369049	0.3057973072406404
0.8107832065298117	0.0954085047468392	0.3055452405526297

0.9382706595662521	0.5930675774327503	0.3067903893864213
0.3122222654303383	0.4201528745914826	0.3095357982186133
0.4359472483354115	0.9242374688143481	0.3056549045328200
0.8105463712990478	0.4221256902004603	0.3055293283788134
0.9383796322307186	0.9256762868983917	0.3067847753083494
0.6848802609967517	0.9267900773253669	0.3050137913343570
0.5614927643951774	0.4253728607725538	0.3051092260677933
0.1873300827515543	0.9231343759158179	0.3086392731872731
0.0606171000473509	0.4208017037469658	0.3116233918344019
0.6847819229114148	0.5894878719884717	0.3050223875263556
0.5615211309463115	0.0907269455442156	0.3050701964277754
0.1870530139322809	0.5947222842757415	0.3081657680563705
0.0606693293258732	0.0980389908129574	0.3119713482059892
0.1788799485798276	0.2653630128902231	0.4084264144380080
0.1797651262335956	0.2821120426440574	0.4781372444336140
0.1232666975222875	0.2599650598652390	0.3387077990777935
0.2396197515338269	0.2576383716548296	0.3357260442533407
0.1376547715703299	0.2298482439556155	0.4987481580161915
0.2228168566301775	0.2320087448598668	0.4977880114585119
0.1790846519697509	0.4365610101363796	0.4970267071459528
0.2102027672554156	0.6284631888079002	0.4898128098733196
0.1856533471590065	0.5780025673738010	0.5663217795648060
0.2032433576881348	0.7025900760384742	0.6529636680029237
0.1617526264776924	0.5439942051377502	0.6630463680273447
0.1758749171986917	0.9497429675274577	0.6660767259681906
0.2212064739131705	0.8919263247200173	0.7247168422105337
0.1762722365884627	0.5666237081629759	0.5139804209624884
0.1985259485222413	0.5905411067831849	0.6370661674815309
0.2153500564504858	0.8849850252711817	0.6763879326472521

Final state cd (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3109006149981576 0.9288824197628520 0.3070494700820859

0.3749300588528283 0.1720405487936436 0.3056239529405617

0.4368410029256033 0.4243719111709744 0.3053169140855759

0.4979582728179409 0.6728641389399460 0.3051894894737944

0.3722550445074860 0.6715871371351698 0.3065322061084105
0.8700100960964444 0.1755884155637269 0.3047817133768789
0.7502824547519820 0.1734429490927858 0.3045154184077559
0.9350415228112406 0.4358552474383625 0.3053670116339816
0.9969985018573292 0.6742631833451795 0.3064871372283455
0.3100533125361150 0.5834976025433304 0.3083015112132533
0.3745096943117614 0.3410971108949377 0.3063676999085520
0.4372109199268067 0.0890543720114549 0.3048750939038324
0.4981294771609766 0.8408631887044767 0.3050390876967873
0.3726157840573961 0.8407295769462114 0.3060351501438948
0.8696547390478695 0.3461818558211021 0.3047441067334049
0.7499852400264597 0.3435876907012202 0.3045098644306665
0.9356305198494040 0.0876318480711785 0.3054184494904440
0.9974838946495578 0.8498731276799898 0.3066059383458943
0.6850236187753309 0.0841949994717380 0.3044605244582931
0.6246447478638959 0.8437550518680901 0.3046242076043398
0.5600533190795206 0.5904957502811571 0.3048226584797419
0.4989217288110771 0.3409033837454610 0.3047135582816009
0.6230918842778252 0.3402357769392479 0.3044750750083661
0.1260379995604081 0.8473146124552459 0.3087119825331346
0.2466031014495366 0.8433145608101021 0.3081042647113291
0.0605746181161041 0.5897408487561677 0.3077760795306051
0.9968451660168096 0.3473824400419929 0.3064123191093007
0.6846721471058242 0.4312592603568088 0.3044733660366955
0.6244799414265862 0.6712527200128808 0.3046455715213700
0.5602381934578710 0.9237614121841552 0.3047289317150466
0.4991062045989614 0.1729753611448377 0.3046304496391171
0.6232656274166104 0.1746096121023328 0.3044488586582387
0.1254415726498404 0.6753490234258964 0.3084917548420247
0.2459975550838962 0.6712936901671761 0.3084826815148511
0.0613894212428889 0.9348685829027492 0.3081954717315855
0.9973328878143248 0.1764805300307068 0.3065477677497089
0.3126955082544058 0.0938002118215963 0.3081420438255725
0.4352467694401714 0.5904730786562278 0.3057853720045365
0.8103575977376251 0.0961763022687954 0.3046311383336033
0.9364843931137036 0.5953834065830499 0.3056052893380017
0.3117075273021193 0.4179041934151124 0.3105247564424815
0.4355532904269912 0.9226750833021664 0.3052314144321545
0.8095269586545599 0.4232192645453852 0.3045906881140165
0.9371272187043992 0.9284351994369816 0.3056418033404929
0.6845068590862985 0.9258488215078278 0.3045398452735527
0.5610224048842224 0.4243470302074137 0.3046692866268583
0.1866853091291258 0.9236775151117724 0.3085429131658748

0.0588419354078305	0.4269676448823528	0.3089370329411287
0.6841874769759480	0.5894289509045333	0.3045586608280634
0.5612110211131952	0.0900375546238622	0.3045708541331167
0.1851236974563749	0.5950167611105985	0.3085442452973446
0.0596738673129916	0.0979813254384636	0.3093780222076637
0.1827181728070916	0.2584488061988638	0.4111963125008196
0.1783775956882825	0.2780361939241844	0.4825521538615276
0.1268642920105632	0.2673745610840858	0.3337169666958810
0.2445822631899914	0.2520499911130489	0.3424598002757764
0.1349567850867054	0.2255631314180696	0.5003738964550615
0.2197420649844567	0.2266546807519413	0.5050796521028998
0.1774686889029407	0.4020742272668782	0.4947988164884543
0.2111216333798859	0.6403032895711752	0.4892745657841088
0.1850081681538288	0.5908686899877257	0.5614359140303878
0.2048905423280065	0.7006606257268132	0.6572022875262256
0.1615973385316326	0.5464345770098664	0.6658998995397422
0.1755227171032352	0.9500549853560940	0.6668444268444699
0.2194809244690091	0.8963857551700753	0.7270521420296753
0.1746800775144918	0.5840598711032668	0.5119579099257643
0.2005461022653798	0.5890234815199022	0.6418930469091447
0.2159214026518224	0.8898481866685990	0.6785221663961433

Final state cd (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3109332210717278	0.9288876859299107	0.3070637741184795
0.3749381219115445	0.1719620255927749	0.3056379957882944
0.4368195558653801	0.4244048159548041	0.3053358508174082
0.4979005706775085	0.6729362024310920	0.3052013353966199
0.3722416363306415	0.6715610559795546	0.3065475425931787
0.8699805582878595	0.1755970033091744	0.3047796270434820
0.7503134284620946	0.1734750027784619	0.3045154735553874
0.9350628543455254	0.4359037380904797	0.3053614605412936
0.9969861983682380	0.6742420839084627	0.3064762180802911
0.3100853176687066	0.5834546901794661	0.3083261491082375
0.3745200438321401	0.3411157349447122	0.3063828751671383
0.4371885643751581	0.0889675609904379	0.3048937214468642
0.4980674505538317	0.8407678973780786	0.3050507085614917

0.3726039793511198	0.8407107353454975	0.3060439121128134
0.8696262829794736	0.3461660421364009	0.3047423242107199
0.7500114418964022	0.3435416948837862	0.3045134131817427
0.9356473576215729	0.0875902274395114	0.3054108019047395
0.9974739700551403	0.8499083929657932	0.3065937618315721
0.6849896153603150	0.0841127134903636	0.3044641746461851
0.6246456153424474	0.8437762662323973	0.3046343246070510
0.5600819841499528	0.5904302204442347	0.3048344935407611
0.4989547813991449	0.3408661974161283	0.3047387659365205
0.6230549253342706	0.3402233009053420	0.3044825825028982
0.1260752334862595	0.8473093054947129	0.3087273404264578
0.2465901526536445	0.8432936021555496	0.3081105043292282
0.0605626939378038	0.5896809964979945	0.3077939599043835
0.9968526267712059	0.3474332688540396	0.3064255034388807
0.6846337672485875	0.4313101004474530	0.3044794770738764
0.6244774287538293	0.6712082561718659	0.3046547601572448
0.5602719311308241	0.9238226187326558	0.3047422253536324
0.4991373723621871	0.1729795699224066	0.3046555499786266
0.6232293940488238	0.1745911682422656	0.3044573974923909
0.1254745964374721	0.6753687257081450	0.3085108898755031
0.2459834151558918	0.6712936007389004	0.3084954249187724
0.0613786098002177	0.9349552909042388	0.3082075828059559
0.9973404075134982	0.1764534078511292	0.3065537694737610
0.3127047768516020	0.0937838560380321	0.3081905597660956
0.4352816630963561	0.5903910883579918	0.3057934696117803
0.8103673125801921	0.0962222282223047	0.3046248828375984
0.9365093613839923	0.5953448979457125	0.3056079696206343
0.3117213647017664	0.4178660945263073	0.3105645787793375
0.4355900916985734	0.9227261482492933	0.3052374976095865
0.8095312326007333	0.4231663883000986	0.3045887647422895
0.9371548070284569	0.9284910837606180	0.3056437005267960
0.6844858451613564	0.9259131632467309	0.3045471954544188
0.5609785689664075	0.4244747317990662	0.3046847901857488
0.1866985793709604	0.9236084486233362	0.3085942636563584
0.0588056772012271	0.4270595539922100	0.3089645471510696
0.6841632207328510	0.5893444046271875	0.3045655806188920
0.5611711470565612	0.0898753628795542	0.3045878398195898
0.1851282648080182	0.5950868432567950	0.3086066720410345
0.0596290160242083	0.0978888539797063	0.3093964122113285
0.1827823720846954	0.2584997753076727	0.4111809759784729
0.1783715976699005	0.2780459134820111	0.4824828753004092
0.1268928124173337	0.2673181374673594	0.3337372498479498
0.2445769213001016	0.2520617834935326	0.3423889029907319

0.1349363375829161	0.2255503566109914	0.5002974491495714
0.2197253442860731	0.2266774701117708	0.5050484382619658
0.1774421804715335	0.4021847131897035	0.4947447343762882
0.2111069210455606	0.6402669483130160	0.4891952515246679
0.1849914787638122	0.5909275044333561	0.5613686222815194
0.2048713782867077	0.7006477135963721	0.6572155571353581
0.1616392022317692	0.5463128591316395	0.6658637048479799
0.1755372981938613	0.9501432461347711	0.6668309942697516
0.2195625738793339	0.8967139303089106	0.7270384923986316
0.1746800520666437	0.5839673398721869	0.5118804234783491
0.2005348426814999	0.5890684765454697	0.6418338820703717
0.2159341432345118	0.8898828227480691	0.6785071115335451

Final state cd (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 18 1 1 9 3

Direct

0.3109659527097234	0.9288825759332119	0.3070911720578515
0.3749548352748639	0.1718992816820632	0.3056653425189810
0.4368001708212179	0.4244319795705584	0.3053655985126233
0.4978541207157334	0.6729735483794665	0.3052125788888151
0.3722286247341465	0.6714793806836947	0.3065659818198381
0.8699485767191943	0.1756000589807759	0.3047762298920430
0.7503388718516850	0.1735094160175890	0.3045162249346049
0.9350841309668823	0.4359207879738872	0.3053603985212833
0.9969928069082379	0.6741632778848438	0.3064631560751647
0.3101107655610987	0.5834310265857139	0.3083558525575285
0.3745316528104530	0.3411408929577671	0.3064113028944203
0.4371705519526634	0.0889036833664657	0.3049190166448832
0.4980198349341626	0.8407056792105257	0.3050607743482068
0.3725923530520211	0.8407515563135755	0.3060565191291029
0.8695923359687658	0.3461366425496230	0.3047387262051989
0.7500332605946979	0.3434819252247772	0.3045157725479257
0.9356626758483246	0.0875670326923613	0.3054065832252464
0.9974761707967698	0.8499793285914563	0.3065773836758386
0.6849575945986192	0.0840721933928930	0.3044684228299557
0.6246419651962244	0.8438112533386098	0.3046444901562197
0.5600894561092280	0.5903578964239948	0.3048460766067654

0.4989742627238080	0.3408316908449907	0.3047659037105404
0.6230051129836905	0.3402362432541460	0.3044900265416552
0.1261124770566338	0.8473252028265905	0.3087435186701364
0.2465799998746360	0.8432713899507089	0.3081320460484460
0.0605477059536298	0.5896097820011715	0.3078232672736093
0.9968554802741113	0.3474986776409474	0.3064514160893062
0.6845972744322359	0.4313144540023508	0.3044856347379362
0.6244704752570808	0.6711456239184296	0.3046642699730664
0.5602814165388124	0.9238820917896698	0.3047553728256808
0.4991578724208145	0.1729887515616433	0.3046829515250075
0.6231797155401709	0.1745448286775593	0.3044647579499985
0.1255129269809854	0.6753997109464066	0.3085358509651298
0.2459732147034623	0.6713052203562213	0.3085182325256086
0.0613727273604696	0.9350527440131108	0.3082193182887917
0.9973401428981589	0.1763898966416602	0.3065703505507152
0.3127291125596577	0.0937586598099392	0.3082364362585886
0.4353006147305200	0.5903564983834567	0.3058012623977578
0.8103657028194404	0.0962380029094925	0.3046193154628431
0.9365379948953257	0.5953122824915871	0.3056031248064091
0.3117371389236223	0.4178306679635571	0.3105951302997820
0.4356097272990866	0.9227432065026602	0.3052450306342129
0.8095287730800974	0.4231264871955330	0.3045869669327058
0.9371949052383746	0.9285065630654934	0.3056374884162010
0.6844426302273801	0.9259648452222344	0.3045549620949872
0.5609455532510712	0.4245508610558121	0.3046988982118085
0.1867218802303462	0.9235408211241887	0.3086695494513046
0.0587711082193422	0.4270969686966551	0.3090048156693818
0.6841184137356386	0.5892675199925181	0.3045721953415624
0.5611411023945666	0.0897646354020219	0.3046050675670571
0.1851337935322539	0.5951792286349618	0.3086857028155407
0.0595802279700112	0.0978463025856037	0.3094084112706146
0.1828644718837759	0.2586447567954364	0.4111456180445244
0.1783878441387431	0.2780816525695312	0.4823828209541277
0.1269354469339290	0.2672867447146475	0.3337749353427130
0.2445693159432094	0.2520308678572145	0.3422925206602433
0.1349297956777648	0.2255585320941834	0.5001659908315695
0.2197209142435100	0.2267134283590888	0.5050012608122154
0.1774314665627131	0.4023634549984740	0.4946809044042738
0.2110866779249509	0.6402033599525221	0.4891187645212677
0.1849674085547037	0.5909364500814065	0.5613059194113041
0.2048522979359194	0.7006448750012414	0.6572226933174072
0.1616817702708045	0.5461963658033405	0.6658254327788459
0.1755565277027556	0.9502194759357756	0.6668210275831321

0.2196408680677102	0.8970234713569829	0.7270175346427044
0.1746928275434773	0.5837743857187161	0.5118022884041126
0.2005182875046483	0.5891244986298277	0.6417601358454782
0.2159393768811812	0.8899317419164202	0.6784963350972308

2.3: Step de ($\text{N}_2\text{H}_3 \rightarrow \text{N} + \text{NH}_3$)

Initial state de (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3107622122135185 0.9294969292410238 0.3067044084306066

0.3748433906955570 0.1725168074006276 0.3051768190927974

0.4368220603472650 0.4248663191691419 0.3047548102550416

0.4978936245472557 0.6733353781654293 0.3048989393053370

0.3722138372523745 0.6721616948321532 0.3058236395129688

0.8699123093266449 0.1751505628431552 0.3045921716294641

0.7502000791859615 0.1734672627323607 0.3045237194425897

0.9350438490764662 0.4352845819485398 0.3050915339298762

0.9969689191243155 0.6736508837149874 0.3060378070446191

0.3100587324394309 0.5840788298212990 0.3074640336871856

0.3744802083080415 0.3416201722709194 0.3056466424242764

0.4371218153367376 0.0895182547104434 0.3044736399710347

0.4980314518633800 0.8412660369894198 0.3047970871240308

0.3725064649938132 0.8413307607192557 0.3055204331416219

0.8696195069050662 0.3457492931060657 0.3045717724782350

0.7499561193446521 0.3436203232433350 0.3045338123558647

0.9355346697844598 0.0870690825134308 0.3051428344909019

0.9973738373155493 0.8492794376027979 0.3061853168476195

0.6849048297109954 0.0843850443002386 0.3045361651787989

0.6245483569017817 0.8440235169565464 0.3046780522593586

0.5600071032056724 0.5908408037357350 0.3047151708263872

0.4988663116682614 0.3413559369394922 0.3044118745464294

0.6230228207081774 0.3405470836662708 0.3044982479341908

0.1259256373324370 0.8469323767123057 0.3083152053173482

0.2464821472859738 0.8437460785534978 0.3076775902137424

0.0605791813246531 0.5891515138970342 0.3073184705204632

0.9968561686324533 0.3468177261076084 0.3061376798749471

0.6846244220588162 0.4314780848778108 0.3045493248799038

0.6244171432517560	0.6715154987726192	0.3046865738740424
0.5601525988066320	0.9241482999677024	0.3046568674632754
0.4990215809372264	0.1733555864496413	0.3043561927162778
0.6231638516142217	0.1748684513647727	0.3044825405797035
0.1254439269602010	0.6749944788459773	0.3079459224474253
0.2459858228574247	0.6717069580243547	0.3077961298423365
0.0612560560205341	0.9342718255376145	0.3078319564812597
0.9972715470745979	0.1758830119892266	0.3062964881972056
0.3125610062190136	0.0944938423758628	0.3080738576173574
0.4352068162396294	0.5909717990321443	0.3052585001558461
0.8102166206154228	0.0959883834733482	0.3045285931870585
0.9364796369326870	0.5947585841101596	0.3052723869859721
0.3117472946201986	0.4185029898476103	0.3096676012246540
0.4354603482835527	0.9231655894161246	0.3048809225984260
0.8095416152128985	0.4229849755269560	0.3045274481357840
0.9370216898359859	0.9278596413784258	0.3053280829832623
0.6843948740350990	0.9261049933066348	0.3046647800036382
0.5609700735147060	0.4247195110863053	0.3045817268618723
0.1864798498324129	0.9237225100774491	0.3083086870466439
0.0588571173687475	0.4263893114865611	0.3086453148966098
0.6841432433379083	0.5896258463192828	0.3046751402319253
0.5611199783939050	0.0903712753309715	0.3045163187224397
0.1852025123893945	0.5950581081869731	0.3078969797377348
0.0595606681762216	0.0973006062864458	0.3091914890490679
0.1830970259775144	0.2637306291237186	0.4113666947788870
0.1792427272732592	0.2847229552268531	0.4833239640433002
0.1268481145135150	0.2662898010740873	0.3338320320149282
0.2449139708522357	0.2535962864004562	0.3426526260000324
0.1357854549411116	0.2331213331736220	0.5016057626701349
0.2207065462212185	0.2332142392769928	0.5056711658278310
0.1786229048010410	0.4022741547602073	0.4951490889094232

Initial state de (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3107976639747475 0.9294903535529113 0.3067157982769422

0.3748612594586807 0.1724441908509349 0.3051911831425657

0.4367964716285380 0.4249042108430320 0.3047833019208239
0.4978415053439275 0.6733931302681069 0.3049076194022242
0.3721994941529302 0.6721284288048753 0.3058503360705863
0.8698930960113838 0.1752010411055086 0.3045945989161545
0.7502332156341698 0.1735243894018358 0.3045188221057695
0.9350622448356168 0.4353621153802655 0.3050834325857166
0.9969582502503835 0.6736719009519867 0.3060300692839957
0.3100834740236048 0.5840175829230752 0.3075132090955500
0.3744930571278534 0.3416263963238052 0.3056758909648022
0.4371019714861222 0.0894179486630945 0.3044929797198661
0.4979772070592334 0.8411735589156564 0.3048033811401850
0.3724986306767537 0.8412899886193635 0.3055343547767972
0.8695982926791698 0.3457561979439188 0.3045680375256634
0.7499837598356678 0.3435719686238906 0.3045266811357079
0.9355534870131914 0.0870673958887281 0.3051403173951734
0.9973665194890645 0.8493408967027056 0.3061777969615156
0.6848824062435873 0.0843169000989564 0.3045282947190158
0.6245569986482009 0.8440491862860471 0.3046747145193756
0.5600412967146702 0.5907836581655898 0.3047145283936992
0.4989052144444157 0.3413071864300220 0.3044328451990733
0.6229940015367949 0.3405292519902768 0.3044864675920473
0.1259616271794851 0.8469539762695296 0.3083365219649853
0.2464712551844896 0.8437125879359212 0.3076895031113128
0.0605617105166593 0.5891268566532392 0.3073376142680641
0.9968601412528264 0.3469024555290501 0.3061458163330196
0.6845931983123928 0.4315343238322150 0.3045410191406154
0.6244222493261322 0.6714777232702650 0.3046839617485109
0.5601910849843322 0.9242009000377633 0.3046565426689394
0.4990622287329208 0.1733694867846677 0.3043755944659314
0.6231369168458192 0.1748724792930662 0.3044721302503282
0.1254696769017910 0.6750489255345585 0.3079690121289188
0.2459658224194405 0.6717023939188108 0.3078237738359039
0.0612454400855830 0.9343973386355421 0.3078491471837638
0.9972756211605569 0.1758840190927939 0.3062995140165827
0.3125813958104390 0.0944530157569123 0.3080994087226698
0.4352450646264291 0.5908809718472079 0.3052722789494700
0.8102298216550632 0.0960409253550119 0.3045265610554689
0.9365015188777498 0.5947553360295118 0.3052753252603921
0.3117530721689753 0.4184496264397196 0.3097398040011181
0.4355011160240349 0.9232151474601992 0.3048896459465131
0.8095465476334328 0.4229676451474010 0.3045177888709403
0.9370493886192820 0.9279538324739739 0.3053359605357906
0.6843821999243711 0.9261680834584807 0.3046596570398777

0.5609272955097526	0.4248434572169293	0.3045756017975042
0.1864975861731034	0.9236692242703022	0.3083672915222791
0.0588206326582933	0.4265102295463974	0.3086718065513423
0.6841266881201733	0.5895578851022114	0.3046700869788834
0.5610823515959298	0.0902160295135145	0.3045126726906678
0.1852013312266359	0.5951349166595140	0.3079720042199452
0.0595193156301378	0.0972520559008012	0.3092068592776614
0.1831615034664246	0.2635756305222497	0.4113186924662348
0.1792327726005198	0.2846897483723825	0.4832147526628607
0.1268657286559551	0.2663196414569654	0.3338383563449852
0.2449039135776657	0.2534994874088520	0.3425458203105614
0.1357701709067686	0.2331219718380254	0.5015170034029214
0.2206877427924906	0.2333302781315227	0.5056401109390209
0.1785690345752266	0.4022957685699310	0.4949567364927672

Initial state de (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3108370851110684	0.9294682160937446	0.3067378661826149
0.3748861163646042	0.1723779714224160	0.3052142244647718
0.4367780267404934	0.4249324957188836	0.3048203474440422
0.4977976422935110	0.6734242199160850	0.3049146044915805
0.3721883104412395	0.6720338113824909	0.3058801958352432
0.8698627480182405	0.1752327394564704	0.3045934080813665
0.7502628232611572	0.1735709443823966	0.3045142726690502
0.9350823088069088	0.4354107965109252	0.3050793381645743
0.9969613797412860	0.6736277106290885	0.3060210355731439
0.3101031080137269	0.5839724143354963	0.3075642916263778
0.3745049622030789	0.3416397016600525	0.3057183593318719
0.4370909551259232	0.0893445869426480	0.3045190300571373
0.4979344099102816	0.8411080124635890	0.3048095091420421
0.3724923005887559	0.8413163427433847	0.3055508776823955
0.8695647942253359	0.3457518694617651	0.3045616776450779
0.7500095548153175	0.3435280154543897	0.3045204177583674
0.9355692977994141	0.0870769082794155	0.3051389112194918
0.9973687199743827	0.8494481805759094	0.3061648503506019
0.6848556147085413	0.0842874128828172	0.3045207755808385

0.6245593662987966	0.8440925310964631	0.3046714750329995
0.5600519224328133	0.5907113803615678	0.3047138976006168
0.4989287836442804	0.3412643581457526	0.3044538538703076
0.6229494895282056	0.3405445501443759	0.3044759042921217
0.1260010324883725	0.8470003861886598	0.3083594825059771
0.2464633455125497	0.8436863910009502	0.3077169992035842
0.0605390160708871	0.5891005773322072	0.3073691300722796
0.9968603895687107	0.3469969809654361	0.3061673966456006
0.6845606714783944	0.4315526013050681	0.3045335999842035
0.6244201393134500	0.6714195804033688	0.3046806741160801
0.5602058037751910	0.9242569685264145	0.3046558853759062
0.4990897644788261	0.1733806148534849	0.3043974247610632
0.6230945872530504	0.1748386456984047	0.3044616913431348
0.1255051671736856	0.6751104991507758	0.3080000283962726
0.2459525468338504	0.6717052764942792	0.3078616508842439
0.0612410108316525	0.9345250821011496	0.3078638629733508
0.9972764510285155	0.1758544800916562	0.3063135195500367
0.3126184910157339	0.0944032249227759	0.3081189077062617
0.4352663131227757	0.5908343006563045	0.3052853432780757
0.8102329944808894	0.0960745011760408	0.3045230724737218
0.9365265166926212	0.5947541097812590	0.3052704419962837
0.3117619317781631	0.4183874009994629	0.3098042822660661
0.4355256241395754	0.9232295880965314	0.3048959481675024
0.8095453198842208	0.4229515855919226	0.3045087061753684
0.9370927376791562	0.9280070896309568	0.3053323720355558
0.6843460209453573	0.9262258275282769	0.3046554503378183
0.5608953662154930	0.4249251031091728	0.3045701937421006
0.1865276544233142	0.9236172499866395	0.3084467715932979
0.0587799783848079	0.4265924113688664	0.3087063060890606
0.6840877594036781	0.5894896349833615	0.3046640250880009
0.5610561393739160	0.0901068524002726	0.3045111162080045
0.1851953449000565	0.5952393407715395	0.3080633068007008
0.0594687995924943	0.0972410310764626	0.3092103278709352
0.1832446440488947	0.2635197239901840	0.4112561262512986
0.1792434385259464	0.2846731208455481	0.4830771276676196
0.1269075351861587	0.2663976083341924	0.3338524868922373
0.2449044566797071	0.2533337376889407	0.3424379261122757
0.1357646332415613	0.2331012508138638	0.5013721413513649
0.2206867156021133	0.2334268880489979	0.5055883198668867
0.1785246228288509	0.4023274180264572	0.4947578681211763

Initial state de (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3107413917599766 0.9294225595673673 0.3066983697421600
0.3748508256478701 0.1725307535085613 0.3051746146245753
0.4368474501005245 0.4247892908137431 0.3047692809036358
0.4979533829384811 0.6732364172398693 0.3049050166092991
0.3722234185604599 0.6721255354222849 0.3058473188572596
0.8699454224860195 0.1751688219748261 0.3045928067970745
0.7501779840475655 0.1734362469013878 0.3045167562734156
0.9350200743743481 0.4352894257572680 0.3050969944896356
0.9969781658460484 0.6737325256880123 0.3060592333235370
0.3100213469848673 0.5840611829032009 0.3074943608317552
0.3744754682218680 0.3415611243883870 0.3056688554257457
0.4371576355281502 0.0895567997099889 0.3044784518108996
0.4980954819821621 0.8413228799515735 0.3048017345780062
0.3725220232755951 0.8412904630266342 0.3055345990782883
0.8696463266872129 0.3458095729135587 0.3045686265403649
0.7499313049070621 0.3436713736761453 0.3045228593770165
0.9355225710006496 0.0871530827099565 0.3051519226683171
0.9973899335371178 0.8492837220829952 0.3062091973636731
0.6849525787911673 0.0844632180215612 0.3045303082440064
0.6245617933585779 0.8439925687534486 0.3046740457344489
0.5599853602037221 0.5908844414041363 0.3047128067128880
0.4988386866473607 0.3413534841903239 0.3044132813180954
0.6230653087005054 0.3405435363614696 0.3044949144836439
0.1258880681251589 0.8469761708460003 0.3083348919804693
0.2465021966352199 0.8437327819955360 0.3077018680567908
0.0605816063151207 0.5892710160569034 0.3073258297950286
0.9968337872422264 0.3468072439973408 0.3061265141366115
0.6846695306472119 0.4314073254837842 0.3045405814905399
0.6244295023861171 0.6715359723330776 0.3046827109718262
0.5601344422084189 0.9240635265136745 0.3046560280824882
0.4989991575483894 0.1733276632440616 0.3043574763534687
0.6232090765837427 0.1748607282825336 0.3044798499011426
0.1254013727172212 0.6750050970591944 0.3079712998281701
0.2459981788586239 0.6716723179741131 0.3078329931013106
0.0612710341629719 0.9342378700170043 0.3078407019451522
0.9972586840321889 0.1759715334564487 0.3062912030167695

0.3125728869468346	0.0944388899606113	0.3079985998586797
0.4351769416725171	0.5910085315675643	0.3052800529996597
0.8102230831217999	0.0959651154941975	0.3045309014134198
0.9364444475906952	0.5948577544141346	0.3052708518203223
0.3117287750891964	0.4184682334163946	0.3096769475512576
0.4354374742174220	0.9230742850290860	0.3048899846622489
0.8095388331023723	0.4230583120960962	0.3045198860193896
0.9369924806987148	0.9278454644605540	0.3053319155306586
0.6844296573785111	0.9260185586008104	0.3046576522320993
0.5610194039244092	0.4246004997658711	0.3045815208440144
0.1864808544908726	0.9237966944219979	0.3082910652745065
0.0588808234050150	0.4263681807683914	0.3086242822623346
0.6841738123188853	0.5897017535771891	0.3046700582971046
0.5611717790856200	0.0904757741889287	0.3045135369454245
0.1851798464837809	0.5949824687755370	0.3078903552894467
0.0596045975951827	0.0974265514486421	0.3091797098410912
0.1830059553118135	0.2633951194818343	0.4113398072481467
0.1791961486596658	0.2847392734368616	0.4833305271824125
0.1268128655391000	0.2664365616843492	0.3337799448911397
0.2449029139986851	0.2533787696800719	0.3426768611120509
0.1357620268422761	0.2331628802163628	0.5016279550554741
0.2206730794421322	0.2333695935582602	0.5056897177085181
0.1785634240345651	0.4023347137299081	0.4950385995130933

Initial state de (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3107619913754978 0.9294024694443492 0.3067338090407506

0.3748600484214010 0.1725383070582819 0.3051616362787659

0.4368732249929030 0.4247005283558078 0.3047744771505950

0.4980295436623718 0.6731524830647665 0.3049344790571595

0.3722572408883515 0.6721178630869181 0.3059206761986783

0.8700098518376369 0.1752240641953981 0.3046112017471372

0.7501929107597460 0.1734191749912189 0.3045083771887065

0.9350170494877926 0.4354098469018871 0.3051284512267939

0.9970358364385409 0.6738586819338017 0.3061355871159688

0.3100221201765294 0.5840109262011736 0.3075461634738275

0.3744666745514460 0.3415145784787115 0.3056693146021155
0.4372077344880875 0.0895981262865281 0.3044655109538383
0.4981830136856386 0.8413524207020466 0.3048257393701166
0.3725605040768284 0.8412192904561592 0.3056002718935221
0.8697097985109175 0.3459370632828059 0.3045766202509107
0.7499429188830178 0.3437590655102239 0.3045065532580111
0.9355212499224268 0.0871943145993831 0.3051974858337703
0.9974433237652895 0.8492842537556365 0.3062901434109968
0.6850383242674813 0.0845014062053448 0.3045199508060462
0.6246352693629007 0.8439805358136553 0.3046675557595218
0.5600122514247686 0.5908935319009175 0.3047239288621562
0.4988455661234273 0.3413181128368955 0.3044053509501466
0.6231494673881637 0.3405061010877449 0.3044984876617356
0.1258917839746043 0.8470090157863389 0.3083856506958227
0.2465534997822407 0.8437412104832014 0.3077460402551014
0.0606329808283636 0.5894084482314181 0.3073909124773838
0.9967990659533016 0.3468063153460376 0.3061457943034108
0.6847509232185356 0.4313703719016201 0.3045263448449834
0.6245013322067519 0.6715225871174550 0.3046751753639545
0.5601610267139165 0.9239848078715580 0.3046617995228672
0.4990094937632209 0.1733013542893929 0.3043388389447412
0.6233000305884671 0.1748636101133314 0.3044773537323026
0.1254105564422184 0.6750345998483551 0.3080290745220610
0.2460481668125379 0.6716517234471411 0.3078893440404438
0.0613107311471305 0.9341578181454132 0.3079070422803941
0.9972176992065822 0.1761012707864527 0.3063221420099618
0.3125800544701748 0.0944308466598162 0.3079473235335396
0.4351800832903144 0.5910294788594876 0.3053276606490113
0.8102785442044599 0.0959787204632478 0.3045433346842360
0.9364539743537033 0.5950135286076763 0.3052933301484505
0.3116853699245375 0.4183889234252701 0.3096698841450405
0.4354435401003242 0.9229896889799717 0.3049209162685769
0.8095764968572304 0.4231814417895782 0.3045111896848705
0.9369970451974553 0.9278367622624970 0.3053732914944969
0.6845080204427154 0.9259196958043471 0.3046422317643983
0.5610930616253534 0.4244884690485589 0.3045949789370765
0.1865191324693182 0.9238961949786136 0.3082594590352201
0.0589185027482629 0.4263748061008854 0.3086288642636144
0.6842396537802514 0.5897898100679770 0.3046467413150954
0.5612583451471509 0.0905492511785437 0.3045108642601264
0.1852086463246764 0.5949245593931117 0.3078799703244895
0.0596350906944971 0.0975101953195709 0.3092067074835190
0.1826310395920668 0.2627340447807707 0.4111927230640982

0.1788913664697868	0.2847500317095805	0.4832106662082216
0.1265870125649471	0.2662984290200890	0.3337043550029727
0.2447321245584305	0.2530905919949573	0.3425920786300649
0.1355572866868571	0.2332557996369343	0.5017490712471535
0.2204708156892420	0.2337253622640825	0.5054700306082992
0.1782442716791704	0.4024493421370738	0.4946760801627375

Transition state de (n = 0)

C N Fe Ru H

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3109649864756420	0.9289468404084921	0.3074783879672761
0.3746840015378514	0.1723647733122058	0.3050184321631910
0.4368689960356119	0.4248953912562355	0.3044927192366391
0.4979101020071471	0.6734890304398312	0.3048927779210437
0.3724384578733912	0.6726223765568562	0.3061703144805321
0.8698469282167328	0.1751831150291288	0.3045333698390613
0.7502089555912861	0.1736206196546291	0.3043838598518087
0.9350186645119891	0.4352506235461581	0.3051728523806068
0.9968929393082834	0.6735823225702007	0.3062370950260977
0.3103179835052952	0.5848707687197477	0.3081904777107919
0.3743689161682011	0.3419797392861720	0.3054247949385405
0.4371461388483888	0.0896838050018400	0.3042251828804318
0.4980390483012945	0.8413121559723231	0.3047972541296413
0.3727189143841950	0.8411302999136095	0.3058608621071050
0.8695625517207315	0.3457080376677527	0.3045005895379471
0.7499712450283361	0.3436260648223114	0.3043778316661383
0.9354884279551589	0.0870083954825099	0.3052218941699053
0.9972817633568917	0.8491906510750854	0.3063523498599950
0.6848358336458769	0.0844240133255539	0.3044065794603166
0.6245461645221481	0.8441412279733547	0.3045792988992629
0.5600790628978288	0.5909212977938605	0.3046493362101212
0.4988751013575475	0.3414814325223688	0.3041361425016025
0.6229472192969202	0.3406484428838431	0.3043823760215134
0.1259677736835628	0.8468175550223971	0.3090206871773749
0.2464655487821800	0.8437017473690720	0.3085290254146533
0.0605273275112520	0.5890905660730259	0.3080539262803309
0.9968112691061867	0.3468629514514783	0.3066595904704125

0.6845671343791634	0.4316211458445671	0.3044042063544317
0.6244232848446885	0.6715835085026716	0.3045785742318000
0.5602183604737155	0.9242717467710487	0.3045944875844517
0.4990075492922486	0.1734122315703736	0.3040793035567206
0.6230762037164390	0.1749498509257789	0.3043678664575778
0.1255025981185808	0.6748305271826146	0.3087737408315913
0.2460042436984836	0.6718003026858933	0.3086749438316647
0.0611838491854469	0.9340675973449208	0.3083909150430792
0.9972126981966321	0.1757099559679771	0.3067497814385902
0.3128286493075221	0.0929795238464965	0.3087846004440051
0.4353510571483567	0.5909655414344016	0.3052605225289871
0.8101587644054564	0.0960772477338280	0.3044106476252573
0.9364814467279746	0.5946716481828866	0.3052216975559433
0.3121037361968967	0.4203167519754195	0.3100791041270287
0.4355745200026456	0.9233842386094605	0.3049142881805317
0.8095140808573570	0.4229802670561335	0.3043768947060010
0.9370018126921801	0.9278484937286560	0.3052527062983985
0.6843783222158623	0.9263563970118970	0.3045229742435175
0.5609432817882278	0.4249049370507189	0.3044634204970220
0.1865017975393898	0.9236850677752563	0.3094415013262292
0.0586981209251757	0.4265977061305825	0.3096092606456329
0.6841404359464645	0.5895721971860539	0.3045060988950070
0.5610979031082239	0.0903656659231852	0.3043984664939774
0.1852803257857824	0.5949180201421753	0.3092067670214804
0.0593835017834563	0.0968510480466094	0.3098127344047249
0.1844901566035608	0.2615026256554591	0.4097191094221604
0.1779236160662598	0.2857612090912388	0.5027478387001454
0.1268958801541721	0.2656688472185542	0.3331836779178678
0.2468800206344068	0.2541206748483502	0.3472774049201239
0.1343252880376855	0.2321811722299087	0.5181286413264398
0.2204050152002111	0.2323434507455362	0.5210203564149455
0.1777147073373244	0.4035984104513730	0.5115613738147445

Transition state de (n = -0.25)

C N Fe Ru H

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3110013001685575 0.9289368383762064 0.3076001150635630

0.3746901827656985	0.1722793738041849	0.3051093023551388
0.4368574308867381	0.4249369452279775	0.3045230728028309
0.4978682429510967	0.6735526126959901	0.3048909576812378
0.3724333132685765	0.6725751922366432	0.3062446953351218
0.8698449094478511	0.1752262393336591	0.3045571607201883
0.7502669700228316	0.1736736440924203	0.3043666837001053
0.9350565649236032	0.4353223956199023	0.3052152554954228
0.9968983942549793	0.6735840862444141	0.3063053999263676
0.3103533344998963	0.5848255480233288	0.3083336150948002
0.3743799427557309	0.3419825583686952	0.3055286050880101
0.4371348151061317	0.0895599904233165	0.3042355367120452
0.4979987279383731	0.8411916727196408	0.3047910151310895
0.3727150824171471	0.8411104140833910	0.3059281142230008
0.8695562617524821	0.3457245248348438	0.3045154662032694
0.7500225896730585	0.3435668624166683	0.3043540703422148
0.9355300299200849	0.0870125272947607	0.3052641249219916
0.9972876875872771	0.8492624652293659	0.3064123936910341
0.6848324829761099	0.0843395324274878	0.3043787087860945
0.6245625591456437	0.8441414441425606	0.3045594682650713
0.5601367398984213	0.5908269391478257	0.3046241514445819
0.4989150021798062	0.3414370426544105	0.3041172491890708
0.6229227365684759	0.3406326956443763	0.3043415623579609
0.1260193540198400	0.8468422207325192	0.3091598823788098
0.2464660697399253	0.8436682970128011	0.3086612012861526
0.0605309328724162	0.5890566078230404	0.3081836535992079
0.9968450167835681	0.3469519967776825	0.3067594889815342
0.6845517827157758	0.4316605804270726	0.3043713438031966
0.6244331111009881	0.6715346349221540	0.3045565845635732
0.5602779954006853	0.9243226758362613	0.3045680206889504
0.4990459872223744	0.1733838970220463	0.3040460576373665
0.6230526294152888	0.1749107984648337	0.3043289915798255
0.1255486579207897	0.6748691318142642	0.3089254459280839
0.2460026255093239	0.6718011089107142	0.3088184836352033
0.0611942682933764	0.9341889178064613	0.3084970324740510
0.9972503856387078	0.1757003852952494	0.3068357563851165
0.3128520482902970	0.0929748505242023	0.3089709387761205
0.4354091536141662	0.5908602948940935	0.3052817703149034
0.8101924315830433	0.0961226896580912	0.3044112860991800
0.9365196512860509	0.5946757262024691	0.3052540082047873
0.3121363924386931	0.4202502914438129	0.3103095643520293
0.4356253263348286	0.9234295488666044	0.3049281784210451
0.8095328419225718	0.4229651851135603	0.3043612376498392
0.9370439826001444	0.9279259838687157	0.3052925736604635

0.6843869463938806	0.9264151581812873	0.3044995801689886
0.5609086448443359	0.4250246611251134	0.3044116082746069
0.1865310368929775	0.9236473277396976	0.3096249143873624
0.0586858143644541	0.4266967898856636	0.3097120310120565
0.6841440587106462	0.5894712867100586	0.3044784813456914
0.5610724383613679	0.0901803917745838	0.3043438099376727
0.1852966132549066	0.5949717231175071	0.3094135121493594
0.0593724657545848	0.0968184764673397	0.3099048617536450
0.1846096696031073	0.2616058079631688	0.4100473193560084
0.1776760506384930	0.2857616048642744	0.5031702729076309
0.1269995822020717	0.2657021031572390	0.3333218854732119
0.2469613593781134	0.2541671298715825	0.3475815796656856
0.1340933875339821	0.2321998683237570	0.5186721758531702
0.2201051328597881	0.2324352544583675	0.5216346728060083
0.1774135373957746	0.4035573019017094	0.5121644874610704

Transition state de (n = -0.5)

C N Fe Ru H

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3110702064522506 0.9289582639875553 0.3081973892055671

0.3747109776563611 0.1722234664845624 0.3055313791341010

0.4368738279499411 0.4249716801382673 0.3046625159025179

0.4978324680144303 0.6735785658754131 0.3048871802755481

0.3724686515540919 0.6725665418732139 0.3065769851361615

0.8698833124691041 0.1752596291459600 0.3046370817126747

0.7503423831529172 0.1736776172805428 0.3043204505963696

0.9351566553547548 0.4353747518730228 0.3053933185293724

0.9969760381158407 0.6735647764078893 0.3065766709848087

0.3104324770124604 0.5848437222344545 0.3089367549596256

0.3744201843913217 0.3420238146229736 0.3059608867482028

0.4371368190244156 0.0894756038698300 0.3043806300610591

0.4979636235125315 0.8410909006501427 0.3047970280343386

0.3727460736120414 0.8411321536704059 0.3062632187770145

0.8695903750936936 0.3457238863780914 0.3045790672124633

0.7500940882249549 0.3434800247369629 0.3042909098065194

0.9356341672239905 0.0870531383553685 0.3054523090419679

0.9973702582995844 0.8493866984669397 0.3066729537697543

0.6848360868642910	0.0842433559122701	0.3042883869481643
0.6245751096009424	0.8441298793426666	0.3044671247142384
0.5601790272697328	0.5907067062050001	0.3045249476332764
0.4989716482445072	0.3413875431334421	0.3040577000131710
0.6229013618162291	0.3405924644746223	0.3041914481596438
0.1261196525293452	0.8468780274518501	0.3097711568536377
0.2465058607989143	0.8436604251870681	0.3093170270951560
0.0605891164183866	0.5890456460312925	0.3087299582380356
0.9969515588947028	0.3470775256796605	0.3072020130142678
0.6845473227193375	0.4316388971412715	0.3042626003861004
0.6244412990680372	0.6714373379883266	0.3044594566356860
0.5603195565135564	0.9243527222381029	0.3044798003763372
0.4990985683086120	0.1733571143829479	0.3039959116801651
0.6230314667764122	0.1748268390297152	0.3041885683488466
0.1256445901586601	0.6749307020815012	0.3095767538159231
0.2460454548565857	0.6718171905798151	0.3094988065782329
0.0612648276890550	0.9343330894119607	0.3089889748300932
0.9973607265460410	0.1756999100518238	0.3072576902955475
0.3129176918633787	0.0929389626451666	0.3097086156112188
0.4354663411207643	0.5907829889470421	0.3053839774521802
0.8102590653606518	0.0961481725670837	0.3044280634080294
0.9366351319358101	0.5946668306890482	0.3053598228980070
0.3122482099773803	0.4203358783505528	0.3110577291612604
0.4356766942087049	0.9234791054558742	0.3050635315007270
0.8095820292373609	0.4229140656451370	0.3043431670049073
0.9371767239692242	0.9280337744827071	0.3054010629058204
0.6843743735926431	0.9264305032533167	0.3044206354266955
0.5608960831741100	0.4250825392196324	0.3042473231356924
0.1866044806362285	0.9236125651315507	0.3103370082187380
0.0587217736732108	0.4268133012984839	0.3103594087969432
0.6841273643629125	0.5893386295530875	0.3043812822052153
0.5610584923192681	0.0900180452984560	0.3042026283791096
0.1853595971114810	0.5950469656668647	0.3101959480037780
0.0594101210412114	0.0968199621328320	0.3104630826622979
0.1848597490129811	0.2618178342043323	0.4108881007737641
0.1769826679280074	0.2857165520952097	0.5052183651481648
0.1271938873019368	0.2657746945542217	0.3340882554792790
0.2472455766794988	0.2543664578139924	0.3487228091151198
0.1333203768996802	0.2318261045972752	0.5202576246847027
0.2193288320979166	0.2325146735221135	0.5239169101733369
0.1765215983074263	0.4034730345011245	0.5142278041322661

Transition state de (n = +0.25)

C N Fe Ru H

1.000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3111417984205700 0.9284716884192062 0.3073494724499393

0.3748981934836306 0.1720546575132356 0.3048553756514225

0.4370025515188828 0.4245465385311978 0.3045613333049085

0.4981131129274744 0.6731272028469375 0.3049340521242981

0.3725787512882919 0.6722854376718725 0.3062987903029803

0.8699654929783303 0.1754283727646918 0.3047167808117262

0.7503073358864073 0.1735608323205999 0.3044228130097013

0.9349948296396045 0.4355958894897546 0.3053320748810639

0.9969083165777737 0.6740045216583450 0.3064455291024049

0.3103659425998442 0.5844615374044468 0.3082443984436667

0.3745094327760504 0.3416003774686904 0.3053863134605220

0.4373424117367521 0.0894384380971302 0.3042054714085571

0.4982661663118753 0.8411367235545152 0.3048153651144329

0.3729104463717395 0.8406405659260892 0.3059223978258840

0.8696330201426891 0.3459921896342540 0.3046534465607964

0.7500327519652965 0.3436671479263069 0.3043945832158419

0.9355476990120873 0.0873613942867547 0.3054197960657266

0.9973661092616924 0.8495268121221862 0.3065880546780184

0.6850325646251870 0.0843727777095371 0.3043904858767260

0.6247402267768836 0.8439675574865145 0.3045564577086113

0.5601930904347581 0.5907627775032224 0.3046398653203324

0.4990049611897486 0.3412147432290017 0.3041482239609137

0.6231317200716127 0.3404729842863916 0.3043392654542804

0.1260399558845210 0.8470897353158252 0.3090053046695690

0.2466153408220713 0.8434558462295499 0.3084949506603627

0.0605187499898889 0.5895947601624592 0.3080024578900515

0.9967531254056334 0.3471737342512118 0.3065982148152864

0.6847257890886995 0.4314465049639949 0.3043752502702440

0.6245978788805995 0.6714467060294581 0.3045591728956968

0.5603639321132575 0.9239791654226932 0.3045730103559954

0.4991673469171544 0.1731750443758062 0.3040697012399478

0.6232856964386255 0.1748020870936356 0.3043237266678982

0.1254988075759943 0.6750463438824765 0.3087436478738437

0.2460735581730505 0.6714732277658478 0.3087021251440119

0.0612903813386883 0.9343172662076576 0.3083797509506876

0.9972285751564695	0.1761200654523413	0.3067085456223752
0.3130730820910120	0.0923258996050678	0.3082259663955267
0.4354525948156548	0.5906834362154948	0.3053520549450966
0.8102994453105204	0.0961401804766227	0.3045407144945981
0.9364441291496470	0.5951141186330499	0.3054306762790183
0.3121794044391326	0.4200119718453871	0.3098880481451030
0.4357288933897877	0.9229940897441875	0.3049245214022289
0.8095569681215414	0.4231768044051494	0.3044500298572124
0.9370389963304951	0.9281301895701378	0.3055001258140915
0.6845792461582879	0.9261248860999725	0.3045073628921420
0.5611225351515866	0.4245588988321556	0.3044266276243962
0.1866872418211293	0.9237327840295252	0.3093849320285078
0.0586740935907489	0.4269877568537958	0.3092027349807129
0.6842981621598715	0.5895421171030096	0.3044856639969543
0.5613029396950895	0.0903101876683909	0.3043482778777709
0.1852486510415279	0.5948184475239927	0.3091723382155120
0.0594995600913336	0.0973310162802795	0.3094170822557372
0.1835384439146829	0.2602288462927662	0.4073584339008230
0.1766067919115952	0.2866632205054863	0.5011517787178620
0.1271414496149708	0.2666160476778382	0.3304423652687733
0.2467341721989513	0.2529262139228816	0.3459315550900390
0.1330400148913673	0.2330247015337730	0.5163775061279507
0.2192543372570563	0.2335024797333272	0.5190206032100609
0.1764054670720176	0.4046963044439456	0.5091070948770415

Transition state de (n = +0.5)

C N Fe Ru H

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3112050750341825	0.9282539474047110	0.3070110524245697
0.3750162962832190	0.1718624162278086	0.3045757532428613
0.4370745951706782	0.4242501527049896	0.3044788354096817
0.4982381741977015	0.6728103305333426	0.3049336651102411
0.3726265656307647	0.6719794096662388	0.3061819346484171
0.8700651747146879	0.1755939376925830	0.3047550260499973
0.7503544809804625	0.1734518275643198	0.3044820558335820
0.9349803532125457	0.4358582000784696	0.3052903545660459
0.9969428049256687	0.6743617753068453	0.3063817534675128

0.3103475641355384 0.5840581726321938 0.3080486226068849
0.3745864841462537 0.3412806312340812 0.3051932460020914
0.4374502317469930 0.0892571022346637 0.3040705481955379
0.4984114466233080 0.8409940307809133 0.3048035661268093
0.3729887178163687 0.8403470274570842 0.3057621284877210
0.8696974469362990 0.3462129435723262 0.3046931064722253
0.7500544881208907 0.3436858479208268 0.3044594153206442
0.9355958527518113 0.0876489207090466 0.3053842691751200
0.9974523830194537 0.8497801184215520 0.3065355833727070
0.6851743540723547 0.0843152938494209 0.3044278524302174
0.6248619030203106 0.8437881363136445 0.3045686920895654
0.5602427077939910 0.5906115658690523 0.3046581700321983
0.4990711729021607 0.3409809207217430 0.3041276856275803
0.6232592082222571 0.3402964197586602 0.3043864005873561
0.1260751860672146 0.8472898810906465 0.3087127978857300
0.2467161085059066 0.8432656665881049 0.3081741418202280
0.0605314781816805 0.5899723737247471 0.3077145930909717
0.9967306256405821 0.3473890273733503 0.3063170269064819
0.6848372728506765 0.4312590523984947 0.3044212005918917
0.6247021061293349 0.6713166431965507 0.3045751201992951
0.5604302992394368 0.9237126105748027 0.3045846970920627
0.4992518755870266 0.1729672153831516 0.3040382746255883
0.6234303477348724 0.1746493403628610 0.3043627693984278
0.1254791703871800 0.6752153538659071 0.3084518859162800
0.2461179180792284 0.6712342325522096 0.3084386929847942
0.0613845594048087 0.9345369541341234 0.3081313012161322
0.9972540695024554 0.1764750856007627 0.3064449904354430
0.3131368529580610 0.0921979179492555 0.3077168222500831
0.4354847621638224 0.5904866956458945 0.3053345461885071
0.8104026622755645 0.0961591378412745 0.3046095131067740
0.9364143939632005 0.5954746303032332 0.3054633567289450
0.3121440586420110 0.4194975274646943 0.3096662164214072
0.4357927459265632 0.9226771492644131 0.3048358656480213
0.8095791730272472 0.4233071947928059 0.3045238187803979
0.9370657882419458 0.9283424782019360 0.3055504576029135
0.6847073521794249 0.9258741700384154 0.3045269347861028
0.5612478410699672 0.4242494948892846 0.3044612777559526
0.1867990687694394 0.9237657700763118 0.3090007117857556
0.0587057909770553 0.4272239780801907 0.3087563428276804
0.6843939391478844 0.5895086071774697 0.3045095436778283
0.5614423526885318 0.0902396589804983 0.3043739132990603
0.1852076323969028 0.5947376128248135 0.3088431916558402
0.0596274042910702 0.0977745163261943 0.3090442671094798

0.1831081785940659	0.2594087144755842	0.4069960657072480
0.1759901312252772	0.2872053769299019	0.4984956373225093
0.1271380542259247	0.2673031256606261	0.3298523492527092
0.2464179851352702	0.2521303464564035	0.3450998636098399
0.1324108557229073	0.2338861932833458	0.5140136754763354
0.2185341549895705	0.2346616037502971	0.5170009803764305
0.1756630066197778	0.4053777880869882	0.5063109209385346

Final state de (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
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0.0000000000000000	8.5216999054000002	0.0000000000000000
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0.0000000000000000	0.0000000000000000	20.0000000000000000
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C N Fe Ru H

36 18 1 1 3

Direct

0.3112869114821026	0.9309711663282626	0.3080835944492968
0.3752627913465350	0.1738221943367793	0.3054133442821246
0.4375110315822854	0.4260349602212533	0.3047320590837017
0.4982580158098801	0.6746362096868038	0.3049629505605254
0.3729956883775913	0.6742694196193633	0.3067995426254830
0.8693832340272659	0.1740497786098041	0.3043021208684655
0.7501369792903027	0.1739257044462944	0.3042936492148384
0.9347995163515588	0.4343725106258350	0.3048198329174518
0.9972978808752027	0.6716763578563204	0.3063836670850418
0.3111773881664727	0.5859296130366066	0.3080858189544102
0.3752358499881367	0.3429865590161501	0.3054107345044011
0.4375543258891047	0.0907016741382414	0.3047229078762461
0.4982894272470919	0.8420893983642551	0.3049572766310049
0.3730406904314939	0.8424735096857833	0.3067971129151296
0.8693084942002524	0.3446629894434079	0.3042948262492238
0.7500638600663957	0.3435035477674427	0.3042889305203126
0.9349052483354851	0.0847377081882424	0.3048345317794625
0.9973761221551919	0.8475079225516161	0.3063960269297788
0.6848201264662199	0.0847203203752506	0.3043462123042159
0.6248461703200832	0.8446433521215068	0.3045291201387752
0.5605593501380172	0.5916083962277432	0.3046363580743365
0.4993662529771472	0.3424424089029656	0.3043052178556552
0.6230060858545392	0.3412785604743373	0.3043540383535799
0.1263677691590024	0.8458282892884254	0.3098771976073398
0.2469526405935505	0.8448378722477420	0.3090753867426734
0.0610560475648456	0.5864302073805617	0.3088817982986840

0.9960676933960251	0.3451339068158499	0.3062585677425999
0.6847292831287558	0.4322496208559323	0.3043461642035885
0.6248021756132696	0.6722522048323596	0.3045303718591915
0.5605980259859805	0.9251591130766247	0.3046280562893492
0.4993834953595867	0.1742780208341898	0.3042967028218510
0.6230496724468227	0.1755420492380534	0.3043504640877336
0.1262759481114905	0.6729954392632391	0.3098507962498616
0.2468657207654673	0.6725042778407129	0.3090639603346887
0.0611750113584634	0.9327284171804272	0.3089165510667633
0.9961219025789388	0.1740682152540908	0.3062762000105629
0.3132655508333661	0.0948129050594239	0.3076436759478647
0.4359514278186982	0.5922080736379262	0.3053346135191989
0.8097974343895874	0.0955905394521311	0.3042365009845308
0.9368150669116568	0.5933645607208508	0.3051206750726189
0.3131938308319546	0.4220040687515215	0.3076441851018847
0.4359940798991944	0.9245160449685753	0.3053275028756869
0.8095782951481558	0.4224856579619379	0.3042269128969891
0.9369258639033295	0.9258089611676216	0.3051404696608284
0.6845597219319706	0.9272467702273117	0.3044332864120116
0.5613232057293326	0.4260076073446371	0.3044555117852659
0.1867270381265078	0.9231624380882575	0.3099721356008941
0.0581117488972206	0.4241120310608528	0.3101470136552204
0.6844714714998095	0.5896926597070089	0.3044345256152853
0.5613524391476652	0.0907646560312546	0.3044447189852900
0.1864781581735443	0.5949467898398246	0.3099290239298112
0.0581854871289790	0.0951017368032290	0.3102183662789030
0.1793622936757857	0.2589899958905910	0.3974645305878546
0.1796719723944697	0.2863474480451889	0.5841811555832869
0.1208756134191526	0.2596186943001909	0.3335520517002827
0.2416354447301779	0.2583737325507883	0.3336038434357800
0.1369431460718339	0.2351406757724305	0.6033505059885397
0.2199435213192245	0.2345427118288383	0.6077079006506545
0.1789630445778052	0.4005615986571536	0.5997781142429295

Final state de (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3112890312259963 0.9309993273144660 0.3080661181844957
0.3752845803417099 0.1738119784797785 0.3054122481187217
0.4375174073239644 0.4261490265366821 0.3047518982005466
0.4982066265318548 0.6747645924073378 0.3049775257679934
0.3729778443477256 0.6743450867633540 0.3068089895251915
0.8693656828492649 0.1740188513769751 0.3042836776698566
0.7501713223229837 0.1739840663706898 0.3042796924473142
0.9348044544969062 0.4342982994633820 0.3048007811305490
0.9972465365006036 0.6715440177695037 0.3063922033260407
0.3111888212626922 0.5859507417349001 0.3080716595501528
0.3752566368247230 0.3430542448007762 0.3054119092827194
0.4375515206051276 0.0906487408345080 0.3047428694400772
0.4982334695286130 0.8420269439540135 0.3049734859313337
0.3730195553106697 0.8424604355096067 0.3068054243589318
0.8692971850886468 0.3446127026832042 0.3042793986702805
0.7501051755555803 0.3434665946399619 0.3042752984408367
0.9349005629569233 0.0846976620105175 0.3048118570292329
0.9973167109788295 0.8475192977441705 0.3064026833509524
0.6847914183720952 0.0846670501782580 0.3043337694471487
0.6248473677767095 0.8446790203624838 0.3045260717970457
0.5606075801533619 0.5915964576078951 0.3046438493075500
0.4993891971260176 0.3424880400301430 0.3043274827750535
0.6229627363916818 0.3413261677320750 0.3043509329972818
0.1263816744365095 0.8457656587390384 0.3098961572828969
0.2469317363978691 0.8448410452035576 0.3090621005555050
0.0610513343863291 0.5863185807303953 0.3089006480738120
0.9960822104889038 0.3451767769740682 0.3062568066086122
0.6847079019526938 0.4323617272934236 0.3043339657737275
0.6248070633882356 0.6722763588662959 0.3045268801120075
0.5606448666238399 0.9252420209747340 0.3046382259288416
0.4994095674514387 0.1743062167356854 0.3043204928795326
0.6230000107280027 0.1755656951095784 0.3043487625435107
0.1262978488649300 0.6729685501214400 0.3098745142089363
0.2468508442582338 0.6725216041145231 0.3090549239661530
0.0611594022612055 0.9327213169274217 0.3089300058072993
0.9961311403544084 0.1739038160748430 0.3062735195987291
0.3133087635240667 0.0948531405880963 0.3075776428771102
0.4359874227185507 0.5922119758538755 0.3053467781552241
0.8097949552817494 0.0955977510433996 0.3042202078013254
0.9368571251119751 0.5933005757765615 0.3051329664158991
0.3132413176876311 0.4220244310233512 0.3075821907036355
0.4360272749628371 0.9245777642385044 0.3053408315461455
0.8095954095735562 0.4224485905937787 0.3042131206596369

0.9369573657846205	0.9257525965021820	0.3051482324978956
0.6845553494217473	0.9273724951838134	0.3044173546984492
0.5612907082598524	0.4261837467924298	0.3044640429620525
0.1867157879522955	0.9231177528768197	0.3099783970436412
0.0580497687498008	0.4240812657335670	0.3101607743614372
0.6844739780738663	0.5896236921427824	0.3044196893629993
0.5613181980238712	0.0906538906937031	0.3044556637177819
0.1864863049437549	0.5949557827561327	0.3099461630332973
0.0581159739945407	0.0950091135382358	0.3102268138283591
0.1794793205675892	0.2589571782168989	0.3972144764879704
0.1796865624558596	0.2863712325322844	0.5842234716183995
0.1207286737929176	0.2595516145983819	0.3337054062970762
0.2417380587582936	0.2584122089239505	0.3335446092749010
0.1369528151710861	0.2351720838208747	0.6033793527688135
0.2199372451752179	0.2345769307964043	0.6077811106665445
0.1789672785490305	0.4005677256042976	0.5998231851325020

Final state de (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3113106410785301 0.9310243254069527 0.3080443455240308

0.3753200521550878 0.1737614179940355 0.3054047242516558

0.4375184867929648 0.4262521999501468 0.3047692826424265

0.4981623890161263 0.6748648456928112 0.3049909378463535

0.3729673109366148 0.6743593719692808 0.3068140346471522

0.8693271753305668 0.1739816405057878 0.3042636353078281

0.7501866100286335 0.1740328496194866 0.3042642621570678

0.9348044171033580 0.4342614924602874 0.3047841031127789

0.9972148838605882 0.6714201686961487 0.3063930491901139

0.3112188248604729 0.5859765669967447 0.3080529690178352

0.3752917794165774 0.3431593114770116 0.3054056609981660

0.4375465799036348 0.0906050939492530 0.3047598812900026

0.4981866453537381 0.8419901403597236 0.3049876363010351

0.3730052449936782 0.8425062832076404 0.3068097866528300

0.8692635072396392 0.3445759338424836 0.3042611817485462

0.7501254590337058 0.3434339996466068 0.3042604422003762

0.9348925807315598 0.0846288592501531 0.3047934551022404

0.9972781361150542 0.8475316230379905 0.3064027815858659
0.6847599312786244 0.0847041880574623 0.3043218533011438
0.6248510503481195 0.8447938112981581 0.3045229353284527
0.5606392273406808 0.5915627355034669 0.3046518937739879
0.4994304298748494 0.3425062456904971 0.3043537665875801
0.6229211001244536 0.3414173250568903 0.3043480518001334
0.1264058980166702 0.8457162939086319 0.3099115141642678
0.2469219398236087 0.8448340819969120 0.3090492166912841
0.0610370229388965 0.5862133166755933 0.3089200407727820
0.9960832226732723 0.3452018958000312 0.3062592752208361
0.6846835012622919 0.4323764806459652 0.3043224472627832
0.6248139136282594 0.6722155459734103 0.3045236918972304
0.5606736348079682 0.9253402077659233 0.3046470131280040
0.4994508388330074 0.1743555628155772 0.3043473126880743
0.6229526853899766 0.1755371575533233 0.3043454217200285
0.1263283175604001 0.6729299800320163 0.3098931888540639
0.2468466720578363 0.6725472501486950 0.3090445119957091
0.0611358926437754 0.9327172705812513 0.3089450813552831
0.9961278106717003 0.1737662733638937 0.3062743919563458
0.3133652461121332 0.0949119425688087 0.3075424930674813
0.4360294836297418 0.5922132907660737 0.3053578868092677
0.8097787694315304 0.0955958619728898 0.3042006423735207
0.9368849661527923 0.5932301095534065 0.3051347537072355
0.3133025430049051 0.4220247580131681 0.3075516958270394
0.4360673203362679 0.9246367637798004 0.3053519263894994
0.8095962606391620 0.4224224258400718 0.3041966567855660
0.9369756616861722 0.9257115100802713 0.3051479590742098
0.6845101247342041 0.9274257043593840 0.3044037222035830
0.5612684494508230 0.4262951930051266 0.3044761995247580
0.1867090392422233 0.9230608869362219 0.3099909420060258
0.0579927337136212 0.4240800329084269 0.3101966337197011
0.6844371910473821 0.5896218513255569 0.3044060013090199
0.5612944270532265 0.0906052009819955 0.3044673970356475
0.1864982024772185 0.5949742385177950 0.3099644966984234
0.0580534607942041 0.0948970354313140 0.3102548195879239
0.1796243841582122 0.2589375413234382 0.3970531451652040
0.1797022001094049 0.2863889332437502 0.5842530275284773
0.1206291879864736 0.2594905773066274 0.3338321002091487
0.2417817682829566 0.2584424511093260 0.3334116579013313
0.1369607560816777 0.2351987022630376 0.6034005781236468
0.2199345787301897 0.2346070944991998 0.6078484991689078
0.1789721159205460 0.4005784012840794 0.5998622997100754

Final state de (n = +0.25)

C N Fe Ru H O

1.000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3112646778201176 0.9309828725215783 0.3080565229906908

0.3752496021801609 0.1738975975528268 0.3054018015956228

0.4375109128799837 0.4259881746159209 0.3047475226118583

0.4983176341187934 0.6745755328410887 0.3049775846478645

0.3730062720077600 0.6742510854750575 0.3068022610282019

0.8693985768309955 0.1739999084938779 0.3042934645754621

0.7500969808152046 0.1738955029591497 0.3042769660025557

0.9347975955488658 0.4343224796563035 0.3048298175066153

0.9973444424505707 0.6717066252010450 0.3064049060681941

0.3111638928079478 0.5859677879448959 0.3080621470259782

0.3752228160836523 0.3429730030299655 0.3054006250021589

0.4375467392701539 0.0908172104287472 0.3047386398070105

0.4983466710015867 0.8422181655927349 0.3049732704631577

0.3730480476179024 0.8425583408702295 0.3068001373177055

0.8693303030063231 0.3446283000426174 0.3042882642465512

0.7500303112987300 0.3435538961391332 0.3042725144751895

0.9348938148438934 0.0846740375062138 0.3048407040457656

0.9974146419318699 0.8473551338574823 0.3064141602165008

0.6848576778156769 0.0848560076041426 0.3043348420590677

0.6248532823549030 0.8446590535626224 0.3045240954739581

0.5605271381531637 0.5916991395296656 0.3046442402136756

0.4993523497721963 0.3424692437195661 0.3043247383395246

0.6230682476817043 0.3413183892955181 0.3043546277530962

0.1263283294005766 0.8457932873333985 0.3098802147874835

0.2469618060853525 0.8448454326869667 0.3090699111008361

0.0610530537473821 0.5864347769114280 0.3088918659196657

0.9960412238788258 0.3449716370136507 0.3062421568602451

0.6847724481340025 0.4321742335498494 0.3043337714715626

0.6248111162296074 0.6722990371700518 0.3045254536844348

0.5605637239950444 0.9251365660485321 0.3046374614702724

0.4993706052737659 0.1743244007436559 0.3043181342184512

0.6231065696242288 0.1755680963896413 0.3043527736007615

0.1262427000378279 0.6729397951606522 0.3098592906029991

0.2468805102837497 0.6725175516142552 0.3090633376418159

0.0611622768319898	0.9326036899732533	0.3089212823390899
0.9960902356070162	0.1741088311643362	0.3062577419601114
0.3132164672202995	0.0948300583891231	0.3076081070966091
0.4359252880550042	0.5922753209686947	0.3053481561852450
0.8097847144127720	0.0955384152525869	0.3042212855171781
0.9367651075058357	0.5933221425965839	0.3051304278195416
0.3131489456724476	0.4220474503969895	0.3076121158659367
0.4359647076444126	0.9245181271358199	0.3053420956370893
0.8095855782743160	0.4225072670532947	0.3042134744120552
0.9368670876585818	0.9257311264855472	0.3051453376375181
0.6845745391017156	0.9271679322496462	0.3044163073930573
0.5613610347073632	0.4259051925111707	0.3044628983925694
0.1867071987318180	0.9231834652951891	0.3099538151657031
0.0581689654529413	0.4240277375923571	0.3101589272348124
0.6844926360308269	0.5898305706977903	0.3044179213236103
0.5613893441554746	0.0909314662632067	0.3044554367726314
0.1864773483404759	0.5948884677591781	0.3099215669293097
0.0582351400348963	0.0950611866501918	0.3102245706420197
0.1793618125959954	0.2589455246301358	0.3976089133932810
0.1796860627864167	0.2863751021221617	0.5842580290138573
0.1209826771038114	0.2595528352399597	0.3334378771343333
0.2414736133738694	0.2584071439510669	0.3333801749299272
0.1369478194896942	0.2351674260903508	0.6033888126132572
0.2199420927336105	0.2345720865490477	0.6077938898936194
0.1789672754958861	0.4005813839198661	0.5998319218726709

Final state de (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H

36 18 1 1 3

Direct

0.3112387694864062 0.9310030655135891 0.3080329383662165

0.3752219330513540 0.1739589824261115 0.3053942844887790

0.4375046475049243 0.4259426286649152 0.3047569152396017

0.4983683292756729 0.6745029690755143 0.3049901461565954

0.3730163410015133 0.6742471452350254 0.3068013795010571

0.8694208001000255 0.1739481908687552 0.3042884460212716

0.7500641062346899 0.1738456406337292 0.3042601432535410

0.9347970104725820	0.4342604395459542	0.3048411668865685
0.9973921910487045	0.6717250031349885	0.3064289577075773
0.3111466051275941	0.5859975038698229	0.3080412531002089
0.3751941691566618	0.3429686582192350	0.3053935367337645
0.4375338236870446	0.0909249646240475	0.3047496719054666
0.4983951690686951	0.8423573915714210	0.3049874528937649
0.3730545089833889	0.8426252352501771	0.3067992322556891
0.8693575517186378	0.3446056054260370	0.3042837124665472
0.7500030214774975	0.3436204161384299	0.3042563936686958
0.9348844746012467	0.0846260915945633	0.3048497838950045
0.9974567029061799	0.8472233713530939	0.3064359630133912
0.6848951557033801	0.0849669016870600	0.3043242631438557
0.6248699449737927	0.8446932158332268	0.3045195479976192
0.5604926228966058	0.5917814613126006	0.3046513603684619
0.4993344198804748	0.3424816056012007	0.3043406241875704
0.6231319254200105	0.3413425628742776	0.3043568346569999
0.1262913839784767	0.8457684602117577	0.3098736951840929
0.2469646116949170	0.8448569655253665	0.3090601526387508
0.0610633752747252	0.5864390774750143	0.3089004976644967
0.9960229909383758	0.3448146669360921	0.3062338697039121
0.6848168643307000	0.4321175130070867	0.3043216293088269
0.6248308770910317	0.6723239462776048	0.3045199962217763
0.5605257543538599	0.9251244178269513	0.3046465071186069
0.4993534931170303	0.1743816358944811	0.3043341467153323
0.6231651021121989	0.1756068047437638	0.3043558956049913
0.1262128148294133	0.6728791272869440	0.3098575569538699
0.2468897089652952	0.6725245497447022	0.3090567702974529
0.0611645640327696	0.9324892299962769	0.3089250073773171
0.9960663367943694	0.1741519656344434	0.3062466408553983
0.3131538115385318	0.0948597766729783	0.3075777810809170
0.4358919986577062	0.5923376858568736	0.3053574078916457
0.8097798239584090	0.0954874083463281	0.3042074855084012
0.9367282090318230	0.5932886130642605	0.3051431045122234
0.3130903157548714	0.4220776038630379	0.3075849865525287
0.4359278821673764	0.9245188905251006	0.3053534112433831
0.8095984339510712	0.4225293372299118	0.3042007853215469
0.9368223248589150	0.9256492868816916	0.3051544612086198
0.6845852163828021	0.9270786726852147	0.3043999684050509
0.5613980074825066	0.4258108053575607	0.3044728887386897
0.1866866363384587	0.9232027193927458	0.3099296705677531
0.0582294911492915	0.4239114035351743	0.3101663914869229
0.6845108671905373	0.5899725757864130	0.3044014280430510
0.5614252680562943	0.0910927905377932	0.3044671912526423

0.1864750426637799	0.5948331742638479	0.3099069846208087
0.0582879537918492	0.0950614414902663	0.3102252740374713
0.1793156729494119	0.2588936359823907	0.3977526559341483
0.1797009630497024	0.2863995091652227	0.5843426275195018
0.1211193800385179	0.2594921047697928	0.3332547478278587
0.2413172896476963	0.2584283912608538	0.3332158578015187
0.1369488445271650	0.2351898278525135	0.6034343227889928
0.2199450101318853	0.2345980568506973	0.6078905744019979
0.1789721393911215	0.4006111316150613	0.5998929317012361

2.4: Step gh ($\text{NH}_2 \rightarrow \text{NH}_3$)

Initial state gh ($n = 0$)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O

36 17 1 1 9 3

Direct

0.3078835132277400	0.9460270833294708	0.3123271767011490
0.3714538715989687	0.1866916292312776	0.3084106490774561
0.4368792743287020	0.4378851808593707	0.3035529960506554
0.4981630327046017	0.6858913171263391	0.3047232129497295
0.3736711906143653	0.6904106118307489	0.3058569336059642
0.8688357514098829	0.1601906983928168	0.3053792560981862
0.7491498625928420	0.1754828316558475	0.3054561214199671
0.9370896214547395	0.4134800023919976	0.3054386894261077
0.9988061300494776	0.6503966789005921	0.3072130330056548
0.3130659141787806	0.6025456081163323	0.3065333540198854
0.3744094863859572	0.3552832512999353	0.3038355288922708
0.4350970736522709	0.1041768477447463	0.3067496834407902
0.4969945587149481	0.8544042736946855	0.3059081098481818
0.3713738074469748	0.8583183503885680	0.3087674734793929
0.8709857412776789	0.3309531621842774	0.3054823390691542
0.7509889485127685	0.3455334332467965	0.3054568850425579
0.9337840910074150	0.0660430686631093	0.3048635120056628
0.9960980732954170	0.8256414359364639	0.3063475263618557
0.6834716065381892	0.0919381582087315	0.3053051732139083
0.6235264874346084	0.8527700836243365	0.3051762083207604
0.5601907195940214	0.6017871515369447	0.3048118591619250
0.4987518504920297	0.3535560876846182	0.3044634264983475
0.6231799764842639	0.3499438048720718	0.3050220780500151
0.1248535461421488	0.8259396124677278	0.3086749553164785

0.2447313984400447 0.8505665590672682 0.3114868043711029
0.0637609916725669 0.5648488127632498 0.3084766602501698
0.9985119673820109 0.3236241982391870 0.3041931254304868
0.6856704670046089 0.4386869538258158 0.3052527640299554
0.6246930333947812 0.6802896801220265 0.3051503534999135
0.5591983562820019 0.9353276595233105 0.3054243864007852
0.4975145191551863 0.1861553297257663 0.3051737714485052
0.6220955544951223 0.1844743216581919 0.3051872899056353
0.1278442117296086 0.6524618065363390 0.3121442336139880
0.2488875520532594 0.6791429205440048 0.3120786358065941
0.0592432109818403 0.9081840670399751 0.3051954560142748
0.9962257459806177 0.1524822403572695 0.3029969961007464
0.3081537203986562 0.1126317606984960 0.3152697116870682
0.4357496849134169 0.6051376169976868 0.3034796222696258
0.8073714839784112 0.0896932090942251 0.3055001993314176
0.9390196753623874 0.5725780168803469 0.3061122685868879
0.3140292327027421 0.4391720469972573 0.3026126786589186
0.4344226242531772 0.9382865177804510 0.3078385066450317
0.8124749287177726 0.4165644116222443 0.3055877867272018
0.9352761299670386 0.9055763124387588 0.3057637300641728
0.6829829478758649 0.9343817458153720 0.3052634053020655
0.5611082999152720 0.4354938180288825 0.3046820079032960
0.1816610775884056 0.9180712301812370 0.3099020749855022
0.0613786767032947 0.4003269273544969 0.3050950177939534
0.6849181024867512 0.5975439864738529 0.3053070197221497
0.5600813912444925 0.1012985472189836 0.3053180392758935
0.1917049664021507 0.5813278514312226 0.3174428274065582
0.0572399251099943 0.0703248956203555 0.3011624549236006
0.1670151219440187 0.2286648113355458 0.3997011233385039
0.1317390252248412 0.2209581215538811 0.3072804124132183
0.2330954347092578 0.3275522001535272 0.3330871194967375
0.1374322495145165 0.2938666226877127 0.4312136957556206
0.1728762896336291 0.1178584553167458 0.4185213360251482
0.2500948839192305 0.2372996439274017 0.4591534661514053
0.3279482562505942 0.2403906867198088 0.4768435134196407
0.2752932255329267 0.2299479609785572 0.5636454761517876
0.3079670798779706 0.1653862255447547 0.6348343904412810
0.2306581693166289 0.2482100798630590 0.6429618696152445
0.1376203068625950 0.1869437659120960 0.6726141188676317
0.1848683476804779 0.2478778150453091 0.7301827698443237
0.2841003100071658 0.2007491377311837 0.4922009059386739
0.2782581634252527 0.2462126784370492 0.6158738735896711
0.1731541957706247 0.2629706253693075 0.6831503007395702

Initial state gh (n = -0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	9	3

Direct

0.3078992408246954	0.9461980556919261	0.3123826761643468
0.3714526992388148	0.1867793973227006	0.3085068935111473
0.4368833919728420	0.4379610444050444	0.3036531050209482
0.4981131628072076	0.6859477108276387	0.3047790453014720
0.3736707435827077	0.6904660395251554	0.3059757074378786
0.8687670312826643	0.1601602332441295	0.3053282417044559
0.7491476689220712	0.1754993230821422	0.3054408087636660
0.9371040998768945	0.4133823011804215	0.3053846851775149
0.9987601435438136	0.6502026617690361	0.3072352621138487
0.3130884640063819	0.6026395209444509	0.3066669820704081
0.3744067204558194	0.3553849333581511	0.3039703232359380
0.4350911613033828	0.1042161305703296	0.3068128694131600
0.4969490027182781	0.8543908910463818	0.3059464990643801
0.3713574931799175	0.8584912227133901	0.3088416446909020
0.8709076954138679	0.3308095244995047	0.3054269685822265
0.7509745497629969	0.3454695382448052	0.3054377602663638
0.9337418015471383	0.0659343546622458	0.3048233211591593
0.9960078696623622	0.8255428749789343	0.3063642716896982
0.6833891520669838	0.0918561584610080	0.3053058359214281
0.6234845360357081	0.8527638774213918	0.3051902724370105
0.5601900129364769	0.6017388171539129	0.3048453035411663
0.4987569720536785	0.3535988079332141	0.3045222014494572
0.6231291801087877	0.3499354115745136	0.3050424137733028
0.1248191886466412	0.8257815839481174	0.3086210180264998
0.2446550551823769	0.8506292602046968	0.3115108760401559
0.0636950518409311	0.5645748479565813	0.3085088370914935
0.9985314930344171	0.3235301965342808	0.3041155297854392
0.6856100119640230	0.4387352752475872	0.3052530979988800
0.6246666674521358	0.6802471224878367	0.3051620009217996
0.5591892664845023	0.9353455835941527	0.3054477968798631
0.4975197587774077	0.1861302414727169	0.3052208399979769
0.6220352298964077	0.1844386059649956	0.3051976118669270
0.1278646514687439	0.6523954613021967	0.3121765625075086
0.2488688763023036	0.6792107656733551	0.3121608568047752
0.0591582292384936	0.9080872793660587	0.3051460304952675

0.9962260302133767	0.1523110597318349	0.3029137882486296
0.3081779408565559	0.1126886671177143	0.3153315633369213
0.4357517038606810	0.6051938045318096	0.3036113413012962
0.8072928782919654	0.0896944965531015	0.3054677384428052
0.9389960728024355	0.5723175671948368	0.3060981849880448
0.3140831070270906	0.4393546001827207	0.3027655161131745
0.4343980605263343	0.9383542358223119	0.3078652605258290
0.8124576167639005	0.4164628644732746	0.3055455248551638
0.9352383071093218	0.9055624247553410	0.3057889626664898
0.6829287617535966	0.9344422848435949	0.3052637491069812
0.5610580687929919	0.4355076096233021	0.3047315850437202
0.1816316124381722	0.9179435654023023	0.3098278407435427
0.0613606142382845	0.4002579001534711	0.3050673356169099
0.6848819861245660	0.5974556955435062	0.3053082880111447
0.5600398328558873	0.1012323572393425	0.3053309341764485
0.1916952974347415	0.5813702633620890	0.3174868142586144
0.0571373497082968	0.0700690744985711	0.3010973971266448
0.1669993551409333	0.2288838316915038	0.3994459267889126
0.1320367338617820	0.2203295793980454	0.3069355304916548
0.2330153286952023	0.3280452491374184	0.3330404037633605
0.1373416083664140	0.2937535338212214	0.4310001844600243
0.1733964872970511	0.1183344179683474	0.4183987220697091
0.2502197678511686	0.2378241435028104	0.4593415497162451
0.3280850945282252	0.2404018633591427	0.4769034732293938
0.2754315522519390	0.2300312359764465	0.5637356229041069
0.3080203960685109	0.1652668852747201	0.6348797088789625
0.2307022838157504	0.2482500686335052	0.6429614944915796
0.1377150764763904	0.1867978810770475	0.6724177761764654
0.1848043058612674	0.2481891817141783	0.7300317629893240
0.2842183066774236	0.2007841855182503	0.4922235258125016
0.2783804726812537	0.2462225901390704	0.6159351155224809
0.1731667810366068	0.2630244653961888	0.6829616082364741

Initial state gh (n = +0.5)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	9	3

Direct

0.3077925901865816	0.9458496990359191	0.3123796607004242
0.3714226894415520	0.1866705913859563	0.3084813606836484

0.4368737615579831 0.4378961227033896 0.3035788883113117
0.4982376135386997 0.6858675258371101 0.3047653471661209
0.3737166409024663 0.6906337033984300 0.3058828168610884
0.8688210555659491 0.1600754711652204 0.3053274074821714
0.7490428021839297 0.1754425574887592 0.3054452305747476
0.9369905869347841 0.4132366748615005 0.3053706507938174
0.9987153351393463 0.6502979807507224 0.3071725111423230
0.3130042842314025 0.6028191944479452 0.3065852874568791
0.3743775232406958 0.3553255778466294 0.3038857544812295
0.4350868441931853 0.1042493722186937 0.3068160887951956
0.4970478068039132 0.8544809509313031 0.3059741006772963
0.3713944476348728 0.8581448517131270 0.3088435968150179
0.8710363884233937 0.3310189541841251 0.3054193916804985
0.7509211274694578 0.3456466316267847 0.3054427301565870
0.9337002229787364 0.0660074305868590 0.3047770256370060
0.9959924366963193 0.8253430021700966 0.3062911271342710
0.6835667453391875 0.0920993831378328 0.3053110969172923
0.6235800905242795 0.8528005335273469 0.3051936098211917
0.5601841346111328 0.6018950567940329 0.3048614925333051
0.4987323806318696 0.3535280919608393 0.3044922302072892
0.6232326724574954 0.3499578501541453 0.3050554827172879
0.1247104128280595 0.8258601203367620 0.3087292538012880
0.2447301339735158 0.8507006833627389 0.3115413494946236
0.0637976056739870 0.5648308480900531 0.3084024818502776
0.9984941283130702 0.3233543897940580 0.3040865333905812
0.6857422497011654 0.4386194941760564 0.3052631623318770
0.6247349911102850 0.6803650494104957 0.3051822059433403
0.5592136156401002 0.9353276210523027 0.3054642449702539
0.4975116285351617 0.1863243474828783 0.3052040464183809
0.6221486934368767 0.1845667528105434 0.3052189545636717
0.1276860200924428 0.6522420294944199 0.3121960875703842
0.2488794575936586 0.6793082408685891 0.3121924569686992
0.0591365293057016 0.9077969784597189 0.3051446786183113
0.9961461998835635 0.1523982588908972 0.3028733283578901
0.3081212334592234 0.1126566092085000 0.3153327671195479
0.4357354541836954 0.6051326861315225 0.3034248288746935
0.8073891822130933 0.0895905564824108 0.3054927885666253
0.9389211788535496 0.5725578461554857 0.3060833934845871
0.3139808477780384 0.4393645435114410 0.3026132280091813
0.4344719768841107 0.9383239120099767 0.3079845165663124
0.8124384553818956 0.4167132216887099 0.3055577425144577
0.9350976519080409 0.9053579019486883 0.3056980094329157
0.6830476045767599 0.9342362214729126 0.3052605354843734

0.5611694412304894	0.4355224120402900	0.3047173451775442
0.1814651677422073	0.9183710385619507	0.3099131670101866
0.0614259036110448	0.3997925466675806	0.3049426366454205
0.6849597754346931	0.5977029001384171	0.3053137539762442
0.5601218351093448	0.1014030410065482	0.3053641739653396
0.1917061014534690	0.5810993200423272	0.3176703344224163
0.0572372450705328	0.0701827259597731	0.3010237820470081
0.1671840757287128	0.2290962639586777	0.4000028760745237
0.1319446242634257	0.2198412097479185	0.3072323992405958
0.2330081521331397	0.3283792065920602	0.3332365295035073
0.1372399470010254	0.2934920674225553	0.4314366034631535
0.1731658334066502	0.1181017802387859	0.4185663168697719
0.2501901221435927	0.2372488542780090	0.4588222974361392
0.3280505950121101	0.2402756351784851	0.4768355771003219
0.2754462216239655	0.2302157231543360	0.5635016476578936
0.3080168164882719	0.1652591047010797	0.6348108898038699
0.2308118800348805	0.2482567926326117	0.6428369181959783
0.1376798457095406	0.1867715417208116	0.6724242637529116
0.1847443346806885	0.2481207926317123	0.7300546532037102
0.2840843636047812	0.2015715549711583	0.4922807633558361
0.2783921272122352	0.2462221316376624	0.6158422281229142
0.1731252242919410	0.2629904739513516	0.6829897408964607

Initial state gh (n = +0.75)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	9	3

Direct

0.3077506212478185	0.9457465619681537	0.3124476785924034
0.3714016886532891	0.1866387760691094	0.3085439164468186
0.4368565389003677	0.4378853266868711	0.3036229755274381
0.4982492922125897	0.6858273115512545	0.3048103773327246
0.3737049223218201	0.6906867068265015	0.3059276124611604
0.8688211410655926	0.1600090792475082	0.3052728827932725
0.7489872268799529	0.1754277240686974	0.3054240728279095
0.9369484869204858	0.4131737999409513	0.3053068110512249
0.9986911856440885	0.6503124269692413	0.3071027163713509
0.3129469455278885	0.6028465136334465	0.3066450788160339
0.3743526297997095	0.3553133346938461	0.3039445852190323
0.4350592058438240	0.1042881978107539	0.3068771007918384

0.4970482314713463 0.8544936043533323 0.3060271439016704
0.3713736486827883 0.8580457197332657 0.3089131657392234
0.8710462462137778 0.3310520002960062 0.3053586220822040
0.7508706973605923 0.3457063655749384 0.3054180333515428
0.9336578933873905 0.0659946877154012 0.3047064808815835
0.9959720984980214 0.8252323522115480 0.3062133284578839
0.6835844692133368 0.0921630224198403 0.3053058767841291
0.6235795877937050 0.8527984990660910 0.3052017259574762
0.5601626914769036 0.6019264996337267 0.3048934354411855
0.4987102012649220 0.3535167601122511 0.3045270789786311
0.6232444574297767 0.3499639029089756 0.3050679288418451
0.1246543767700320 0.8258796685933274 0.3087657453225991
0.2447315227113231 0.8507128355244576 0.3116026958218625
0.0638103109590634 0.5648661854065986 0.3083652249765554
0.9984707527584022 0.3232545746093642 0.3040435594896747
0.6857800949327094 0.4385706618163243 0.3052572211958753
0.6247391298864801 0.6803827784399546 0.3051953535312413
0.5591951599332888 0.9352835934811208 0.3054894161061773
0.4974868190937377 0.1863759827550361 0.3052395512744527
0.6221597972397461 0.1845894085584946 0.3052314882070150
0.1276230089252072 0.6521712064554352 0.3122214535143983
0.2488641427913856 0.6793037733161531 0.3122634414350873
0.0591246681612130 0.9076794555042100 0.3051230365236057
0.9961101338892870 0.1523944284216269 0.3028268542140607
0.3080833191691785 0.1126502799344987 0.3153925288518808
0.4357017803858438 0.6051285679367127 0.3034455271849579
0.8073774156849983 0.0895440914715849 0.3054626367369626
0.9388795962970251 0.5725729249176676 0.3060050250723473
0.3139332060210028 0.4393484419541928 0.3026700986765268
0.4344729534482643 0.9382964342366154 0.3080941078308791
0.8124290569415027 0.4167692613196312 0.3055167894561435
0.9350374770145984 0.9052576182672679 0.3056036689126378
0.6830576657774347 0.9341551777392694 0.3052551843441026
0.5611941879802900 0.4355016402868419 0.3047447636695515
0.1814156549484635 0.9184901303128399 0.3099605962011873
0.0614372594907835 0.3996265304104824 0.3049056199030528
0.6849700250057886 0.5977991198200800 0.3053081047609474
0.5601161099873011 0.1014472643948359 0.3053934008272297
0.1916777891705444 0.5809975941977523 0.3177762014637928
0.0572431289158096 0.0701912129044863 0.3009910631372910
0.1672154224252442 0.2290771576736406 0.4001867514632601
0.1319116956894789 0.2196729745149092 0.3073122479994302
0.2329812770269344 0.3284655011198611 0.3333559515643117

0.1371967558088854	0.2932882461289580	0.4316074969078562
0.1731779357024317	0.1180073342193630	0.4186593216165500
0.2504395306641416	0.2375579257146472	0.4585937323399775
0.3282799891466683	0.2402880580436077	0.4768254037099406
0.2756434882766434	0.2304987990600445	0.5634393012192560
0.3080954579291516	0.1651780305915898	0.6347927739187695
0.2309339505568961	0.2482716257587931	0.6427190046518646
0.1377064632552858	0.1865094115360511	0.6721822320366634
0.1845476500079703	0.2483857655280195	0.7298762379743088
0.2842349692610611	0.2021435332264158	0.4922715770040693
0.2785396415352340	0.2462894372741781	0.6158294290312938
0.1730741856132442	0.2629088211314082	0.6827579322717982

Transition state gh (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 9 3

Direct

0.3092079206516194	0.9467318323324441	0.3133297695687351
0.3726704884544663	0.1876032034943685	0.3086768679777300
0.4380746262097560	0.4390303384565492	0.3037962137191841
0.4993866697536462	0.6867756941917132	0.3052032727229734
0.3750558760571510	0.6914036143370560	0.3066687876250584
0.8700710115317175	0.1600538091095174	0.3058504302577584
0.7503905404754839	0.1761055271026279	0.3053409795718118
0.9387491335282725	0.4130180011668818	0.3067362021798932
0.0002684136161987	0.6498456860220996	0.3090629901851657
0.3142892300256523	0.6034652874389808	0.3074174072914073
0.3755336066711017	0.3562904117523807	0.3039370486564563
0.4363604023748917	0.1050167152319375	0.3070846531386922
0.4982306633734544	0.8551464706569413	0.3063717153989077
0.3726967122556016	0.8589702707208871	0.3096147990303237
0.8723977433677272	0.3306953305903359	0.3059240821175035
0.7523705496400552	0.3460642403877293	0.3053766769338664
0.9351024366502820	0.0657235897830885	0.3062433618169114
0.9973808500171930	0.8252363188050081	0.3082633309891260
0.6846233302936156	0.0927297394313945	0.3051966149612506
0.6247135898349341	0.8536053129316371	0.3052502585855489
0.5614329159719745	0.6024712694916670	0.3051122839707639

0.4999272410454995 0.3545070345595563 0.3047293062207965
0.6243875499345640 0.3507752217750334 0.3051140503831268
0.1261104040453646 0.8260770961515870 0.3114182253113072
0.2460059803815030 0.8515330198008333 0.3131545885795259
0.0652998424696540 0.5645417572941542 0.3112763311538315
0.0002296141467136 0.3231763747268047 0.3071257137131904
0.6869529516808253 0.4395315189691375 0.3052244979971055
0.6259076858054848 0.6810135768588618 0.3052608172098062
0.5604305124386670 0.9361085866062546 0.3056655128625682
0.4987213630131433 0.1870624260215091 0.3054078034736791
0.6232829486698174 0.1852965280475214 0.3052170321823385
0.1292320924303116 0.6529468826874928 0.3144899302760811
0.2501683480077525 0.6799515183111723 0.3135347449237261
0.0604411312062313 0.9082066847903058 0.3083575351595164
0.9977585595752849 0.1520692956848984 0.3060701125994192
0.3095917042052241 0.1133639685715407 0.3157119121316272
0.4369711008693316 0.6059905524359582 0.3041087346944088
0.8085340782463587 0.0899667006358848 0.3055563101624186
0.9405425358903666 0.5719546124266740 0.3071721068968886
0.3151869298091736 0.4403586520139505 0.3031785723646242
0.4356981832541103 0.9393065902122409 0.3084114965374327
0.8139887384766924 0.4166566165224433 0.3056538530015191
0.9366403926978708 0.9053990966769285 0.3068334152169559
0.6841484160839824 0.9351919594067328 0.3051549567070203
0.5623149904197702 0.4363503106073950 0.3049802520716885
0.1828559813625163 0.9187785919369097 0.3122773350405555
0.0632689062384359 0.3996359262632190 0.3091577095688963
0.6861328496254688 0.5982252622270323 0.3052859211652446
0.5612407304906433 0.1021356494072479 0.3054701677604698
0.1931562146606173 0.5820191551853373 0.3189764013906916
0.0585496568022656 0.0699661917626829 0.3057135619932831
0.1764234834566703 0.2219312843403766 0.4100523470722941
0.1346169541079311 0.2210927458779711 0.3103938229827186
0.2349747011549475 0.3285744243234539 0.3346685321635779
0.1382551414106892 0.2749041112082824 0.4364472112646738
0.1734018695927415 0.1028542309454294 0.4166510871057245
0.2321582068437865 0.2464951730559306 0.4531042126397553
0.3162910774887858 0.1986618618587293 0.4708862494669308
0.2747320445908105 0.2489452620154990 0.5395826573192551
0.3051301252797576 0.1434482872210027 0.6240559855277260
0.2379328488210034 0.2420241763929459 0.6392982989392341
0.1377396356833831 0.1830551236280804 0.6801872309055867
0.1853186384124357 0.2511837647874070 0.7350213108135941

0.2792009384930193 0.2655184717707070 0.4866989162482342
0.2801452694277382 0.2370448425212715 0.6105909073114951
0.1722753579186549 0.2628389536402940 0.6882395550027558

Transition state gh (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 9 3

Direct

0.3093984291819609 0.9468036551168026 0.3132643649742590

0.3727454415926630 0.1875828940389255 0.3085304276972138

0.4381603485122483 0.4390314755645903 0.3036778682900945

0.4994693679247959 0.6867646024361420 0.3051683191796215

0.3752149417534625 0.6914004815675270 0.3065768091803989

0.8701569024919067 0.1601387670247192 0.3064749383865646

0.7505340499329520 0.1760590194976004 0.3057438182324717

0.9388969980841750 0.4131120216723758 0.3072709155032882

0.0004196500264229 0.6498470388833724 0.3094980030654995

0.3144661834460720 0.6035728086554784 0.3073322412951427

0.3756061853018764 0.3563021613613770 0.3037929587284225

0.4364835629873198 0.1049777649154606 0.3069721040175040

0.4983297640872237 0.8550823766767337 0.3063540795147688

0.3728411991884428 0.8590351804479681 0.3095091869847053

0.8724651314984797 0.3306908097263559 0.3065342005661051

0.7524943252113445 0.3459476270672042 0.3057809979757451

0.9352389281147779 0.0657272868556760 0.3068859624365174

0.9975301725233834 0.8253435914363507 0.3087831659319136

0.6847008249323920 0.0926165272176007 0.3054227056203729

0.6248162054526034 0.8535870676930202 0.3053525798024239

0.5615498275973678 0.6023801482851852 0.3050967645818830

0.5000352570968047 0.3545247891987842 0.3046484792649835

0.6244591039492207 0.3507414051128563 0.3051984683807305

0.1263439531739365 0.8260473485219890 0.3117210533412305

0.2461495799237099 0.8515602110234397 0.3132172450638748

0.0654170220096049 0.5645348750623498 0.3115847136576804

0.0003764713142331 0.3233214269530436 0.3075668093478043

0.6870216434153136 0.4394950418081649 0.3054336716881849

0.6260123089386767 0.6809145042383875 0.3053326488131702

0.5605527077161341 0.9361062685514767 0.3057265912836726

0.4988361511477351	0.1870043277693370	0.3053621279995369
0.6233610945667181	0.1852156499491215	0.3053378623000214
0.1294370410277708	0.6530160389917015	0.3147380668616293
0.2503498782171576	0.6800079312167924	0.3135464080849957
0.0605698253579590	0.9083818486447583	0.3087938959108740
0.9979225985845730	0.1520701139031360	0.3066668509083499
0.3097731767423895	0.1132189854005574	0.3155725685196344
0.4370954796486117	0.6059797973815577	0.3040432140790017
0.8086461642710603	0.0899745284627755	0.3061093401664294
0.9406934466561054	0.5719599442361698	0.3076447083924805
0.3153115017322250	0.4404991007701327	0.3030769169587160
0.4358116643877139	0.9393296125222648	0.3082668319226585
0.8140810368925884	0.4165987681084928	0.3062039914321630
0.9368281887707823	0.9055552011015848	0.3075029460061032
0.6842333365814852	0.9351908310460146	0.3053435618887477
0.5623935166565985	0.4363256362510910	0.3049296991994410
0.1830574422351035	0.9186556091225526	0.3124408152950693
0.0633637866361383	0.3998456318826129	0.3093102256263123
0.6862140475364953	0.5981066130877721	0.3054610008797525
0.5613306025078231	0.1020741188678471	0.3055300197321245
0.1933706459298818	0.5820117716331055	0.3190415508022042
0.0585995854378965	0.0699018588106597	0.3063270102923852
0.1761023960193882	0.2240397578989928	0.4099482628071698
0.1350012904563087	0.2214859382006651	0.3095227655143518
0.2347847673696890	0.3303062606252212	0.3346321841950513
0.1377477410157439	0.2773223954716357	0.4359635143138334
0.1728403604514952	0.1050027430375451	0.4165886638880281
0.2314115227023095	0.2483361150712753	0.4525140591264929
0.3158403118486532	0.1999509507274695	0.4702179206441244
0.2745039458236889	0.2500078055398234	0.5387091415165060
0.3043088081572520	0.1399544133762518	0.6227033391223955
0.2376670980512046	0.2396305269998180	0.6386308610202178
0.1375847294203325	0.1788421655799297	0.6801215373156424
0.1849570753481657	0.2512330101598437	0.7341525780094784
0.2790124122107471	0.2675751717967145	0.4860490547244609
0.2799663409104696	0.2350589181717524	0.6100301343968653
0.1718810339398402	0.2596736401596331	0.6872502593082785

Transition state gh (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 9 3

Direct

0.3091623953202053	0.9464449029793225	0.3135016552245373
0.3726774909936985	0.1874587132479475	0.3087615667119099
0.4381022705051613	0.4388422054339272	0.3038613889354539
0.4995091696937405	0.6866092806273446	0.3052786086275737
0.3750849217440304	0.6913877573679407	0.3067679332705934
0.8701816439227784	0.1598841101903830	0.3059116289616714
0.7503879063781723	0.1759500600804567	0.3053833076177553
0.9387086523914845	0.4128640737085843	0.3067895372784758
0.0002817543668922	0.6498396101399667	0.3091101244459688
0.3142747479815346	0.6034751100155308	0.3075194553164958
0.3755514895227806	0.3561641637106809	0.3039831026612145
0.4363752267967686	0.1049853134364116	0.3071958175032509
0.4983256039696287	0.8551145989941512	0.3064807300803751
0.3727248362501029	0.8587086784017307	0.3097853998943791
0.8725220714242695	0.3307318700216877	0.3059867910985686
0.7523770761591785	0.3460700260761350	0.3054259334735222
0.9351173989110080	0.0656806406802404	0.3062654598956747
0.9974143968489767	0.8250135522898994	0.3082892870013580
0.6847806136140264	0.0927403579827746	0.3052205112929612
0.6248162623504521	0.8534937045431324	0.3052662567681924
0.5614911070180182	0.6024986988516845	0.3051751179251316
0.4999609106233776	0.3543590181013197	0.3047994365083697
0.6245187417476907	0.3506686940840879	0.3051674336224289
0.1260605962382633	0.8260955129445965	0.3115725468621954
0.2460785765604787	0.8515001308721275	0.3133509323448688
0.0653995928295430	0.5645720542268002	0.3112828730082962
0.0002160632005735	0.3229395899935342	0.3071165103199687
0.6870962626721576	0.4393479127958399	0.3052628461734572
0.6260051677633552	0.6809971476122696	0.3052923134410806
0.5604844318260657	0.9359806469166477	0.3057204346277523
0.4987484184443021	0.1870646879867486	0.3054737518165561
0.6234100537295054	0.1852761645507756	0.3052636203185226
0.1291667438163026	0.6527245401611018	0.3146009709169437
0.2501975204345646	0.6799856978187229	0.3137236594687767
0.0604964633092471	0.9078794779504165	0.3083855215233324
0.9977301009191178	0.1520464685710044	0.3060219293708326
0.3095490139473616	0.1133188025628155	0.3158344016892515
0.4370126443292995	0.6058633551879243	0.3041012313590575
0.8086382090476367	0.0898009431276549	0.3056122912995884

0.9405304080220689	0.5720164676254323	0.3072564919170981
0.3151364271703668	0.4402857788755324	0.3031182109900014
0.4357679771552858	0.9391392335987460	0.3086317007183295
0.8140284187782847	0.4166918994409687	0.3057182399656613
0.9365810196642524	0.9050933703476384	0.3068510635934755
0.6842787554303466	0.9349512222530338	0.3051567246120275
0.5624322465015856	0.4362390191877484	0.3050378601268779
0.1827770142947941	0.9190543426160188	0.3124934480650498
0.0633314799738406	0.3992344485516128	0.3091074455130634
0.6862606375699016	0.5982902905864455	0.3053027224957490
0.5613320469999505	0.1021358628353233	0.3055276473225079
0.1931866889900297	0.5817791764445127	0.3192171287621449
0.0586982314026349	0.0700281400784022	0.3055576300897865
0.1759081364642399	0.2226848021758719	0.4096757352405332
0.1343449863861266	0.2206205947987222	0.3107559494550693
0.2348951444944403	0.3286831624538489	0.3346900958116148
0.1380484461172795	0.2757673975398898	0.4364257481215684
0.1733583126266547	0.1037500314597552	0.4168123039674699
0.2329891921917154	0.2479029579312172	0.4536007852627254
0.3161193551932733	0.1986693140036671	0.4706733240957789
0.2745268449329125	0.2491166504185104	0.5396827428071668
0.3044494861316620	0.1428435001964315	0.6233899142503819
0.2374377869066054	0.2421988502477901	0.6386456936047654
0.1376641927209716	0.1827935743261920	0.6797810066619596
0.1854014447619627	0.2522696514273472	0.7342141975700519
0.2792387172724138	0.2660034708644730	0.4866082940271156
0.2798069205608700	0.2370622636599750	0.6100913137936731
0.1721129727023290	0.2629690193419214	0.6874588632323739

Transition state gh (n = +0.75)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 9 3

Direct

0.3091362136663906 0.9462680008818504 0.3135878209708561

0.3726830832977253 0.1873536140709197 0.3088005770233515

0.4381220704504213 0.4387242883866173 0.3038687149315858

0.4995641861825590 0.6864881858106022 0.3052987291856040

0.3751017386937556 0.6913400144815397 0.3067976775890562

0.8702242632285014 0.1598207229675210 0.3059600721555615
0.7503767836272044 0.1758742153588106 0.3054291127473903
0.9386880936088763 0.4128146767296409 0.3068178371944956
0.0002874745625451 0.6498576880321616 0.3091367449061254
0.3142670233637039 0.6034213789197044 0.3075726609214616
0.3755646913709338 0.3560680439513893 0.3039983343391227
0.4363797708380157 0.1049409480355493 0.3072356987996987
0.4983648321131163 0.8550724767639657 0.3065206956288378
0.3727410352042137 0.8585447815915531 0.3098552959258571
0.8725693813732410 0.3307807595857016 0.3060317950892724
0.7523620753329179 0.3460949687124225 0.3054671171209807
0.9351056772990736 0.0656774926562116 0.3062841415637606
0.9974252862828884 0.8249215900446116 0.3083076006225655
0.6848497417736036 0.0927407027636232 0.3052597085002348
0.6248628254916410 0.8534367406958538 0.3052866814199955
0.5615128251901917 0.6024854754558198 0.3052021676053946
0.4999814379846542 0.3542655494023786 0.3048156528889805
0.6245829657613141 0.3506126730207099 0.3052058331768902
0.1260426127611643 0.8261140504303432 0.3116702086370331
0.2461193380983106 0.8514647333476562 0.3134532898450227
0.0654499611167229 0.5646139404450884 0.3113033124437078
0.0002047942671335 0.3228591602129701 0.3071097837445469
0.6871742231401188 0.4392306048006189 0.3052954547023725
0.6260555313864945 0.6809573342791850 0.3053164478668342
0.5604967847504324 0.9358893012970303 0.3057504630398555
0.4987646278310834 0.1870270048854259 0.3054958281162218
0.6234715549128432 0.1852344474832556 0.3053076028004156
0.1291266387388240 0.6526194278110699 0.3146902654474005
0.2502077195931776 0.6799296862376527 0.3138316038318281
0.0605115881604417 0.9077669521589291 0.3084092750052256
0.9977070704415825 0.1520531834395134 0.3060024889126443
0.3095326122581210 0.1132585512648332 0.3158972641760316
0.4370246723489205 0.6057699499248832 0.3040606971269110
0.8086773899183972 0.0897353168319560 0.3056637886157354
0.9405238789610841 0.5720680995886107 0.3072967276753740
0.3151246163195850 0.4402192338420905 0.3030907846316658
0.4357893277449482 0.9390139400297665 0.3087159289328105
0.8140471023809143 0.4167314105636601 0.3057647927484389
0.9365506797884455 0.9049855057968504 0.3068654192478175
0.6843309315360827 0.9347985310827146 0.3051772132550959
0.5624996889413069 0.4361448940546929 0.3050595933979703
0.1827430778333154 0.9191339216130971 0.3125905235572659
0.0633591915489959 0.3990577431170733 0.3090855266850522

0.6863118149840888	0.5983427119553983	0.3053213388162846
0.5613649818658450	0.1021321714083090	0.3055629886355535
0.1932099048218075	0.5816489203304167	0.3193592694601289
0.0587301677908161	0.0700402077716873	0.3055045299320160
0.1757797053564470	0.2230405654871057	0.4096574999776439
0.1342518146417181	0.2204902321721006	0.3107876002541032
0.2348550425489450	0.3287683897760147	0.3346847402542341
0.1379006082967535	0.2761392369718990	0.4363612491402595
0.1732698889081194	0.1041321236611814	0.4168717129977743
0.2332193897098760	0.2487513332696097	0.4534830314413840
0.3160950647729618	0.1986878802847876	0.4705051664863454
0.2745381141825283	0.2493265038835127	0.5397540751090960
0.3041802478951319	0.1426659607680249	0.6230838316750561
0.2372341605981218	0.2423471366739876	0.6384090736626741
0.1375837989837560	0.1826425173612187	0.6795891468311352
0.1853379654594025	0.2528184483586441	0.7338719348373267
0.2793811634516827	0.2663526500313247	0.4865599453828968
0.2796837848615218	0.2371959183981954	0.6099216109206455
0.1720629603260678	0.2628479528322826	0.6870908202734234

Final state gh (n = 0)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	9	3

Direct

0.3080330948592803	0.9428991708016581	0.3105611571198834
0.3713435402993586	0.1841466082204798	0.3081495759757010
0.4360400114586742	0.4357578410787021	0.3048137823276583
0.4974298286830212	0.6839327543400858	0.3054869613598505
0.3726097085626796	0.6862826433535716	0.3059962982592826
0.8696564831260917	0.1689383010995164	0.3055982084472508
0.7496212883943517	0.1775740853600917	0.3055014633418578
0.9369812608497086	0.4243252806389052	0.3054845871621989
0.9987053148894107	0.6617926819816184	0.3067580528315159
0.3114037837127897	0.5975923895442016	0.3054958153415999
0.3734119020223901	0.3525675483553644	0.3044293531283031
0.4349117987466110	0.1012843729164454	0.3071378342418922
0.4967099117903900	0.8521780062398389	0.3063216071194300
0.3711410473969787	0.8546416192837150	0.3082516263892383
0.8708909560342074	0.3394641519360763	0.3056662246280220

0.7507107007408097 0.3475400875044045 0.3055404707441390
0.9354457208058627 0.0770685755636889 0.3052669428870629
0.9973253771308206 0.8378957316411180 0.3063980952464240
0.6837416165194998 0.0918854034050669 0.3053839125845774
0.6233140287311355 0.8524241693372796 0.3053950204145005
0.5595785957764025 0.6003604035812812 0.3053976057762297
0.4980297138231333 0.3518043971244807 0.3054471606983465
0.6226320911618666 0.3491789741344143 0.3053735449201104
0.1254122804166821 0.8352048380609171 0.3069796838607424
0.2451641660582020 0.8499827174019816 0.3090737499247149
0.0630008700787302 0.5761538359425645 0.3066727263159173
0.9989612471935064 0.3350270340376916 0.3038109595770436
0.6849255011457621 0.4388865841376443 0.3054134103768323
0.6239729213185217 0.6797089916175372 0.3054115167565459
0.5590158956833303 0.9339661704233928 0.3057636033221456
0.4972140007801946 0.1840987011432330 0.3058871329456276
0.6220152800508699 0.1837090825937978 0.3054328774505152
0.1269923414131939 0.6626373526840528 0.3094776769475769
0.2476173775384585 0.6776215673898591 0.3093089961751247
0.0606036828868976 0.9212068515767430 0.3048621817324439
0.9980370185996095 0.1642691944239192 0.3034211926932380
0.3081745668316053 0.1093681515623667 0.3130962152396024
0.4348707824061513 0.6024261607415097 0.3047296831327531
0.8088058354158717 0.0950957588142450 0.3055714319550132
0.9387239043031581 0.5835223182663707 0.3059949576313454
0.3119992378705287 0.4333462154971357 0.3020024209122351
0.4341426271020689 0.9354469703356714 0.3078541150520532
0.8115262300346632 0.4217985692414393 0.3056858808650643
0.9366276779317023 0.9176531790202127 0.3062231998703450
0.6830652166398815 0.9342349655148329 0.3053060339899273
0.5604548573178586 0.4340818524824585 0.3053828079271702
0.1833520149572926 0.9214089331696682 0.3071414407157610
0.0612907656187406 0.4125383658912871 0.3024261075970779
0.6841319742191057 0.5971514721357722 0.3054157598113652
0.5598101682807571 0.1001273221528809 0.3056692167120701
0.1892737786813924 0.5876824439868653 0.3126406444112443
0.0598188589732548 0.0841323043546443 0.3014400004203071
0.1887165782730096 0.2088067296396260 0.4177771404217989
0.1335644272008099 0.2431767856322319 0.2806102958671751
0.2342631573245119 0.3007145733238580 0.3299538652234100
0.1482419576968609 0.2716575997037164 0.4353576973561307
0.1742301273823950 0.0940378895563915 0.4136276421893341
0.2283464925937499 0.2166500197334376 0.4523804565987817

0.3440525652883762	0.2029631408391377	0.4836172323811330
0.3001094829712246	0.2464864218928595	0.5468686451281540
0.3142633034128379	0.1301938135812511	0.6456795949322153
0.2486428805403127	0.2326067588462398	0.6555369692255396
0.1419631390290953	0.1768682134233307	0.6932086646393304
0.1894219157192014	0.2357267412915242	0.7498207648017292
0.3049695393915102	0.2646585606856136	0.4976741659556466
0.2928377397921341	0.2272230579848845	0.6310008819656888
0.1769984381204082	0.2541393288232855	0.7032852990469822

Final state gh (n = -0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	9	3

Direct

0.3080440920212756	0.9430193745114804	0.3105466996271631
0.3713500725242829	0.1842012712837763	0.3081645084414095
0.4360362937379431	0.4358202782030976	0.3048541932387011
0.4973914401934935	0.6840003298583353	0.3054989409988557
0.3725917443170738	0.6862797317817869	0.3060205960035259
0.8696064197271853	0.1689729899215043	0.3055843870064734
0.7496325884822833	0.1776073675771220	0.3055005872776820
0.9370362109782552	0.4243886246690204	0.3054634249640947
0.9987187573957247	0.6617933752617111	0.3067549569370766
0.3114105205426741	0.5975793595499154	0.3054902711685382
0.3734125645607184	0.3526232485646993	0.3044375052614717
0.4349051052151792	0.1012561598675949	0.3071477359920084
0.4966808389470716	0.8521423117965448	0.3063301157073239
0.3711387730913583	0.8547197487869007	0.3082505748215665
0.8708127860056545	0.3393394654640246	0.3056481794950526
0.7507005911952633	0.3474494687252260	0.3055393664790737
0.9354589857995300	0.0770378478378052	0.3052555544163640
0.9973138031003421	0.8379101980695081	0.3063874374379380
0.6836779607470705	0.0918186611380355	0.3053893392857716
0.6232925892320742	0.8524166042957442	0.3054024866084966
0.5595824713621315	0.6003331765263283	0.3054027046077828
0.4980291397020963	0.3518452867867332	0.3054764178240700
0.6225821026083491	0.3491619109226397	0.3053748264689221
0.1254334654848941	0.8352519897397798	0.3068967063784830
0.2451413432591396	0.8500853828991521	0.3090346147117292

0.0629293572978822 0.5761204891340510 0.3066777406211279
0.9989957633122341 0.3350835472543356 0.3038123837076305
0.6848666557809731 0.4388994986483498 0.3054162735835924
0.6239525407764958 0.6796696933765217 0.3054143027092398
0.5589989868551816 0.9340040402698579 0.3057745298761705
0.4972001716094526 0.1840307303768634 0.3059076321832740
0.6219600692500606 0.1836734789682641 0.3054408085071120
0.1270457685773970 0.6628798555391311 0.3094371968286962
0.2476029271449253 0.6776944808951416 0.3092985282530121
0.0605735459277596 0.9213347696770646 0.3048352798390407
0.9980681460900184 0.1642581454759311 0.3034275589071578
0.3081989880464772 0.1094046344482110 0.3131271837810232
0.4348825229283765 0.6024586636590356 0.3047690224014905
0.8087681898376476 0.0950942333019892 0.3055668396542163
0.9387098900089309 0.5833443595735209 0.3059869620724930
0.3120180763729246 0.4333596236604599 0.3019391664872729
0.4340975747449328 0.9354654658219299 0.3078452344932072
0.8115300022928742 0.4217033247361022 0.3056766225833952
0.9366475599020739 0.9177552799275284 0.3062210706011233
0.6830199138749740 0.9343047305081701 0.3053111193166803
0.5603948744972205 0.4340773999125927 0.3053894764703930
0.1833854757053565 0.9214348523200246 0.3070918455675343
0.0612871456576527 0.4127493852806895 0.3024814009541656
0.6841081197957323 0.5970630144642139 0.3054179888406461
0.5597703576311033 0.1000764495797928 0.3056816599326339
0.1892444406170550 0.5879916549264720 0.3126909544274505
0.0597590936991275 0.0840507943079926 0.3014980180509668
0.1887686515027575 0.2086158954107045 0.4177685017990920
0.1337937276056116 0.2431973628895091 0.2804288825805378
0.2344027004736388 0.3004545389696516 0.3300802507174891
0.1482524416277425 0.2714399233926734 0.4352973721919419
0.1743438784671547 0.0937797857801053 0.4137521602294213
0.2283927065577752 0.2166883138496403 0.4524063889703177
0.3439864052692954 0.2028156954359782 0.4836524247106048
0.3000911425081497 0.2465257611277080 0.5469064488054128
0.3143010291880783 0.1300579310305855 0.6456658745641336
0.2487306575163823 0.2326197755274903 0.6555560577805014
0.1420049439382110 0.1768617651519233 0.6931279270843703
0.1893588555076687 0.2359097095723386 0.7497871370617937
0.3049079912156545 0.2645731954809845 0.4976900595137246
0.2929314213723903 0.2272048728676996 0.6310309353725029
0.1770272287834968 0.2541514504303986 0.7032108878077561

Final state gh (n = +0.5)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	9	3

Direct

0.3079759285171193	0.9426690480180657	0.3105707945390913
0.3713323363480595	0.1840227006830583	0.3081310997003663
0.4360553743846265	0.4356351163160347	0.3047678963111259
0.4975027562738236	0.6838491394624774	0.3054967245104450
0.3726060847036556	0.6863280003750758	0.3059851808193880
0.8697360470288418	0.1689563245487920	0.3055949444208594
0.7495915566045105	0.1775668064778219	0.3055058617807609
0.9368678767337224	0.4243470538920582	0.3054677117371364
0.9986425136660559	0.6619794361260011	0.3066793336118840
0.3113651599686408	0.5976170409523468	0.3055222020908612
0.3734110299427492	0.3524660634151624	0.3044107674479737
0.4348920499853376	0.1013119680042339	0.3071547334590687
0.4967334208843836	0.8522056149019512	0.3063554606589979
0.3711085742090750	0.8544018827332213	0.3082852589665055
0.8709769006548304	0.3397452175216223	0.3056623178646048
0.7506721064762385	0.3477403790786520	0.3055423430264144
0.9353876897271242	0.0772527884838424	0.3052426625259038
0.9973016679660853	0.8379871532547059	0.3063447714458871
0.6838328114071518	0.0920135774679556	0.3053919493597755
0.6233520923956978	0.8524427023786749	0.3054045812655684
0.5595765371908515	0.6004730407519728	0.3054120652789145
0.4980160912842410	0.3517488976406394	0.3054236662843446
0.6226881016374408	0.3492262812361548	0.3053919480909023
0.1253295127609062	0.8353468489881254	0.3070145264282273
0.2451793851056217	0.8498840440319824	0.3090737593950748
0.0630580402628366	0.5763917441914317	0.3065761268562691
0.9988632499182754	0.3350552595376066	0.3037476427541096
0.6850291707190928	0.4388602506999534	0.3054220429764001
0.6240236041619421	0.6798341364604252	0.3054255092492171
0.5590372188476670	0.9339406182265776	0.3057836858606202
0.4972194272364408	0.1841873054535296	0.3058832057107656
0.6220908862894071	0.1838070579611124	0.3054509213464014
0.1268638919402793	0.6624409579012347	0.3094652356526864
0.2475987883166206	0.6775807002480596	0.3092908812254848
0.0606258857950943	0.9211151096877969	0.3048137306377723

0.9979501837750301	0.1644492681461791	0.3033384155439200
0.3081110064324342	0.1092699225973269	0.3130358434384394
0.4348495203116645	0.6023566061149096	0.3046742201691769
0.8088445708442539	0.0951468338590400	0.3055780253808410
0.9386856267644681	0.5839110126513422	0.3059524673698478
0.3119775687096627	0.4333352054069203	0.3020959355215229
0.4342170292538952	0.9353699036426660	0.3079391684598954
0.8115143295973531	0.4220224583260654	0.3056860388219245
0.9365464218722872	0.9175693796443519	0.3061625612283100
0.6831494601040128	0.9341636997167198	0.3053092512503816
0.5605735097744712	0.4341140503440747	0.3053914045955350
0.1832617791935378	0.9215817599221570	0.3071481360328195
0.0612523675555349	0.4123716252164642	0.3022869453566811
0.6841788849544143	0.5973458575645388	0.3054163459092177
0.5598242241377126	0.1001755931848676	0.3056944666389817
0.1892599187647625	0.5873049722926267	0.3125465542570018
0.0598947577740116	0.0844380771631318	0.3011892529416586
0.1887324961025087	0.2085881361295259	0.4178602747239999
0.1332645002677064	0.2428285388376026	0.2811372026162398
0.2340533936394929	0.3010960073022397	0.3298389614954529
0.1481460018286305	0.2709344048709084	0.4354783425350781
0.1744300380155992	0.0937337812707571	0.4134465855984203
0.2282994402717656	0.2165495047282234	0.4524558266263639
0.3439758022598871	0.2027143837228013	0.4836453575665067
0.3002351701372630	0.2464751906423068	0.5470070282204039
0.3143067016098655	0.1299362407476193	0.6456875064151901
0.2487588193659074	0.2325882106964082	0.6556021319014728
0.1420164915090067	0.1768563381375255	0.6930824143098342
0.1893133523893135	0.2359877069644859	0.7497838459546025
0.3051026420983318	0.2649260151132468	0.4978471362379616
0.2929957986967241	0.2272049016801901	0.6311464439964803
0.1770250226439559	0.2541568832545300	0.7031946065959791

Final state gh (n = +0.75)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 9 3

Direct

0.3079447721217743 0.9425935339630827 0.3105767193818794

0.3713419838155850 0.1839780842971966 0.3081341196996964

0.4360618697596590 0.4356111709706294 0.3047576104596536
0.4975277017452511 0.6838258017255282 0.3055070574802298
0.3726004875717803 0.6864073837713355 0.3059768250463790
0.8697588291411790 0.1689430899343592 0.3055821916918189
0.7495520047499989 0.1775471723855545 0.3055138631703487
0.9368181483530076 0.4243889764319100 0.3054444770786955
0.9986098947067464 0.6621129834382643 0.3066335568528932
0.3113258544927786 0.5976362238449472 0.3055168428215925
0.3734154747173291 0.3524628767616590 0.3043954017239648
0.4348812105692214 0.1013476153317598 0.3071724509180823
0.4967488050433438 0.8522181217243163 0.3063813062709344
0.3710890393044901 0.8542925044654309 0.3082987533337068
0.8709867684695820 0.3398824682671537 0.3056514177607473
0.7506145993257002 0.3478613070272667 0.3055460525409260
0.9353431607314161 0.0773429397516303 0.3052160239046070
0.9972786398417940 0.8380098129267360 0.3063088727018726
0.6838746861398340 0.0920736453344183 0.3054042688276482
0.6233764894069858 0.8524469896144278 0.3054190878132338
0.5595717708582709 0.6005232517500503 0.3054251466599073
0.4980128939814144 0.3517358845709392 0.3054250648470881
0.6227153128932453 0.3492372817682990 0.3054062166214317
0.1252776949403911 0.8354712378550943 0.3069984180749351
0.2451707058749091 0.8498710205710522 0.3090641940952609
0.0630619506968576 0.5765209277076392 0.3065187082859385
0.9988165212929374 0.3350741563818220 0.3037003113902043
0.6850870401744890 0.4388220927099699 0.3054286207760243
0.6240553474558919 0.6798593404248109 0.3054384499784212
0.5590306713612220 0.9338948163977812 0.3058075194435258
0.4972141091190367 0.1842036097752732 0.3058916454249183
0.6221182372500678 0.1838269061388411 0.3054703068294784
0.1268034930773151 0.6623931359786748 0.3094410975163948
0.2475894798140406 0.6775622181918434 0.3092790926582602
0.0606424243615272 0.9210912788099751 0.3047693652171654
0.9979118084644766 0.1645584708180770 0.3032895889766161
0.3080857999960355 0.1092388603739750 0.3130329373589554
0.4348443670241529 0.6023661627956347 0.3046488120613903
0.8088464000399589 0.0951639599730273 0.3055829518181020
0.9386494402907618 0.5840528858727639 0.3059230992195486
0.3119764484838614 0.4333501888850366 0.3020827209761869
0.4342326713944128 0.9353210644682297 0.3079932805417694
0.8115114272206967 0.4221248868003025 0.3056866480075326
0.9365083744094043 0.9175468854391015 0.3061242037556924
0.6831731463766055 0.9340818239021006 0.3053181680496028

0.5606079450128003	0.4340944138497755	0.3053981116747925
0.1832296197482964	0.9217041157717831	0.3071352588304826
0.0612341851173902	0.4123545034257243	0.3022018225876545
0.6841959728237765	0.5974777624277268	0.3054204635422312
0.5598289631060984	0.1002032708351757	0.3057235638928130
0.1892301622216576	0.5871668113616160	0.3125349193258814
0.0599105986332651	0.0845970954182071	0.3010684306326170
0.1887685858187602	0.2083152224979031	0.4179222352836414
0.1331902754440227	0.2426918176933618	0.2813674227412005
0.2340064333294514	0.3012621660674227	0.3298078119011559
0.1480973143341266	0.2703235157281513	0.4355341095035000
0.1746202774160006	0.0934010528035364	0.4133797041613984
0.2282889271255554	0.2164779718094591	0.4525131578897404
0.3439179285174127	0.2024819882123589	0.4836979935646373
0.3003422569548720	0.2465087268873598	0.5471376117546516
0.3143455749622263	0.1297755586076889	0.6456847701841868
0.2488454270657859	0.2325956116662901	0.6556468340215403
0.1420411529547971	0.1768353399466478	0.6929500440247774
0.1891932722193649	0.2362717676551420	0.7497149462483781
0.3051980014805222	0.2650995243935043	0.4979922704546653
0.2931203448874097	0.2272490257085990	0.6312609183649700
0.1770194239668602	0.2541704239047394	0.7030743723518147

2.5: Step ha ($\text{NH}_3 \rightarrow \text{NH}_4^+$)

Initial state ha ($n = 0$)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3088335697228928 0.9444088878428900 0.3123155044518882

0.3720749818999280 0.1857127096973059 0.3086550456074590

0.4370756539726628 0.4373292845379453 0.3041184630783675

0.4986562572753996 0.6855219838338300 0.3048362138095015

0.3738565016309678 0.6886183560842625 0.3063246033796290

0.8707217362390267 0.1679336107608123 0.3059634499016894

0.7504611319504733 0.1781534947224159 0.3053703094406259

0.9379875857083846 0.4228241536634272 0.3061925970432853

0.9998384566442766 0.6605423562000965 0.3078846105853401

0.3126909153217312 0.5997695540221173 0.3066924453487729
0.3743494686911930 0.3542172286955036 0.3044350245123795
0.4357338444471210 0.1033395325286577 0.3069361451094892
0.4977703858486819 0.8540616963356555 0.3059251381601698
0.3721219674765379 0.8562737975025811 0.3089645428830750
0.8721357944631549 0.3390270681829293 0.3061024421548950
0.7517053170408445 0.3486524706984042 0.3054557766154460
0.9362276902050652 0.0757792392076198 0.3058643524185527
0.9982886013850063 0.8361962290115272 0.3074586487596562
0.6848619128036262 0.0933473778837097 0.3049938374359087
0.6243992287700308 0.8538420567999481 0.3048285095094272
0.5606752010112643 0.6021312570596677 0.3046370466567936
0.4990461133666670 0.3534516743169078 0.3045536234311186
0.6238442072066874 0.3506768610544739 0.3047541990585572
0.1263001397383405 0.8338681740960538 0.3092669408510389
0.2461635342194199 0.8507192016539236 0.3114304940719208
0.0644359026794703 0.5747468221552339 0.3082786849340948
0.9999616909567806 0.3332760989178141 0.3046562041986434
0.6863032909016482 0.4399724006342538 0.3050259386064411
0.6251950314774888 0.6812048064548719 0.3048183331777992
0.5600124612940505 0.9354648472765916 0.3052093793652091
0.4981611627090459 0.1859644580375104 0.3051757131532682
0.6231266657029124 0.1852782281309544 0.3048939895856648
0.1281093261138153 0.6604143311869137 0.3119333335628838
0.2489860882722326 0.6785646809487744 0.3116049851445837
0.0616450073296448 0.9191254853952060 0.3062356414955900
0.9989406213332330 0.1627956694343169 0.3041508938251454
0.3088290089149623 0.1111461772180178 0.3150121100626677
0.4359736815810535 0.6042457778755406 0.3040069181357410
0.8096439759126781 0.0950092049750992 0.3056994226740812
0.9399258450265577 0.5824370731091904 0.3067478199856311
0.3131670482828781 0.4358676513215300 0.3028773165594387
0.4352198626834465 0.9372369695432639 0.3080162286229111
0.8128284248262787 0.4220389548091958 0.3059344091592493
0.9374232310005439 0.9158732989595677 0.3068565916579118
0.6841297659751007 0.9352021544136875 0.3048649974008626
0.5616968600136190 0.4356363631526818 0.3044539503931745
0.1839270009908773 0.9214606820979085 0.3100220254017216
0.0624270108080012 0.4104744428037677 0.3035638407987733
0.6853667366605762 0.5989295957606160 0.3049897165752284
0.5607885994357318 0.1018894862556365 0.3050618853446778
0.1909827937863895 0.5858494422614982 0.3159110778746239
0.0608838228918600 0.0827549583702663 0.3021603447363077

0.1822113077756384	0.2091480912658952	0.4155915664338110
0.1342931428211074	0.2413791994740038	0.2816083671157017
0.2336517989806381	0.3113702778202452	0.3316035742987324
0.1396717953157705	0.2664484754169507	0.4318229476108755
0.1695964114662019	0.0944062418283451	0.4068960757168298
0.2169038811672692	0.2107760055446519	0.4536245315103358
0.2094698047820103	0.1941167758485136	0.5718094856351854
0.2589404709987519	0.2392915978875152	0.6298194792925358
0.1609267462946633	0.2237838561561034	0.6570764335794692
0.1008351690216855	0.3568461917773007	0.6753902247048202
0.1246823583344465	0.2369713536146918	0.7380025846657858
0.1763732240231093	0.2546901224266520	0.8236741247274537
0.0973243193539588	0.2540604155332673	0.8333988703703028
0.2185143903855717	0.1777171852251982	0.6191855608101591
0.1160739414528038	0.2498625134361774	0.6852152864508128
0.1341622502261046	0.2091785238519179	0.8068818833699325

Initial state ha (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3088760836320356 0.9444124802132924 0.3122425997203596

0.3720385357072220 0.1856327049079426 0.3086830590109266

0.4370369376318367 0.4372224097287197 0.3042418609893842

0.4985705977088795 0.6854597122742276 0.3049439593189589

0.3738168875098944 0.6883090197218238 0.3063858184482545

0.8706654517526324 0.1682849780270105 0.3059040253225381

0.7505375419792295 0.1783008632889430 0.3053759472617234

0.9380204720384505 0.4231501760863757 0.3060995303549899

0.9998129693060830 0.6606965962856056 0.3078444733010489

0.3126962637187109 0.5995630592008870 0.3066642189297252

0.3743196762625354 0.3540790422051466 0.3045144902043886

0.4357505274424214 0.1030753845081663 0.3070270096207587

0.4977228734017969 0.8538613216218905 0.3059923599063983

0.3721238664501844 0.8562819348356926 0.3089875370522570

0.8720666488309716 0.3390958697539262 0.3060175071466014

0.7517874092019090 0.3484938270719546 0.3054436623636346

0.9362975881437157 0.0760055179075634 0.3057941795063716

0.9982730333251286 0.8365826707406467 0.3074121965506092
0.6847568748927780 0.0932406863878034 0.3050595772160342
0.6243392673251856 0.8537875327987232 0.3049237919467611
0.5606573786357035 0.6019396669357501 0.3047621896654587
0.4990239076949232 0.3533498649991376 0.3047087140275879
0.6237401111398300 0.3506169036138219 0.3048462674870571
0.1263570781740117 0.8339409169506840 0.3091258397801409
0.2461473024614971 0.8506777658957534 0.3113315569131667
0.0643363073390337 0.5748880158539819 0.3081918922894480
0.9999892084302032 0.3336516142033210 0.3045462885551027
0.6861470141711880 0.4400670532161005 0.3050767757743605
0.6251055896861080 0.6811410102948428 0.3049161934365837
0.5600135404882293 0.9354566168918387 0.3053223504207165
0.4981366088790050 0.1857508750390827 0.3053359833734814
0.6230514010494941 0.1851729850226798 0.3049896759355099
0.1281495169196810 0.6608263678322113 0.3117770662321085
0.2489411403875939 0.6785293899969259 0.3114920014483447
0.0615859914757904 0.9195884706832477 0.3061522522346214
0.9989894794663007 0.1630041262924901 0.3040520409952536
0.3088689423866503 0.1110897493240091 0.3148702703746214
0.4359460687717573 0.6040636987209822 0.3041652971273260
0.8096409776963130 0.0951961227903410 0.3056513018410326
0.9399056077647989 0.5825891094822303 0.3066945645952999
0.3131131662052764 0.4356129844136193 0.3028375232708195
0.4351713791699013 0.9371697720363725 0.3079999413520301
0.8127730418155885 0.4220819250453681 0.3058448342380430
0.9374691226144698 0.9163306991686488 0.3068184149942405
0.6840890330142416 0.9353908618706106 0.3049417183812030
0.5615928563798481 0.4355841099420064 0.3046269193855845
0.1840003848967226 0.9213205634992567 0.3098898666683702
0.0623881578423823 0.4109635386143982 0.3034778015291211
0.6853074869028658 0.5986439312929742 0.3050735543449004
0.5607659801109264 0.1017153003746687 0.3052245709126175
0.1909123247290191 0.5862776838562812 0.3156654965531363
0.0608397933520918 0.0828514076042164 0.3021029551130499
0.1824969413196167 0.2087182356398302 0.4153238194297179
0.1343065973424481 0.2422651806335175 0.2810021581596155
0.2337100478419560 0.3103877580975176 0.3313465277239863
0.1399483102327346 0.2658707897998643 0.4316545160091483
0.1699457833689622 0.0939104302895972 0.4066873431584319
0.2172817441736669 0.2103201628618996 0.4532927842210369
0.2096221659058051 0.1933308924885394 0.5722563666362459
0.2589805724776821 0.2397022440864184 0.6302436730822908

0.1609326179062299	0.2238246646797690	0.6573038989100299
0.1008790646674880	0.3570703455583114	0.6754319313738367
0.1244973301427250	0.2371295821259534	0.7380843745107863
0.1763146277077983	0.2548184986711592	0.8236001764044765
0.0973020159696416	0.2537956689478369	0.8335465366258458
0.2186051242546255	0.1779573916231459	0.6197127089422092
0.1159503202778988	0.2499879736406881	0.6852798367254491
0.1341034570976392	0.2091964365317618	0.8068861376648935

Initial state ha (n = -1)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3089118851618188	0.9445277872562762	0.3121785552897013
0.3720349707637057	0.1856508189846852	0.3087011474108481
0.4370006006643212	0.4372605281836353	0.3043695391149688
0.4984673867417108	0.6854766530402729	0.3050149416458710
0.3737801589433652	0.6881563052497343	0.3064468179627997
0.8705806821965452	0.1684797288842212	0.3058676586319293
0.7505625979880847	0.1783727052101953	0.3053809833688026
0.9381027859656951	0.4233700076457763	0.3060439352103010
0.9998251161298464	0.6607551140855389	0.3078395858272461
0.3126898108960942	0.5993998084303368	0.3066489207147450
0.3743072169159863	0.3540876096557308	0.3045851721198668
0.4357592494375109	0.1029464708272644	0.3070682095227084
0.4976757194341236	0.8537459386500890	0.3060286986855513
0.3721254275956696	0.8563771191234344	0.3089793714250844
0.8719619700942189	0.3390195660338439	0.3059710506099320
0.7517999294699461	0.3483484627695003	0.3054442619493665
0.9363540848604206	0.0760802965107815	0.3057592515028167
0.9982691293163373	0.8367797470190749	0.3073933660412729
0.6846490996130115	0.0931081941544703	0.3050957163257231
0.6242952828133367	0.8537545926432323	0.3049830133731555
0.5606372581910672	0.6017881684751004	0.3048327137793478
0.4990116937544418	0.3533438999912659	0.3048284052239331
0.6236471406587758	0.3505644386538640	0.3049002414343806
0.1264288356971141	0.8339805090335624	0.3089733564263021
0.2461208336382594	0.8507258994895609	0.3112433015171803

0.0642272554199143 0.5749300596607575 0.3081577759376794
1.0000463295314728 0.3338911035335979 0.3045043761622719
0.6860123167909051 0.4400981378322895 0.3051064845177806
0.6250417678495105 0.6809962126517273 0.3049680365360340
0.5599783330361262 0.9354340860975218 0.3053791273666461
0.4981142753176678 0.1855799754832226 0.3054262171420023
0.6229536928890531 0.1850507356585454 0.3050400306339552
0.1282183025413443 0.6612238136778785 0.3116341469941065
0.2489020423449389 0.6785018017165716 0.3114128042032608
0.0615481585518074 0.9199417148214505 0.3060917697341088
0.9990514433815302 0.1630774166669721 0.3040244648858699
0.3089168544051151 0.1110987355655173 0.3147883406637497
0.4359421728055985 0.6040348629461382 0.3043149705451943
0.8096122191736524 0.0952805283804497 0.3056321072395004
0.9399092337266983 0.5824789212087568 0.3066704547452646
0.3130991410239957 0.4354916706447756 0.3027983541637689
0.4350920889984440 0.9371409545426085 0.3079612886171920
0.8127440184370649 0.4219901703548596 0.3058139125738061
0.9375373505965241 0.9166719074225703 0.3068202894035011
0.6840009127417668 0.9354825204758241 0.3049900688031538
0.5614570715394898 0.4355150037952016 0.3047302897016680
0.1840838784476069 0.9211719724175130 0.3097720370518363
0.0623777386196653 0.4113888116859659 0.3034789347452099
0.6852290929096254 0.5984179593930617 0.3051144024663619
0.5607239507951098 0.1016074341545871 0.3052790197053841
0.1908529823026096 0.5867504850814552 0.3155362928496052
0.0607763934678559 0.0828102359569355 0.3021680788991826
0.1826812627225310 0.2083929290915376 0.4151497150600704
0.1345275676502182 0.2429386448810063 0.2803887187335701
0.2339067706420756 0.3093695372935810 0.3312573495444812
0.1401669149032572 0.2657449136535365 0.4314911900927684
0.1700915563129900 0.0935416448625800 0.4067803271127878
0.2175189248550047 0.2101795405859143 0.4530873195479644
0.2097528117001746 0.1928936664933089 0.5724751755678963
0.2589931043466035 0.2399760681694208 0.6304744967962883
0.1609272070675463 0.2238895629979287 0.6574300975700028
0.1008928325131721 0.3572243225438252 0.6754697030949043
0.1243975514849336 0.2372033673747226 0.7381387228803715
0.1762900160157801 0.2549105147451062 0.8235667346019141
0.0972944443370370 0.2536650985960933 0.8336276232163140
0.2186832668036783 0.1779535356463106 0.6199629556979103
0.1158951468422753 0.2500881824558374 0.6853207442013800
0.1340748642161800 0.2091760137810793 0.8069095478795026

Initial state ha (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3087933275471557 0.9443388898622015 0.3122890392575035

0.3720917743478787 0.1856367170729828 0.3086689750320658

0.4370884027874881 0.4372385371179052 0.3041505805064779

0.4986828454157916 0.6854294128570284 0.3048916289500501

0.3738496608171236 0.6886281005981740 0.3063218859327953

0.8707417631248618 0.1679789846209922 0.3059327910510884

0.7504197194868187 0.1780981669057752 0.3053766461556623

0.9379187836032572 0.4229524230623602 0.3061469561907120

0.9998167568285077 0.6607187686671981 0.3078509334925716

0.3126682703214817 0.5997337991727474 0.3066518544703902

0.3743714215986351 0.3541638892315569 0.3044317287486936

0.4357212246633634 0.1032927376768006 0.3069812075396884

0.4977836100110179 0.8540360361664017 0.3059632084601168

0.3721166778895885 0.8561568597401653 0.3089859125514556

0.8721367669209902 0.3392454511382753 0.3060558589515277

0.7516497787933125 0.3487657459202035 0.3054481163623202

0.9361961160806285 0.0759487297092968 0.3058323303355320

0.9982870291392628 0.8363188086387786 0.3074334604524682

0.6849131164190674 0.0933884900239548 0.3050318106417553

0.6244165323386248 0.8538223431106168 0.3048670651400727

0.5606620041218671 0.6021527965816537 0.3047068043704698

0.4990581510605493 0.3533657071520870 0.3046196774911502

0.6238782839356815 0.3506405898422498 0.3048065888652930

0.1262540316722753 0.8340322228011458 0.3092404931076943

0.2461618963850339 0.8507021446701341 0.3113822248991428

0.0644503523141833 0.5749301454186766 0.3082103960981132

0.9999092734979749 0.3333901918296138 0.3046048922440774

0.6863576470814262 0.4398958524516360 0.3050554190276250

0.6252182936222676 0.6811973227337328 0.3048717258880531

0.5599985922977885 0.9353817597538838 0.3052595327307036

0.4981642389666730 0.1859071968316098 0.3052387630776245

0.6231644565365430 0.1852523226471338 0.3049506809524427

0.1280477906204603 0.6603964282884213 0.3118900556452652

0.2489807638500982	0.6785156860404233	0.3115547041751390
0.0616669231016101	0.9191977423333677	0.3061920311104114
0.9989024552668319	0.1629864627346895	0.3041081776082405
0.3087887010095156	0.1111314785477071	0.3149975557212514
0.4359661753141973	0.6041974427290883	0.3040130934221348
0.8096573540290235	0.0950395207284941	0.3056764988286659
0.9398796372552753	0.5826964730545668	0.3067222937775817
0.3131673600212265	0.4358332155863353	0.3027546909971429
0.4352249507091872	0.9371277367644941	0.3080831668564886
0.8128061898222838	0.4221931096984928	0.3058814467058054
0.9373981964631789	0.9159471982941638	0.3068222162999700
0.6841569386191850	0.9350481310261390	0.3048985268492029
0.5617297128026292	0.4355443460470511	0.3045349899713859
0.1839160032714785	0.9215943280136090	0.3099897316062349
0.0624061009300924	0.4104969148238361	0.3034597604205255
0.6853814697901938	0.5990582180138729	0.3050328320299739
0.5608066496850925	0.1019045548370932	0.3051669034742888
0.1909641396197173	0.5857170118879313	0.3158525226387322
0.0608971958080077	0.0829961328800640	0.3020302109172987
0.1823077886197887	0.2088356064135480	0.4155110020262879
0.1341771569781920	0.2415065555762996	0.2815787476397710
0.2335891451637231	0.3114431518882336	0.3313876008706225
0.1397502963283276	0.2659702641784228	0.4317714538124477
0.1697647326279624	0.0940963814621768	0.4066254012968874
0.2170528307213865	0.2104219219488092	0.4534921618179357
0.2095306136845466	0.1937026234903338	0.5720495863321924
0.2589650561343588	0.2394758010365787	0.6300334698066049
0.1609324757623030	0.2237778375808662	0.6571901958164376
0.1008604578692159	0.3569453989413813	0.6754042804811878
0.1245927692266549	0.2370593809767119	0.7380422090921974
0.1763359612934568	0.2547414116528129	0.8236367544484674
0.0973093509999207	0.2539161259044000	0.8334803854087893
0.2185476171245554	0.1779207462345249	0.6194738194384897
0.1160100172969808	0.2499168991565834	0.6852509350966173
0.1341303495522155	0.2092117622215081	0.8068741115840431

Initial state ha (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3087552346725613	0.9442595201746021	0.3122734888295914
0.3721030821024915	0.1855863983585027	0.3086679929199929
0.4370929796793233	0.4371815096274185	0.3041673794904139
0.4987077501817622	0.6853601202594547	0.3049337296470570
0.3738495998225995	0.6886901113623539	0.3063106896422497
0.8707602944006353	0.1680007145134451	0.3059050428681687
0.7503740098486753	0.1780486725636135	0.3053789737320912
0.9378609139310133	0.4230383364251253	0.3061146825577248
0.9997897109803759	0.6608724207384200	0.3078143508252408
0.3126420074630004	0.5997284576815275	0.3066029148394992
0.3743842204930837	0.3541578897958426	0.3044000752749474
0.4357119477779935	0.1033150299291235	0.3070209727725989
0.4978055161856356	0.8540393025618146	0.3060103323174707
0.3721116863466431	0.8560498663566078	0.3089998043464461
0.8721439487046228	0.3394263186450484	0.3060217888203910
0.7515856223736537	0.3488817951923880	0.3054420080991241
0.9361494185568214	0.0760962969113731	0.3058023503761268
0.9982750908964417	0.8363996402270903	0.3074028913853409
0.6849715748733067	0.0934128553075278	0.3050609200258051
0.6244489200100032	0.8538070296645277	0.3049050302325605
0.5606602318397649	0.6021715499062751	0.3047644373148591
0.4990656821189710	0.3533098902797461	0.3046732854020919
0.6239176002495074	0.3506065832784703	0.3048583192783944
0.1262168409137328	0.8341798817878804	0.3092268116358051
0.2461648620490586	0.8506963964863182	0.3113551375808217
0.0644627971374643	0.5751173636042743	0.3081510164851728
0.9998565904207403	0.3334780208638737	0.3045528528778936
0.6864176308792068	0.4398202590440401	0.3050812172547803
0.6252527710545126	0.6811709063947121	0.3049175564940356
0.5599902932018739	0.9352921179754212	0.3053051538843450
0.4981680236428368	0.1858997412394924	0.3052895068616016
0.6231984215033417	0.1852301541075256	0.3050024820379598
0.1279805981396050	0.6603510761510430	0.3118568845209042
0.2489706658105827	0.6784753790618713	0.3115121521878139
0.0616847049097521	0.9192301102727244	0.3061480982800214
0.9988573315512395	0.1631361127790014	0.3040597927523475
0.3087544280821871	0.1111122343841671	0.3149750213814460
0.4359732608316774	0.6041993083213795	0.3039989302057537
0.8096728005419749	0.0950517763809191	0.3056667841678979
0.9398502604811823	0.5829029247188585	0.3066915714179768
0.3131637908240460	0.4358651709295971	0.3026501053446159

0.4352338915898059	0.9370406130408593	0.3081643863613543
0.8127915615343083	0.4223190599235639	0.3058536210125007
0.9373703683546600	0.9159821949285647	0.3067926679581364
0.6841815739963092	0.9349023745553560	0.3049280375345869
0.5617638700182769	0.4354592734681558	0.3046007430883992
0.1838876256967032	0.9216946646491394	0.3099783594367393
0.0623811266340657	0.4104780383655774	0.3033361160179210
0.6853984985538428	0.5991747246562821	0.3050622675962660
0.5608274973850021	0.1019365317200456	0.3052343359363841
0.1909547590708099	0.5855709479841725	0.3158159064377399
0.0609031684354022	0.0832122838074144	0.3019268717994826
0.1823871104923631	0.2085444868736673	0.4154437192162446
0.1340721511946492	0.2415433554591105	0.2815958345581326
0.2335246974321038	0.3116429334545103	0.3312542707347089
0.1398053268540110	0.2654758362022390	0.4317449371927725
0.1699156888352251	0.0938454210260919	0.4063388347024949
0.2171533310138258	0.2100529454270079	0.4533975672163853
0.2096012893375786	0.1933444011706204	0.5722465220938786
0.2589825702129898	0.2396762002686480	0.6302149292203506
0.1609395522908725	0.2238091723669278	0.6572860581441677
0.1008681414248532	0.3570463799048002	0.6754170495131838
0.1245098598313513	0.2371282765234398	0.7380750923211982
0.1763206772344663	0.2548006017239838	0.8236164334385986
0.0973008609582790	0.2537977878349340	0.8335504872635052
0.2185895481795251	0.1779743767336057	0.6196989227239214
0.1159671380404372	0.2499880589871995	0.6852824236723680
0.1341071269143752	0.2092149596806679	0.8068937814392902

Transition state ha (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3094322271992982	0.9353800716465737	0.3124995655453099
0.3725847487223998	0.1779220085325191	0.3112210349848479
0.4358332473165670	0.4299153129613153	0.3081562542728741
0.4974476582139841	0.6782898382535890	0.3071232011119693
0.3720991229002764	0.6790273667848680	0.3090372598551057
0.8701867312322542	0.1745199966304173	0.3067218904270190

0.7499485782017052 0.1763245185148769 0.3062632903473172
0.9362497163409667 0.4328170253002059 0.3070094303293794
0.9981134861781911 0.6708979175363246 0.3081261751660067
0.3099842292071958 0.5899460728093429 0.3113824529363573
0.3729228046451943 0.3468693267018020 0.3104215886871526
0.4356523090580992 0.0951764962730745 0.3087496043395551
0.4972863124295492 0.8466641763301629 0.3073266721427582
0.3718342856013130 0.8464972966617061 0.3095981863468730
0.8704295060978499 0.3452949041385969 0.3067257670992017
0.7501587594407151 0.3467693578896757 0.3062570044058644
0.9359839588293012 0.0855373707491578 0.3069513577702422
0.9978735867845875 0.8472204081950405 0.3080662268789267
0.6844872881855643 0.0887405381430173 0.3061183868040932
0.6238564726123021 0.8485605954862088 0.3062192806363296
0.5594944081374298 0.5957962841141812 0.3065272677051110
0.4978691729845010 0.3464324377679761 0.3071691451894630
0.6226745470348033 0.3449946563308212 0.3061807841395148
0.1255927814257037 0.8450714631238163 0.3102422346960461
0.2458770327248261 0.8478252034416943 0.3121952256578235
0.0618909413919209 0.5861305144127194 0.3085519020139976
0.9982349286118021 0.3441907845095916 0.3067204799608603
0.6847329620095091 0.4353778494969609 0.3061082960153653
0.6239933515550118 0.6758185238603029 0.3062163515272131
0.5593970528082923 0.9289108023606831 0.3066299072074912
0.4977203084181436 0.1785703211297709 0.3073096864857561
0.6225549417896835 0.1795537763595212 0.3062038030323235
0.1258343968970587 0.6725726518865994 0.3107924612480294
0.2462823480052897 0.6751979089375431 0.3122564249452424
0.0614373275570551 0.9315434715578624 0.3081409006610643
0.9980872416301430 0.1737917683911042 0.3065746293317909
0.3102607387690872 0.0996858912905088 0.3152035418065362
0.4346801742239389 0.5961690706678747 0.3077707545322947
0.8099707051440991 0.0972218010865646 0.3064970948954560
0.9376867376869557 0.5925305414753006 0.3072083306773421
0.3108026062389616 0.4259586159300157 0.3132502955887058
0.4346404145478466 0.9289409998644005 0.3085173258657224
0.8104874730593625 0.4242691853385935 0.3065007324647676
0.9372589858768153 0.9258804377993062 0.3072441336928120
0.6837460095335346 0.9301932455180534 0.3060569729170896
0.5604303921322673 0.4291553680035481 0.3063862458408150
0.1853506326515481 0.9258227485460010 0.3111345155837164
0.0607137054741005 0.4221478712998861 0.3064426281768735
0.6839348273891267 0.5940587974264703 0.3060677731933240

0.5602595076025838	0.0955994270418967	0.3064836358546901
0.1864501918998612	0.5938358270352017	0.3122589043223414
0.0605503253699199	0.0953598540284601	0.3060339461358429
0.1974660454370529	0.2070290264276394	0.4613799021579422
0.1342585978241665	0.2578808921894527	0.2940702122210951
0.2369255673280638	0.2677797263301187	0.3380766548251856
0.1637536077885150	0.2957554827332318	0.4546731196592121
0.1840091366804992	0.0990136950069478	0.4445913334898284
0.2477371118488909	0.2339888157767029	0.4628994752344442
0.1969604529671442	0.1875301146277281	0.5549242175063477
0.2489549508400691	0.2279886060291864	0.6129803436482459
0.1553849279346433	0.2233160743232495	0.6489679490304066
0.1010584554238542	0.3630179783977438	0.6757885691821940
0.1271578592726039	0.2384223949021592	0.7350571194849214
0.1783887185656816	0.2597930705991741	0.8227841717349649
0.0994596125177631	0.2477413649435976	0.8317896633133863
0.2059145910844864	0.1749389984979418	0.6040245259351161
0.1151790623615842	0.2542453486859091	0.6833503669166968
0.1375247110147621	0.2106130126292356	0.8047640318305493

Transition state ha (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3095658930252382	0.9349619652527175	0.3126286571210598
0.3725798396616685	0.1775783932690617	0.3113687604785186
0.4357496613823535	0.4296440681528597	0.3086056334713204
0.4973536791256442	0.6780381162303627	0.3074270682653214
0.3720717720198585	0.6785110619394655	0.3095047753788329
0.8701354233674159	0.1749664135431792	0.3067824000831183
0.7500346142035743	0.1763978957157946	0.3062160309300270
0.9362637406314964	0.4333784868293311	0.3071676611791652
0.9980173698776317	0.6714172334674692	0.3083998057759020
0.3099480786562066	0.5895017764908195	0.3117532132377821
0.3728084851092363	0.3465218409182936	0.3107610686228946
0.4356446122354232	0.0947071003592104	0.3090483899589477
0.4972393934831048	0.8462121010011683	0.3075875962418221
0.3718843080377826	0.8461255560778689	0.3099294183079495

0.8703124253472262 0.3454024292119511 0.3067822620150721
0.7501933202477600 0.3464427427144186 0.3062096931074434
0.9360779534703046 0.0859453420866597 0.3071205387848274
0.9978551743846497 0.8477795231870819 0.3083599701197564
0.6843483142110616 0.0883919877873205 0.3060328687356743
0.6237925123998175 0.8482699648427402 0.3061489176839516
0.5594711210022530 0.5953663356347016 0.3066113601908081
0.4978033189499408 0.3460813718749018 0.3074435420453850
0.6225352033045485 0.3446947419523186 0.3061564672389887
0.1257131743872789 0.8455092426661071 0.3106354298116417
0.2459009935624186 0.8475758494984018 0.3125614770210006
0.0617322658656174 0.5866659228079468 0.3087797633393811
0.9982606639762718 0.3448053519190887 0.3069258791009999
0.6845307022909447 0.4352380494756029 0.3060345612195386
0.6238934116318088 0.6755417623602493 0.3061496565327315
0.5594044944530649 0.9286899580474932 0.3067037139246305
0.4977011819494936 0.1782128537356803 0.3075558620056308
0.6224502281664225 0.1792525989346660 0.3061773998327276
0.1258845844950015 0.6733610886278262 0.3109560848711148
0.2462004945053485 0.6751767119985848 0.3125252180078366
0.0614262682565207 0.9322557568634776 0.3085047842800690
0.9981716616039878 0.1742776533517219 0.3068021032658816
0.3103590328528635 0.0990626334353676 0.3150550271100639
0.4346641501843688 0.5956732152469482 0.3083993248553749
0.8099843496045540 0.0973790718879361 0.3065005668653942
0.9376095641580701 0.5928059305311231 0.3074722905633958
0.3106900267210170 0.4255694892677180 0.3135624715968815
0.4346466297986286 0.9286991943099855 0.3089353320131769
0.8103746776383159 0.4242405421141500 0.3064966367931550
0.9373144215742961 0.9265646660050020 0.3074764457102936
0.6836952346517665 0.9302278167944921 0.3059269995206493
0.5602916942077620 0.4289677622040062 0.3064880351697111
0.1855356297372515 0.9260255198967995 0.3117161971325142
0.0606432671996959 0.4231146036916451 0.3067489084286625
0.6838361321460504 0.5934957776266870 0.3059597283609237
0.5601792593408279 0.0951331514874500 0.3065790052606345
0.1863177946496245 0.5942774641109038 0.3123231124816274
0.0605586025693358 0.0957116091531863 0.3063823332536768
0.1979875855733321 0.2077718531071185 0.4633699022187199
0.1341066291312059 0.2590845790669811 0.2938244171842785
0.2370051365432737 0.2658889602901979 0.3375224281551790
0.1645057541368904 0.2965030383867039 0.4553381396917248
0.1845922521745142 0.1001146926091857 0.4459835275885099

0.2482857185528574	0.2352386759289135	0.4627292034853735
0.1970789806558861	0.1883927917744924	0.5528734360724460
0.2481126665615290	0.2265963246221279	0.6124328729511194
0.1554631976310178	0.2230620749520419	0.6468529796376271
0.1011120363997296	0.3634567855210417	0.6748730403250249
0.1271465459983163	0.2382131024586110	0.7332285929280021
0.1784876493629750	0.2603717698182575	0.8218923911442069
0.0998093978784717	0.2463544383083913	0.8311396921605936
0.2049565628836055	0.1750959081233324	0.6025098570049409
0.1151831155579231	0.2545044044415256	0.6819795299968348
0.1379063966537147	0.2095342246388421	0.8040744760242376

Transition state ha (n = -1)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3096634685598044	0.9348163146990276	0.3126691673621842
0.3725877026243688	0.1774521045798160	0.3114149364595870
0.4357172238195038	0.4295655372290269	0.3088450381620903
0.4972727824841798	0.6779418886753118	0.3076193290814947
0.3720830026140151	0.6782278039557706	0.3097542193534082
0.8700846617568866	0.1752663953097679	0.3068677641879550
0.7501095363236346	0.1764828155671824	0.3061930415836147
0.9362835549392727	0.4337137246318809	0.3073189436790439
0.9979429581236225	0.6716553995173548	0.3085952920685933
0.3099780469653560	0.5892827281215416	0.3119791843690394
0.3727769652563566	0.3463829617404053	0.3109443993633298
0.4356488817264226	0.0944147459959341	0.3091609509571616
0.4971962980125019	0.8459454451580350	0.3077202900133809
0.3719374896532289	0.8460177246926089	0.3100698482938122
0.8702228944542365	0.3454781818887189	0.3068642847109076
0.7502331851850590	0.3462272352684205	0.3061888376573078
0.9361355353095649	0.0861922836119073	0.3072812124424852
0.9978112325120621	0.8481441009239036	0.3085685591997819
0.6842196480527786	0.0881496597472923	0.3059985620356842
0.6237233747099719	0.8481072117742612	0.3061512439374821
0.5594530622408118	0.5950859981783326	0.3067273261993468
0.4977799718107485	0.3458941436090491	0.3076513983984923

0.6224167642685201	0.3445284960743674	0.3061893864660329
0.1258223980530588	0.8457408626790578	0.3108489065537615
0.2459293245404212	0.8475015296355696	0.3127374648396138
0.0616516600518556	0.5868887611778807	0.3089438464071366
0.9983256583973364	0.3452300250330134	0.3070902358546396
0.6843553560244009	0.4352025659049437	0.3060043072946996
0.6238002393506586	0.6753823995307991	0.3061549930509464
0.5593942655612877	0.9286154824586990	0.3067842496394586
0.4976925574765532	0.1780087579502000	0.3077221303505736
0.6223488770246854	0.1790607075383214	0.3061978644196690
0.1259652211176108	0.6738272760428536	0.3110691899901468
0.2461691233792425	0.6752248889704978	0.3126813213660617
0.0614053966390219	0.9327087463615870	0.3087452195485769
0.9982591976828595	0.1744813381463264	0.3069940229916195
0.3104512869351915	0.0987923523735775	0.3149310009241983
0.4346731402744461	0.5954109341963574	0.3086834280708300
0.8099783898311211	0.0975288536021014	0.3065201373355205
0.9376210969200244	0.5929205093840922	0.3076451821258530
0.3106909695676536	0.4254542662763200	0.3137710910624802
0.4346276051148552	0.9286322354643241	0.3090267224998428
0.8102873706531637	0.4242103204271547	0.3065175608088808
0.9373880279940759	0.9270205747034376	0.3076412721584562
0.6836188284508092	0.9303278971895070	0.3058747673622875
0.5601815528758862	0.4288792012457575	0.3066272785590114
0.1856607073398081	0.9260955372890581	0.3120223855434610
0.0605777108258056	0.4237286162993886	0.3068956117324094
0.6837405867609629	0.5930997868994743	0.3059022671991715
0.5601207843173081	0.0948371716093323	0.3066761010777506
0.1862951322330394	0.5946489544591055	0.3124122489440390
0.0605058407175817	0.0957953659111619	0.3065980317375924
0.1980164710739332	0.2079722775863595	0.4653889860018340
0.1340339580517505	0.2596018200088896	0.2931560840799656
0.2371389759666672	0.2648692407102067	0.3369363953144874
0.1649866908206205	0.2966863490441307	0.4552483738353355
0.1849002129029928	0.1014142306096352	0.4463723394088175
0.2482659361246413	0.2359605658764634	0.4621302105034981
0.1971246280503264	0.1886832489057343	0.5522415088391913
0.2478250289528149	0.2257168746251121	0.6125668189422038
0.1557406623707029	0.2226647487073546	0.6455960394311002
0.1011572787060633	0.3637641030474110	0.6742072391684122
0.1270062873171680	0.2381631275850219	0.7320839379464207
0.1785907979935094	0.2605274018594117	0.8212209194707436
0.1000210630046531	0.2452802588315440	0.8306060431854464

0.2046110237822098	0.1748867685123021	0.6022480659496388
0.1150061766115112	0.2546022826386202	0.6810693139703505
0.1381550280966360	0.2090083955393875	0.8034537642344608

Transition state ha (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
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0.0000000000000000	8.5216999054000002	0.0000000000000000
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0.0000000000000000	0.0000000000000000	20.0000000000000000
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C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3093722417950094	0.9353977839480094	0.3126225908245437
--------------------	--------------------	--------------------

0.3725544051933337	0.1779318905939443	0.3112711022642886
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0.4358285418237185	0.4298936828771303	0.3081935595115702
--------------------	--------------------	--------------------

0.4974612965923998	0.6782776520074872	0.3071774451165497
--------------------	--------------------	--------------------

0.3720711839801218	0.6791365098242409	0.3091223132859799
--------------------	--------------------	--------------------

0.8702048308963126	0.1744390353227677	0.3067287643556955
--------------------	--------------------	--------------------

0.7499067322972820	0.1762446900594392	0.3062535882853819
--------------------	--------------------	--------------------

0.9362023962223348	0.4327646598804085	0.3070339971330203
--------------------	--------------------	--------------------

0.9980987914366671	0.6709145384044025	0.3081894375698480
--------------------	--------------------	--------------------

0.3099478204167109	0.5900381398834561	0.3113961783010026
--------------------	--------------------	--------------------

0.3729153754485565	0.3469179956043622	0.3103966837542914
--------------------	--------------------	--------------------

0.4356421052042020	0.0952754340908094	0.3088608656031477
--------------------	--------------------	--------------------

0.4972914443843765	0.8467275407425036	0.3074106721343816
--------------------	--------------------	--------------------

0.3717915012596296	0.8465036297620663	0.3097489307900648
--------------------	--------------------	--------------------

0.8704542544670232	0.3453669475845217	0.3067319725668387
--------------------	--------------------	--------------------

0.7501223623036875	0.3468693141304589	0.3062470734343736
--------------------	--------------------	--------------------

0.9359437814726187	0.0855831924324420	0.3069676475769129
--------------------	--------------------	--------------------

0.9978645859990012	0.8472164098375824	0.3081204360191461
--------------------	--------------------	--------------------

0.6845436286316972	0.0887983577029857	0.3060962949438704
--------------------	--------------------	--------------------

0.6238746136461246	0.8485698233780511	0.3061849073844199
--------------------	--------------------	--------------------

0.5594830456064472	0.5958729482730851	0.3065161379542103
--------------------	--------------------	--------------------

0.4978566075507299	0.3464862563586049	0.3071691749647043
--------------------	--------------------	--------------------

0.6226997306844290	0.3450258098927058	0.3061740648249958
--------------------	--------------------	--------------------

0.1255590284910979	0.8451486116993064	0.3103457278076883
--------------------	--------------------	--------------------

0.2458624118677210	0.8479066256988378	0.3123219930217789
--------------------	--------------------	--------------------

0.0619163491395941	0.5861849514082725	0.3086172215441481
--------------------	--------------------	--------------------

0.9982131857648276	0.3441762391164576	0.3067188425736199
--------------------	--------------------	--------------------

0.6847927623351687	0.4353514849682253	0.3060921223827041
--------------------	--------------------	--------------------

0.6240126388706255	0.6758378103900246	0.3061855522328087
--------------------	--------------------	--------------------

0.5593842600375675	0.9288745548768534	0.3066320615922113
--------------------	--------------------	--------------------

0.4976982974395602	0.1785860221396889	0.3073295508696198
0.6225794239971376	0.1795700901925790	0.3061972314832947
0.1257895272404061	0.6724522997701342	0.3108917741281445
0.2462739886020176	0.6751701616724685	0.3123390293988513
0.0614578530748980	0.9315169966507825	0.3081791702083980
0.9980667741153522	0.1738225355484720	0.3065562864753598
0.3102190478834259	0.0997723916148399	0.3152401809945227
0.4346542277817307	0.5962784207263117	0.3079128957350168
0.8099756801919344	0.0971615318958038	0.3065008517261565
0.9376599127282109	0.5926240211954368	0.3072745412655489
0.3107906878025538	0.4260330200510680	0.3131292130069284
0.4346254370565189	0.9288970319622568	0.3087839875976967
0.8104920438385244	0.4243348383169077	0.3064988636965118
0.9372338132201269	0.9258068484478419	0.3073136002614111
0.6837650323680442	0.9300855002190530	0.3060105799205584
0.5604635031058051	0.4291128964202546	0.3063864002472065
0.1853050302464201	0.9259114532296928	0.3112940729919527
0.0607099682053650	0.4220389126190429	0.3064792581074030
0.6839565581983631	0.5941920492453769	0.3060381396348800
0.5602838832728307	0.0956859532022363	0.3064978333911896
0.1864448580676791	0.5937165250762078	0.3123535863119375
0.0605642200644045	0.0954745009432793	0.3060341844140336
0.1976362503246990	0.2068262741573743	0.4609541530261654
0.1342689252073840	0.2579167341867993	0.2943244403849185
0.2367316514072750	0.2682839296716343	0.3379042155110019
0.1639819244209447	0.2956319415840319	0.4542828592073323
0.1842377316393018	0.0989926036186801	0.4439880825794215
0.2478663149606557	0.2337348526702228	0.4627819658028962
0.1969351809151278	0.1870524214256078	0.5551207922651494
0.2489481343637941	0.2278160259769901	0.6129579614542956
0.1551812862747761	0.2234272012188161	0.6491283850119904
0.1010642718627362	0.3631625547381090	0.6756416275576189
0.1271302316071897	0.2385165336507338	0.7349757825143461
0.1784003206829130	0.2600124134058975	0.8225046041621816
0.0995229958035225	0.2474318281916518	0.8315885591561157
0.2059268158168414	0.1746057567721467	0.6041399169828935
0.1150719039415800	0.2543670646811363	0.6833080250303889
0.1376098142858120	0.2102790596862034	0.8045958716123363

Transition state ha (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 17 1 1 10 3

Direct

0.3092843008047500 0.9356132569534994 0.3129233518339082
0.3724936446674488 0.1781282902766456 0.3113948870298558
0.4358403139892797 0.4300343575174422 0.3082178483162396
0.4974772020479095 0.6784213329641405 0.3073166052119344
0.3720704291223297 0.6794655210251477 0.3093068181007041
0.8701974789811072 0.1743381249971945 0.3067540052005992
0.7498475640911452 0.1762365491546757 0.3062362764827986
0.9361366244754141 0.4326616181681479 0.3071005255080854
0.9980631492383131 0.6708979454038216 0.3083204038120009
0.3099529140054163 0.5903889624822571 0.3114545733722648
0.3729350480421334 0.3471421854062691 0.3103638923430017
0.4356187606238141 0.0955428348458837 0.3090415850818247
0.4972884162935941 0.8469244762311342 0.3075954172722005
0.3717437079759646 0.8467317164828730 0.3100636912387629
0.8704677462399329 0.3454261038874378 0.3067663932935699
0.7500778887536923 0.3470050286882836 0.3062343275579612
0.9358627031885735 0.0855506903506614 0.3070166952426911
0.9978096298650363 0.8470931980601718 0.3082444527418216
0.6845865408143544 0.0889365587144118 0.3060576926504726
0.6238882542112423 0.8486683614928240 0.3061502691351305
0.5594860411892426 0.5960656207228964 0.3065562650349891
0.4978608758326332 0.3466677272451987 0.3072052338294107
0.6227220455054484 0.3451562063120114 0.3061778035316925
0.1255015458117202 0.8450929298561265 0.3105551291518833
0.2458405849594840 0.8480845941745584 0.3125864994460646
0.0619374411975258 0.5861452188399334 0.3087640331104992
0.9981717848456447 0.3440806875211931 0.3067573902431587
0.6848490680555245 0.4354150572634070 0.3060569848547494
0.6240332277487378 0.6759645264050083 0.3061515641582865
0.5593720692898391 0.9289656406764513 0.3067054715407658
0.4976730584403203 0.1787561566789349 0.3074156235021582
0.6225926734239065 0.1796760991287940 0.3062096968890640
0.1257441690037961 0.6722126170664886 0.3111173850570084
0.2463000983526271 0.6752663992275850 0.3125249099428692
0.0614337188907297 0.9313728925618359 0.3083004592140779
0.9980144904918172 0.1737809561771149 0.3065844828336497
0.3101218796584728 0.1001670752170624 0.3153881107784148
0.4346515263566626 0.5965644146557152 0.3080486256978254

0.8099546332689309	0.0971250851305073	0.3065052029349846
0.9376310771953698	0.5926471514872842	0.3073772008844737
0.3108221235992464	0.4263337907530816	0.3130133281793113
0.4346074853105047	0.9290509626348356	0.3090616990878373
0.8104910612324373	0.4244158708539849	0.3065133572127589
0.9371726828189506	0.9256869066623000	0.3074123926128110
0.6837845754476596	0.9300738281707911	0.3059180105898012
0.5605009761929926	0.4291943393970252	0.3064079174566657
0.1852014429598061	0.9259256561337764	0.3115498470373212
0.0606695324925990	0.4218644312487693	0.3065334191868271
0.6839930102519248	0.5944052732813553	0.3059625695040351
0.5603038351333373	0.0958673605531601	0.3065602906907766
0.1864862528950987	0.5935600656202132	0.3125676028523230
0.0605128284136899	0.0954131792675892	0.3060920864085397
0.1981439840964550	0.2063280978488722	0.4593601198157202
0.1341837750773281	0.2575599821527679	0.2945695761248499
0.2364084115988782	0.2696332912370977	0.3377422646562373
0.1643710659586250	0.2951692697174294	0.4536344998587318
0.1847106723262737	0.0983814160337358	0.4426251044448836
0.2482911686680831	0.2328321261094852	0.4626738182457641
0.1968852110683590	0.1857654973925781	0.5554218806996699
0.2489575112802317	0.2274498949204509	0.6129728708537867
0.1548667676841099	0.2233391537237145	0.6493550095794498
0.1010180723750772	0.3635437648111680	0.6754878937868237
0.1269030596913135	0.2386719506374722	0.7350286756565967
0.1784372662882883	0.2604291842176839	0.8219123159282925
0.0996141683030167	0.2466238341904613	0.8312763023920073
0.2060274405835770	0.1736094847584746	0.6043044129602846
0.1147652777280371	0.2545994698807471	0.6832397820184336
0.1377309769809009	0.2098926025721729	0.8042024590819041

Final state ha (n = 0)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O

36 17 1 1 10 3

Direct

0.3084249759535922	0.9445843905583970	0.3071323434674227
0.3715241160376124	0.1863354613733108	0.3068139985409815
0.4366542202126666	0.4376814560657962	0.3064205781075415
0.4982889902829086	0.6856070063694517	0.3060338157851064

0.3737102775630490 0.6888898863299246 0.3067754362817965
0.8700289202902596 0.1649703024178919 0.3063565958767356
0.7500077712747526 0.1773391823693444 0.3058129863809853
0.9384567819698546 0.4195137430998059 0.3066875656932737
0.0002368315065553 0.6557488914949801 0.3070248991117737
0.3127028755413761 0.6010287874311970 0.3071380303913429
0.3738020009810441 0.3550472061358647 0.3068183248020802
0.4350626297253228 0.1037215703928638 0.3063960116917954
0.4972801047518232 0.8544206423607719 0.3060080732556330
0.3718308145831841 0.8573037874186085 0.3067680344927979
0.8719931287067411 0.3355156557237677 0.3063458330135376
0.7516178970948459 0.3473352184561165 0.3058204279043650
0.9355523763837184 0.0716256119835350 0.3067523999071895
0.9979215472739966 0.8323905618463385 0.3070612297504667
0.6841136130718652 0.0929708156451383 0.3056350048402194
0.6239512046959135 0.8535348455714384 0.3055943185900958
0.5602443653375317 0.6018749689425746 0.3057700343962182
0.4986675469296102 0.3533987952598636 0.3060619061214425
0.6234718618134778 0.3505115683074536 0.3056625397095303
0.1258026881100207 0.8330451295534687 0.3074656734020493
0.2454841736751874 0.8516337821616062 0.3073565040346580
0.0651023733352289 0.5714037490526209 0.3073115873738459
0.9998034452950506 0.3290645293017178 0.3070522602853956
0.6859245790705586 0.4394805429217925 0.3056608458705412
0.6248970223459764 0.6809170149828319 0.3056113051991929
0.5594143767497570 0.9357295325123403 0.3057341115344698
0.4977085622287305 0.1861973254861624 0.3060415705886186
0.6225753811023012 0.1849823489275622 0.3056436186608238
0.1281589481303769 0.6598306943586962 0.3074685856588459
0.2483287426031353 0.6802030412750497 0.3073815889405438
0.0609106613751038 0.9158394837936328 0.3073475723809835
0.9976166833832281 0.1593716243953622 0.3070995922736657
0.3078475576102946 0.1104952106267874 0.3072047787241630
0.4356889706031453 0.6042955791065054 0.3064029518339311
0.8087992199068310 0.0930776344838975 0.3060739914363921
0.9401151545858326 0.5786672838505851 0.3066830845939563
0.3131155526814098 0.4385059076971913 0.3071827907185138
0.4345865242979414 0.9378878722108865 0.3063728415623288
0.8130239981414888 0.4196242482014156 0.3060667144937526
0.9369757011705886 0.9114484579409918 0.3067793911472521
0.6834420964652779 0.9350891477334287 0.3055790053619702
0.5612738867828924 0.4358116476132210 0.3057463910652984
0.1829835334796570 0.9236072012120502 0.3074969366951379

0.0638627784853441	0.4042314770517521	0.3073148482146166
0.6849605479330236	0.5983437506374401	0.3056080290816467
0.5602859148504891	0.1016119149303734	0.3057169995357469
0.1910676604572359	0.5859312553926088	0.3075464398772070
0.0598234730829290	0.0792341810663402	0.3073966978297875
0.1878734085669507	0.2094605217141137	0.4986048123227533
0.1302931208762388	0.2343382219121253	0.3073083602298468
0.2294093371973176	0.3005844036750176	0.3075624564101531
0.1530275796106721	0.2979065554447331	0.4935530097987666
0.1676597074318167	0.1069147031275932	0.4808306430515046
0.2306524662048801	0.2368060393227012	0.4718354482169929
0.2012275196909243	0.1957262189193472	0.5500224585099360
0.2597868135157668	0.2380976567660085	0.6421319811269797
0.1819521249747922	0.2036160837202559	0.6563552166495370
0.0990868634176678	0.3587147152913275	0.6866212313372628
0.1182678717505752	0.2400186727279774	0.7441917130273694
0.1761788685069661	0.2554111961861238	0.8393505445779041
0.0985192428173391	0.2592527788204322	0.8529268442867846
0.2225983950433417	0.1688227339596864	0.6293931199441545
0.1107402338701107	0.2492670531868342	0.6947706082299590
0.1332158126039147	0.2080329471929616	0.8258664737924519

Final state ha (n = -0.5)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	10	3

Direct

0.3084959657628480	0.9447931714149614	0.3071952615854890
0.3715419668123526	0.1863180246760921	0.3068825140364039
0.4366590824517526	0.4376741228566196	0.3064114653032966
0.4982077203514472	0.6855889225792599	0.3060075892797509
0.3736567631487083	0.6885686293256472	0.3067740104433168
0.8700349070661058	0.1650213139805675	0.3063815293380367
0.7501016334122017	0.1773356436190318	0.3058347248054668
0.9385594279237824	0.4195581174765809	0.3067231412574016
0.0003292030862345	0.6555475459071340	0.3070481540835255
0.3127018913122206	0.6007139519249037	0.3071697400806303
0.3737927020717116	0.3549737565969701	0.3068690641307306
0.4350712103953076	0.1036537742935783	0.3064214886664786
0.4972157304314287	0.8543729899781753	0.3059992672470960

0.3717872385064174 0.8575272713220503 0.3067849482148348
0.8719467160346721 0.3353991904015739 0.3063642256645310
0.7516829504857132 0.3473098650513105 0.3058301406816964
0.9356030191134855 0.0716346335169233 0.3067710201309965
0.9979879690551710 0.8326452491549425 0.3070722393907337
0.6840548978360449 0.0928923481456966 0.3056481281941373
0.6239333105701487 0.8535651312323518 0.3055888559064069
0.5601971557700114 0.6017864780846218 0.3057520106862824
0.4986555075406966 0.3534370343758860 0.3060282422393988
0.6233932815020096 0.3505124564110065 0.3056611661240674
0.1258471824510122 0.8332343675971652 0.3075127629889019
0.2454219303578706 0.8516983602952081 0.3074343154838881
0.0650481258324165 0.5711645682399727 0.3073392514045706
0.9998235694468475 0.3291950035434956 0.3070926591750821
0.6858544377820391 0.4395754879840131 0.3056682811452657
0.6248631323515876 0.6808336996644214 0.3056107216579289
0.5593650995035504 0.9357952128972031 0.3057280777588059
0.4976898507084453 0.1860375540032491 0.3060364924421328
0.6225051045408718 0.1849462525010424 0.3056550562119741
0.1282644249688135 0.6600717816332339 0.3075075368293421
0.2482756348498800 0.6802549082386400 0.3074336865229774
0.0609408463538542 0.9161151440339279 0.3073769346284076
0.9976693591861141 0.1593022277503846 0.3071250331929480
0.3078978059881759 0.1104258171077661 0.3072747192127482
0.4356177946913227 0.6043390944120842 0.3063722353859865
0.8087835291167464 0.0931228667236747 0.3060861527046526
0.9402155827170761 0.5785532526396475 0.3067211750724945
0.3130934386996707 0.4383400877213455 0.3072483613496835
0.4344856210711642 0.9377630456811460 0.3063623961846505
0.8130575208987542 0.4195263348282087 0.3060655098359109
0.9371045279378972 0.9114633718038873 0.3067810734150038
0.6833492604155311 0.9352236060701260 0.3055625016394317
0.5612103758335246 0.4357748213636147 0.3057080245434913
0.1830861352195507 0.9233812900305921 0.3075827082070500
0.0638854642640626 0.4044546390577759 0.3073477595085570
0.6848749358389763 0.5982230759393699 0.3055963279706168
0.5602598619433897 0.1015128755301918 0.3056982669475599
0.1909956871068791 0.5865834998350117 0.3076020266766513
0.0598097603357783 0.0794340854505239 0.3074364089653931
0.1879577016443918 0.2094570580624481 0.4983493941454004
0.1304515931793052 0.2344257923283983 0.3073396044061226
0.2293916091953312 0.3001338551766350 0.3075650856691314
0.1530492778576674 0.2978148780582542 0.4934977088659369

0.1676508210577325	0.1068835507809186	0.4807115620020980
0.2306000318429562	0.2368632345894103	0.4713869702461151
0.2015127896039818	0.1958153829118044	0.5497426521968362
0.2597564225415078	0.2379523788979214	0.6421915950571230
0.1818732060265315	0.2036814992745975	0.6561787567446489
0.0989987758348678	0.3586858886177415	0.6866645450207417
0.1182317698587739	0.2400408910536731	0.7442417314570997
0.1761578234416725	0.2553735336280247	0.8394640756970174
0.0985242671104294	0.2590112683452185	0.8531427246887587
0.2225176714599807	0.1691482563777028	0.6291450551425294
0.1108295532323462	0.2493302576497470	0.6948043718189160
0.1332048610602341	0.2080887453446883	0.8259508002887245

Final state ha (n = -1)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	17	1	1	10	3

Direct

0.3085441964153141	0.9449500283473568	0.3072123527620511
0.3715740022496244	0.1863022514223939	0.3068963582077116
0.4366493755938455	0.4377497103871790	0.3064086043219219
0.4980824446665794	0.6857150857802569	0.3059990681914803
0.3735622970125807	0.6883881149213137	0.3067785955136340
0.8700133860366182	0.1650424696878447	0.3063878416370358
0.7501640755933771	0.1773456079669770	0.3058386009488859
0.9386165210002955	0.4196856557242719	0.3067326659445042
0.0003822559165690	0.6554357205209627	0.3070559244363524
0.3127206281092524	0.6005966417243458	0.3071849484311692
0.3737961711835715	0.3550659789517830	0.3068821141282019
0.4351070194581800	0.1036177269849133	0.3064267907952818
0.4971706452704682	0.8542072526615749	0.3059946250984695
0.3717713465362119	0.8576930495001434	0.3067910525746018
0.8718833660210779	0.3353605340134669	0.3063705001940216
0.7517302168891771	0.3472932457685538	0.3058324849509315
0.9356279295863070	0.0715401949099960	0.3067766756987721
0.9980184076433297	0.8327914021428189	0.3070781323862713
0.6839964105896050	0.0927239185276185	0.3056496015952542
0.6239184398981378	0.8535741271476512	0.3055851498545198
0.5602556045045410	0.6016714515839964	0.3057434745646703
0.4986976465540137	0.3535417308712149	0.3060216869300920

0.6233148329670501	0.3504978100794079	0.3056574624362356
0.1259174327905977	0.8333753649767250	0.3075271526218419
0.2453845495020816	0.8517798680353355	0.3074553559677478
0.0649819451448189	0.5708864221052726	0.3073495748120387
0.9998484140397331	0.3293246817048492	0.3071030437793951
0.6857997188306640	0.4397399201840825	0.3056684447451526
0.6248384591659962	0.6807243127112149	0.3056055891395502
0.5593655981346732	0.9357630549341669	0.3057243551201550
0.4977051123669072	0.1857852878876111	0.3060348362643067
0.6224153895119729	0.1848583265621099	0.3056526305920351
0.1284022990420695	0.6601735134648145	0.3075190214828589
0.2482542595608643	0.6802796958994708	0.3074519465439320
0.0609390297132195	0.9163584463274203	0.3073865407647954
0.9977227282304092	0.1592164378336924	0.3071346630950819
0.3080378372855763	0.1104932819392080	0.3072945997648014
0.4356683910192445	0.6044490065159953	0.3063677183140561
0.8087592563924904	0.0931929490465896	0.3060927542285269
0.9402734793975474	0.5784546021720326	0.3067303924481561
0.3131432304405150	0.4381668510060456	0.3072730882996820
0.4343823392492212	0.9376213558007095	0.3063672235676305
0.8130812353398553	0.4194334313685934	0.3060709915804519
0.9371920131202652	0.9115084250383809	0.3067852476003618
0.6832860482193414	0.9352889649268127	0.3055636331917211
0.5610789204781539	0.4357489423108267	0.3057072205312829
0.1831603962103410	0.9231433428976547	0.3076065569970907
0.0638571429022092	0.4046349525362528	0.3073590568124899
0.6848536520149522	0.5980853005376244	0.3055963199245927
0.5602217058075417	0.1014042266905773	0.3056986376379176
0.1909255750682637	0.5870870532453450	0.3076141571374419
0.0597534428378286	0.0794875015409710	0.3074464323787549
0.1879794355013337	0.2094624271391076	0.4982659538809036
0.1305702266834227	0.2345202361782297	0.3073424518684285
0.2293017891082669	0.2999026504862199	0.3075376436417944
0.1530536329931237	0.2978021647101057	0.4934779312168691
0.1676514445809352	0.1068578955489933	0.4806830628014125
0.2306021345560151	0.2368763616119191	0.4712891687306517
0.2015976954896634	0.1958537672439473	0.5496591159246218
0.2597479557796996	0.2379027462162406	0.6422036368011034
0.1818474842729940	0.2037206428819396	0.6561147970505266
0.0989736456951348	0.3586721319640340	0.6866831214430391
0.1182330170734422	0.2400537668887016	0.7442552105279747
0.1761549739996537	0.2553735025820328	0.8395009863852174
0.0985230640138195	0.2589344217937752	0.8532112369980871

0.2224904961097706 0.1692724783703930 0.6290489342665836
0.1108439849896790 0.2493398739754951 0.6948135314569875
0.1331966236399419 0.2080821285824099 0.8259833380599162

Final state ha (n = +0.25)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 17 1 1 10 3

Direct

0.3083827388170094 0.9444743646645978 0.3071582086794595
0.3715098653232387 0.1862906465186840 0.3068435980676750
0.4366575731748286 0.4376393311164565 0.3064179348170418
0.4982978784102047 0.6855621905522438 0.3060231281895393
0.3737022635934136 0.6889923643733032 0.3067770518004233
0.8700514403650631 0.1650004301047204 0.3063692499984425
0.7499738224613753 0.1773255724274467 0.3058254000418564
0.9384267511788268 0.4195039286595228 0.3067021871731854
0.0002274185003587 0.6558440019292492 0.3070349561570220
0.3126842321911582 0.6011168819066037 0.3071470619860165
0.3738067448819148 0.3550511048627045 0.3068373060877361
0.4350474269207611 0.1037466585718816 0.3064087255139862
0.4972851714832612 0.8544277507635020 0.3060074595041537
0.3718155786183549 0.8572405819476961 0.3067778560833850
0.8720222239225526 0.3356171414078499 0.3063513535884740
0.7515892329129639 0.3473798910440912 0.3058242527657694
0.9355344408049653 0.0716697397413692 0.3067588842806974
0.9979037413741697 0.8323210475839189 0.3070633922746193
0.6841375386964915 0.0930220953802368 0.3056429156062506
0.6239339055667340 0.8535340780865667 0.3055938674623472
0.5602458631879783 0.6019170515858255 0.3057667929429614
0.4986681227482246 0.3533698433203070 0.3060471901773548
0.6234997857387063 0.3504850862130243 0.3056634635412164
0.1257778550768073 0.8330374321085547 0.3074807952161390
0.2455267718963485 0.8516184754695535 0.3073891690345373
0.0651425550533649 0.5715148887719202 0.3073227144762861
0.9998144689095252 0.3289897144595672 0.3070698003816480
0.6859569045413174 0.4394472934222598 0.3056661823004115
0.6248855982844711 0.6809331944340523 0.3056165901803692
0.5594240113685512 0.9356543677800445 0.3057335415729653
0.4977012869916521 0.1861964849692548 0.3060435253102752

0.6226042803707407	0.1850030478093967	0.3056504034165403
0.1281137658267681	0.6597354722831926	0.3074819772749511
0.2483599950363060	0.6801351879391588	0.3073983146010055
0.0608963830802161	0.9157684232212000	0.3073607744129846
0.9976098387295135	0.1594433621790533	0.3071036429031432
0.3078085535380388	0.1106084670292092	0.3072272827397177
0.4356886047130721	0.6042783031234468	0.3063889376577552
0.8088205606230904	0.0930872622826969	0.3060739726160208
0.9400918468267357	0.5787014681841287	0.3067007456803933
0.3131340191733121	0.4384827440783210	0.3071976697297632
0.4346129920025129	0.9378672285314369	0.3063599358774026
0.8130185505672777	0.4197112904193065	0.3060596351045298
0.9369078489956379	0.9114561377625261	0.3067780792462804
0.6834757364537292	0.9350241986794872	0.3055666576224843
0.5612876974199423	0.4357837989519955	0.3057254413643480
0.1829419050553864	0.9236971303612841	0.3075284531458293
0.0638840661102954	0.4041348686473278	0.3073219488539154
0.6849900631158122	0.5984304344978991	0.3055983890171723
0.5602657239060391	0.1016674450866963	0.3057016964627352
0.1911002847208044	0.5856898382949837	0.3075739571445108
0.0598439860900696	0.0792451074356886	0.3074177048632145
0.1879150040475880	0.2094584161082789	0.4985145815170176
0.1302808263820607	0.2342583471810265	0.3073254061362763
0.2294324114342197	0.3006572451802433	0.3076188975031537
0.1530401585601683	0.2978508831437531	0.4935256828385196
0.1676544699730262	0.1069304488105793	0.4807713133803791
0.2306050492310995	0.2368333736880219	0.4716103247686924
0.2013307686737450	0.1957546650562703	0.5499173456649061
0.2597751674091511	0.2380504426507641	0.6421567029366904
0.1819247133201917	0.2036314716521531	0.6562983381241003
0.0990526693596345	0.3587017630673818	0.6866317184224248
0.1182447785508276	0.2400209324962998	0.7442135195403315
0.1761779870658950	0.2553978849180353	0.8393947255015028
0.0985275193738345	0.2591553662993954	0.8530012038855661
0.2225768944269822	0.1689247700287024	0.6293267323365832
0.1107830303392273	0.2493060573770479	0.6947827617132594
0.1332030625024685	0.2080755073665949	0.8258925887836780

Final state ha (n = +0.5)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O
36 17 1 1 10 3

Direct

0.3083395495355118	0.9443568841618436	0.3071824595726382
0.3715023773442498	0.1862620911153152	0.3068637606466993
0.4366666826650186	0.4375908381646565	0.3064161955983881
0.4983100123184960	0.6855458317872207	0.3060164781323010
0.3736887403083752	0.6890749386363387	0.3067802926950781
0.8700728340194027	0.1650044593850877	0.3063757597332141
0.7499410414284704	0.1773272875452738	0.3058325114200892
0.9383886965511005	0.4195066660736184	0.3067152895807994
0.0002141768881017	0.6559270755930771	0.3070456714194397
0.3126689816739725	0.6012089687873873	0.3071597510775913
0.3738121123756807	0.3550809251197268	0.3068505312942147
0.4350367384006315	0.1037965813008360	0.3064173583926025
0.4972949484995725	0.8544217167880932	0.3060040133781847
0.3717967152686471	0.8571939347651480	0.3067859651058559
0.8720522365178505	0.3357155326905371	0.3063585121354814
0.7515555445981621	0.3474392414300823	0.3058275686127165
0.9355086817374350	0.0716997548706182	0.3067643944457678
0.9978933268285548	0.8322544213197306	0.3070704795247438
0.6841673764393834	0.0930475871329333	0.3056468151994409
0.6239266780780489	0.8535411062400153	0.3055925344308495
0.5602655816071942	0.6019592413678330	0.3057596534265528
0.4986724762350747	0.3533646170376593	0.3060390305849178
0.6235335947420912	0.3504740288904240	0.3056633038988888
0.1257528116873937	0.8330173214801182	0.3074995851733351
0.2455597373351309	0.8516168099796179	0.3074150676527692
0.0651703272724515	0.5715962603697118	0.3073351513915807
0.9998076009193035	0.3289165876852331	0.3070821279069497
0.6859959025616240	0.4394332028657521	0.3056674685514295
0.6248832960900611	0.6809454771626596	0.3056146783657762
0.5594392634683855	0.9355858544281714	0.3057310601871469
0.4977034474332389	0.1861932867578320	0.3060418980891954
0.6226369228956223	0.1850193012672194	0.3056535896300072
0.1280711148430195	0.6596105592395571	0.3074989545172534
0.2483891680239491	0.6800741898141099	0.3074188887230158
0.0608872081691834	0.9156724395980360	0.3073745341426460
0.9975924509746411	0.1595045744064641	0.3071161254866975
0.3077759993630751	0.1107415189623683	0.3072554550009596
0.4357001816640362	0.6042905429841728	0.3063778407287285
0.8088301088232976	0.0930958282263463	0.3060795388973787
0.9400619967880189	0.5787510803161372	0.3067141174160264

0.3131500083799483	0.43844425556643166	0.3072092458773770
0.4346323581753523	0.9378272073523621	0.3063565089135232
0.8130132135716506	0.4197945781869261	0.3060600292369254
0.9368461405323358	0.9114501678082512	0.3067795482063286
0.6835193286981911	0.9349506682759233	0.3055634962210866
0.5613123546780254	0.4357319712910925	0.3057070523068469
0.1829000870961386	0.9237588366045630	0.3075565341885133
0.0638956963227998	0.4039993269965327	0.3073326446520182
0.6850299847274108	0.5985127318289697	0.3055941808686040
0.5602583598274368	0.1017270108761910	0.3056918207066335
0.1911209871293689	0.5854422252564786	0.3075988832889270
0.0598706201389204	0.0792655979721784	0.3074364375965841
0.1879453918242414	0.2094588351857236	0.4984237459755215
0.1302323176512832	0.2342087688170428	0.3073453685109913
0.2294337099529496	0.3007566313445735	0.3076819970753894
0.1530497229453139	0.2978212839927136	0.4934901434118778
0.1676544955040171	0.1069321132315592	0.4807099212760969
0.2305506241864576	0.2368550345799787	0.4713822474661688
0.2014377357077090	0.1957847172857239	0.5498003169508905
0.2597669806285147	0.2380082509087193	0.6421778540339288
0.1819025679300446	0.2036585769551804	0.6562435326966287
0.0990206661999840	0.3586871900427981	0.6866431090847022
0.1182328029414429	0.2400375241531431	0.7442331171720875
0.1761740310397585	0.2553814225207436	0.8394363761642962
0.0985260033684347	0.2590701824012168	0.8530809070157065
0.2225618217480416	0.1690124477891170	0.6292676185677450
0.1108089918173280	0.2493386353922954	0.6947979520155133
0.1332007809034547	0.2081076675387082	0.8259170163517452

3. HER

3.1: Step a_i ($\ast \rightarrow H$)

Initial state a_i ($n = 0$)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3079784253393700 0.9297570477919720 0.3040212507853476

0.3706836270242284 0.1731509338435758 0.3033387238102033

0.4335999892321702 0.4248694264446700 0.3043116569301768

0.4952755569634739 0.6733299019363060 0.3051503275070561
0.3701599807062376 0.6737308001963539 0.3048362466818047
0.8679173294594112 0.1722270843167575 0.3052512929851040
0.7478486249316423 0.1725192042240733 0.3052450135492596
0.9338369814994728 0.4310606479230317 0.3055440796021539
0.9958707653208650 0.6691879857816192 0.3051996230688183
0.3080386257094834 0.5855604595243333 0.3035047537218919
0.3707218651931805 0.3422036110943576 0.3030097511547929
0.4335787460433245 0.0904175290122114 0.3044841570921874
0.4952661092581176 0.8418855292255247 0.3052090735163793
0.3701341048430705 0.8415953402806123 0.3050004249430029
0.8679293831651254 0.3424769661463789 0.3052442792995100
0.7478626747528541 0.3424389784252515 0.3052406482196242
0.9338176599773284 0.0835698259039230 0.3055586586732350
0.9958538873838186 0.8454154971577322 0.3052113689029988
0.6822424868514102 0.0842869428346651 0.3053283038676927
0.6217771533105974 0.8439336928721487 0.3053638612486687
0.5573282886631555 0.5908312649846835 0.3053022782393422
0.4958156907141984 0.3413318835972913 0.3049026736537971
0.6203851166034376 0.3402955323448859 0.3053593790933300
0.1238897421054771 0.8434752069398376 0.3053624449788435
0.2441372487567094 0.8433470882725108 0.3042046907003561
0.0594032834949459 0.5847231289431822 0.3061314219538786
0.9956844859540488 0.3425342688922418 0.3066807494975843
0.6822631100571247 0.4307800622139478 0.3053279174758965
0.6217903349276456 0.6711585604058309 0.3053659344326738
0.5573124755737513 0.9243188186198512 0.3053244372883042
0.4957972057549133 0.1738821658406645 0.3049268712143628
0.6203718481245025 0.1748144541177533 0.3053604388187950
0.1239247012625042 0.6711853240107729 0.3052418596188387
0.2441676811858453 0.6717953713722959 0.3039450889289887
0.0593754458702497 0.9298507770013414 0.3061979319015773
0.9956767404946276 0.1720791142913024 0.3067050142498857
0.3085030460329776 0.0930557379247787 0.3021831249988731
0.4326934145090617 0.5909402994761056 0.3047327856103580
0.8078714929810239 0.0939018884713633 0.3051973659468363
0.9352537370878520 0.5905176442503453 0.3051324442615836
0.3086092529104751 0.4224528294390776 0.3010684950773524
0.4326627116504952 0.9243337957745053 0.3049789959702421
0.8079137652239357 0.4209214109437407 0.3051827113009037
0.9352292524205116 0.9240893407586940 0.3051310974320586
0.6815913623623269 0.9259005400123336 0.3053583751497080
0.5581816970373785 0.4245190591760744 0.3053346860044718

0.1840420372297963	0.9234107249533788	0.3049747054143559
0.0580834430401066	0.4214903614927750	0.3082134032143926
0.6816160675244475	0.5891772966411797	0.3053616293604155
0.5581791280600611	0.0906384051904651	0.3053487075544932
0.1841260899938442	0.5914810106444172	0.3045794238232876
0.0580682191506559	0.0931287887711384	0.3082676244184985
0.1284969532947221	0.2573093070815283	0.3267953234183722
0.2325155471732418	0.2578365714985716	0.2942308396204226
0.2590471377204495	0.2855351445085990	0.4016626792578615
0.3115812144779277	0.2199448801170226	0.4562414774847908
0.2227355014245744	0.2743261195418162	0.4906929940417675
0.1493698857917091	0.1732827087509934	0.5070765396802859
0.1854896391291466	0.2543524308847227	0.5737884040524923
0.2334945788624613	0.1908753042119100	0.6596006893516234
0.1544423544264830	0.2018353381371040	0.6668229451573687
0.2758275821919132	0.2983540267483054	0.4498488631306117
0.1760869934278354	0.2640650355893357	0.5216089735760107
0.1937118943562393	0.2506581462258057	0.6453702800842213

Initial state ai (n = -0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	16	1	1	7	3

Direct

0.3080060580152809	0.9298867434910461	0.3040038847424676
0.3706796680464753	0.1731618166321162	0.3032869637980752
0.4336069959567607	0.4249231435931645	0.3042561711500817
0.4952726640570611	0.6733499245850172	0.3051131208299357
0.3701737571042548	0.6736437767063038	0.3048070353194467
0.8679066848575581	0.1722432746627695	0.3052764632617359
0.7479243802420380	0.1725154157000956	0.3052534134211154
0.9338724947154151	0.4311766115605329	0.3055844707954056
0.9958718599142691	0.6691473176695396	0.3052389748751435
0.3080673237749806	0.5854537484809815	0.3034914802467250
0.3707173157620531	0.3421923869114609	0.3029627173359934
0.4335900392240618	0.0903726661711705	0.3044369443337601
0.4952628923738461	0.8418861849160149	0.3051739325597446
0.3701477513431160	0.8417068713745127	0.3049715608370787
0.8679190788096044	0.3425117746439836	0.3052720809386897
0.7479403029086052	0.3424684183292342	0.3052485568147949

0.9338566526019911 0.0835322347088308 0.3055955385343739
0.9958548149580493 0.8455448695547333 0.3052497387880337
0.6822396662085429 0.0841968623698349 0.3053313465101957
0.6218039859454451 0.8439630025922967 0.3053546489003948
0.5573424833597943 0.5907805383347239 0.3052792104172680
0.4958304011255441 0.3413622011353113 0.3048596512587195
0.6203859914418326 0.3403060451724533 0.3053536745592951
0.1239588331792018 0.8435279741324548 0.3054178696625043
0.2441214872507189 0.8434012723997849 0.3042208339403045
0.0594205960546440 0.5846529698253772 0.3061564233891529
0.9957451058445083 0.3426505281526057 0.3067315013409610
0.6822611539353884 0.4308893111780331 0.3053286082250900
0.6218184480128839 0.6711349254425714 0.3053504580442146
0.5573266972515499 0.9243832700210636 0.3053020986752146
0.4958119826619646 0.1738633194461332 0.3048869618775917
0.6203716802497545 0.1748257981421201 0.3053540935325285
0.1239941266552312 0.6712047588478649 0.3052955270041846
0.2441511062394978 0.6717671477429846 0.3039551910741993
0.0593918301893826 0.9300060343166368 0.3062234297069661
0.9957379889474909 0.1720491163731823 0.3067560262175610
0.3085123022586391 0.0931088023158014 0.3021469254285911
0.4326928979659212 0.5909447085866714 0.3046922035197631
0.8078926793964105 0.0939691967174544 0.3052172130872652
0.9353185714679368 0.5905090108380450 0.3051821395473465
0.3086149839860589 0.4224150181097378 0.3010866346193625
0.4326611798657694 0.9243441528100306 0.3049372397511668
0.8079309350004257 0.4208956114581656 0.3052028893957830
0.9352949227333124 0.9241847756349054 0.3051765005584824
0.6815741642381644 0.9259851133237189 0.3053592560895039
0.5581722862853473 0.4245520072054305 0.3053184164918792
0.1840784782861049 0.9233472225301367 0.3049982716379461
0.0580876022370721 0.4215809273990370 0.3082384800619453
0.6816040431910169 0.5891048347947158 0.3053569712287751
0.5581743841254985 0.0906218932729343 0.3053324982932145
0.1841598396996357 0.5915999089504294 0.3045999075858066
0.0580745006189850 0.0931303395951040 0.3082868308508832
0.1285939808197992 0.2573719681440766 0.3267424185474765
0.2325782056189202 0.2578612670882010 0.2939885249174611
0.2591077650623609 0.2856736142335750 0.4018537484161903
0.3112361548071266 0.2192844792513242 0.4563491486214124
0.2221182089534574 0.2742150434675911 0.4909497510694113
0.1493238779805738 0.1724694227315051 0.5071229198009296
0.1853081007205051 0.2543500399381504 0.5736852600774648

0.2335783576273075 0.1908263684752453 0.6593559967062893
0.1546059576043886 0.2024135209489828 0.6668834187673602
0.2758381389631756 0.2983740934675198 0.4498599966242135
0.1757719495117431 0.2636345224729374 0.5215714085648541
0.1938526077555034 0.2509044549215880 0.6453026388203037

Initial state ai (n = -0.5)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 16 1 1 7 3

Direct

0.3080454984603395 0.9299738170547284 0.3039868733633033
0.3707002443464719 0.1731722637291334 0.3032855705157321
0.4336117525175168 0.4249481630011649 0.3042395528781728
0.4952417616141263 0.6733840128202518 0.3050944341361329
0.3701746655168408 0.6735670291757609 0.3047799530421879
0.8678864138008132 0.1722716940152771 0.3052805507319410
0.7479502084089072 0.1725301546282152 0.3052512590617477
0.9338871185519710 0.4312283382682383 0.3055949250371505
0.9958510427454871 0.6691313483377611 0.3052387928404116
0.3081042327376591 0.5853809072024186 0.3034793221474764
0.3707366817768737 0.3421913853759507 0.3029660611165436
0.4335951501046926 0.0903553510212774 0.3044212537120430
0.4952319124903204 0.8418584817715479 0.3051533723131681
0.3701492084436829 0.8417906015643130 0.3049456830056662
0.8678972612657887 0.3425138286279915 0.3052791165446760
0.7479647944322119 0.3424674073318891 0.3052477360953945
0.9338731129698145 0.0835131210841800 0.3056026555545450
0.9958343153185690 0.8455956317969903 0.3052491806870657
0.6822103562855800 0.0841382279509027 0.3053255626514300
0.6217865004574422 0.8439788739883496 0.3053431502822508
0.5573458145979471 0.5907474741170740 0.3052629573933579
0.4958491057043209 0.3413941320806579 0.3048349220024031
0.6203608035778890 0.3403246929389591 0.3053439887553004
0.1240244383536026 0.8435449472765616 0.3054493404619842
0.2441332177286563 0.8434219292937066 0.3042107477835714
0.0594250987266683 0.5845822574906334 0.3061660639572938
0.9958147105366850 0.3427465718657716 0.3067844506881107
0.6822307158205507 0.4309576614404257 0.3053247641938285
0.6218007364421693 0.6711276215481446 0.3053401184012583

0.5573304111886048	0.9244220290936013	0.3052849544389983
0.4958318958440385	0.1738375309771520	0.3048641629785956
0.6203471358083698	0.1748122390415160	0.3053443577847419
0.1240605151613073	0.6712206950150177	0.3053269538864015
0.2441616757803899	0.6717652084342257	0.3039472071599159
0.0593973559785046	0.9301096224500657	0.3062346762843184
0.9958084879613897	0.1719837746114515	0.3068055230946076
0.3085373414906709	0.0931560778004218	0.3021408989923027
0.4326935460159497	0.5909623071730150	0.3046717366012529
0.8078886394616994	0.0940264032604502	0.3052184863335657
0.9353701136706012	0.5904453740124304	0.3051893233290921
0.3086363176616781	0.4223760683860921	0.3011016376951899
0.4326619914869440	0.9243339219554075	0.3049155068953946
0.8079240097823076	0.4208606135010563	0.3052083769455280
0.9353469531405130	0.9242815678137296	0.3051790468581934
0.6815466762045006	0.9260340398873450	0.3053514299165917
0.5581492377607964	0.4245896560892618	0.3052952307173668
0.1841233019582926	0.9232448483155764	0.3049546188191165
0.0580474290787844	0.4216963228755920	0.3082866280290967
0.6815759887180735	0.5890641014838270	0.3053514690482874
0.5581514477638785	0.0905889500336780	0.3053130797531694
0.1842007324163745	0.5917294101115481	0.3045582848538023
0.0580350151777639	0.0930472420812456	0.3083321869726499
0.1287300864505226	0.2573845241461581	0.3266948161610263
0.2326184220232387	0.2578598434881658	0.2938137750997264
0.2592115480875800	0.2857623201230210	0.4019990350418358
0.3111256356083527	0.2189531311013391	0.4564286534671391
0.2217894554248115	0.2741693802589179	0.4911245842555343
0.1492870514774344	0.1720594908737232	0.5071553924519658
0.1852131196668308	0.2543098087416508	0.5737604979955458
0.2336212770328771	0.1908483955653318	0.6592145556052176
0.1546687876156462	0.2027095522542403	0.6669006397599478
0.2758642229357454	0.2983662364800168	0.4499161224011476
0.1755836631144212	0.2634905814405733	0.5215965949527287
0.1938850133174652	0.2510153783248462	0.6452154080658944

Initial state ai (n = -0.75)

1.0000000000000000		
19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
C	N	Fe
36	16	1
		1
		7
		3

Direct

0.3081004571166267	0.9300032865967447	0.3039888149485295
0.3707471089299966	0.1731783398523291	0.3033270051466750
0.4336165106971223	0.4249799221200038	0.3042564853995136
0.4952006474081429	0.6734316110708294	0.3050924315252238
0.3701850455448790	0.6735201045172807	0.3047642830580339
0.8678660638050683	0.1723326654065058	0.3052715068498710
0.7479399938240338	0.1725882987106687	0.3052366629673151
0.9338947662025573	0.4312066086627098	0.3055809198742996
0.9958344541491160	0.6691169346766159	0.3052210730591934
0.3081526772701050	0.5853506978576583	0.3034841939722036
0.3707810624234609	0.3422030247956080	0.3030115455367882
0.4335985598596154	0.0903340111116757	0.3044231530808288
0.4951937350780203	0.8418096214751747	0.3051462697453111
0.3701621807346409	0.8418320405432069	0.3049246710337508
0.8678765605475144	0.3424653622097065	0.3052635240600409
0.7479526464237420	0.3424162594970155	0.3052311415948209
0.9338797745674471	0.0835266849635374	0.3055969350713530
0.9958202141694847	0.8455880868163839	0.3052347886206191
0.6821595655088877	0.0841284208678537	0.3053084056276824
0.6217374882364353	0.8439926558149051	0.3053330952247744
0.5573519675580011	0.5907221137269184	0.3052558612719333
0.4958853901638560	0.3413953531281367	0.3048328787976515
0.6203243293510159	0.3403387206397573	0.3053286220739835
0.1240740697450140	0.8434961514635120	0.3054567031749633
0.2441667365761983	0.8433949980594001	0.3041917187098864
0.0594084309687415	0.5845403610245254	0.3061661143466162
0.9958632735480532	0.3428220997702867	0.3068117541508403
0.6821766125580301	0.4309727506030950	0.3053064070800141
0.6217491103594309	0.6711306353942575	0.3053341365584871
0.5573375670446451	0.9244543911994378	0.3052759201575461
0.4958695124847155	0.1738460975698506	0.3048566842921661
0.6203127838925172	0.1747993063955991	0.3053291371128333
0.1241080276778721	0.6712692909139468	0.3053387695639573
0.2441933422891288	0.6718098397743729	0.3039358278394558
0.0593833560397810	0.9301335464073976	0.3062332099578864
0.9958558988383870	0.1718962007359479	0.3068353729098739
0.3085804382024215	0.0931767300301341	0.3021840456468659
0.4327132978265630	0.5909409880979261	0.3046741031463663
0.8078688170139612	0.0940641312721125	0.3052069019622896
0.9353978480942415	0.5903674181791165	0.3051636580759964
0.3086721487789963	0.4223478352098887	0.3011295214671244
0.4326832736287784	0.9243597995159962	0.3048960956204738

0.8079029560925107	0.4208298740433127	0.3051905911295236
0.9353769980370419	0.9243452307278149	0.3051646882617094
0.6815194378656610	0.9260637179397800	0.3053396639279406
0.5581200403005310	0.4246552573220043	0.3052852825826997
0.1841636254603090	0.9231394176001402	0.3049086181488458
0.0579863076175351	0.4218115302619221	0.3083048853725856
0.6815416956962741	0.5890431867906809	0.3053390069239441
0.5581195053837275	0.0905317876068037	0.3052955740805852
0.1842385038300876	0.5918438027356240	0.3045203482562528
0.0579706497121224	0.0929098452141047	0.3083561944704937
0.1288377682048465	0.2573471593120096	0.3267650000813021
0.2326976148681470	0.2577948910128788	0.2936876241587744
0.2592062873987756	0.2857587450778418	0.4020559728108312
0.3111252731359267	0.2189626734472852	0.4564980263968192
0.2218874927883391	0.2742194033879868	0.4910689309781657
0.1493020930744862	0.1720928750681974	0.5071744736693343
0.1852077848010517	0.2542959572729922	0.5739369683447566
0.2335664073373233	0.1909812964806421	0.6591897715107239
0.1545709418758832	0.2025491579721022	0.6669007381389417
0.2757811932719463	0.2983048048793063	0.4499889061340674
0.1755834992283202	0.2636194503213490	0.5216312067980606
0.1937595548818644	0.2509711128471588	0.6451353895096389

Initial state ai (n = +0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	16	1	1	7	3

Direct

0.3079662049691665	0.9296945087248146	0.3040116451912249
0.3707048807055473	0.1731358190981954	0.3033304144639086
0.4336193011238690	0.4248314114204979	0.3043007595102210
0.4953056706011357	0.6733142533903574	0.3051274973901770
0.3701609773666475	0.6738238850547013	0.3048231049571692
0.8679486668786538	0.1721887518600862	0.3052648134950870
0.7478199331596225	0.1724956372138861	0.3052424094039580
0.9338213887292908	0.4310701838227809	0.3055578903870200
0.9958652046762317	0.6693151706843238	0.3052238247891870
0.3080241152905041	0.5856362743354102	0.3034988084618730
0.3707417738323174	0.3422276066057593	0.3030015723393024
0.4335966733641455	0.0904643769342379	0.3044700666611989

0.4952943848073731 0.8419095288158918 0.3051854424963934
0.3701348609097594 0.8415087124053185 0.3049849775970469
0.8679578893473840 0.3425442116099370 0.3052574829803699
0.7478316968117711 0.3424815402938242 0.3052379615122426
0.9338026704467872 0.0835979586943977 0.3055725779739354
0.9958480328448306 0.8453282384279581 0.3052350416488628
0.6822953865150374 0.0843328573595278 0.3053199912907750
0.6218124124602584 0.8439248412924047 0.3053521646641150
0.5573439527173553 0.5908895496606591 0.3052872302411969
0.4958245359755230 0.3413318002143967 0.3048873028699350
0.6204133493558476 0.3403056754259609 0.3053478716165806
0.1238804588821701 0.8435468126565129 0.3053752688983651
0.2441739736527020 0.8433660186477244 0.3042050578173315
0.0594364210134156 0.5847988845859794 0.3061661132139657
0.9956932711983582 0.3424874407322773 0.3066970858928844
0.6823162582965214 0.4307468624658469 0.3053196937019290
0.6218259104409629 0.6711828248959496 0.3053545928890632
0.5573307329854268 0.9242731316822597 0.3053084024969940
0.4958081169481334 0.1738930739278250 0.3049099866296298
0.6204016383589086 0.1748185323649054 0.3053488870423808
0.1239158866454434 0.6711496965016187 0.3052547472344022
0.2442043365579500 0.6717908706843133 0.3039467783734182
0.0594129008431663 0.9298122894362190 0.3062325753482336
0.9956870968551165 0.1721632538682441 0.3067222079123907
0.3085069703640770 0.0930529686771407 0.3021535056144524
0.4327139579847369 0.5909908184581292 0.3047043977764703
0.8078887933643480 0.0938776140454601 0.3052029912198735
0.9352362376338682 0.5905596775949139 0.3051510773829800
0.3086155288909642 0.4224641187972471 0.3010333466725048
0.4326877814319683 0.9242911817169862 0.3049509230856147
0.8079300444135418 0.4209690021783056 0.3051877888627307
0.9352133646588262 0.9240804871166099 0.3051505787344643
0.6816401743490189 0.9258308035650428 0.3053507711725663
0.5582229193521374 0.4244956898564002 0.3053225858844903
0.1840492009076436 0.9235206778049767 0.3049663131607635
0.0581106424583120 0.4214832427576062 0.3082682366287610
0.6816618519798273 0.5892614506146027 0.3053546274019237
0.5582164192517628 0.0906730639564689 0.3053355793788352
0.1841287444360486 0.5913979647679197 0.3045730346335949
0.0580990660426462 0.0931806039877129 0.3083294765543589
0.1285033532622029 0.2573367362211005 0.3267693129278102
0.2324613407838068 0.2578588942997526 0.2943923093574288
0.2589373676758091 0.2856402946542306 0.4016371413043315

0.3113643247102879	0.2196171777917667	0.4563174877223046
0.2226630868032558	0.2743183952181078	0.4906141731601324
0.1493474247365009	0.1728535784780790	0.5071099501813249
0.1853647371576740	0.2543509412358452	0.5737327646933276
0.2335172361012730	0.1908777932082888	0.6594776626235758
0.1544859762171569	0.2020384364396810	0.6668655307430105
0.2757006966205404	0.2982618875885610	0.4499430187120758
0.1759128620808222	0.2639000624084690	0.5215747525540871
0.1937403067635657	0.2507885247655680	0.6453466244634666

Transition state ai (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3087395430887199	0.9304128664782993	0.3045610794070157
0.3714408370421438	0.1737729314151650	0.3034905256702061
0.4343801005935859	0.4254954902725885	0.3041551018602959
0.4960284243824518	0.6739386963992828	0.3048696222429896
0.3709659233626468	0.6743756621152883	0.3048490642806243
0.8685375681416971	0.1726070060085902	0.3053782754526893
0.7485276715534610	0.1730284309024270	0.3051859713873881
0.9344755555811659	0.4314504566679886	0.3057747767594705
0.9965902364943418	0.6693653915678510	0.3057275752151867
0.3088917949118937	0.5862182113857415	0.3037846798667871
0.3715207923186341	0.3428620014342769	0.3030156983539030
0.4343175131233821	0.0910399528343220	0.3043680362169070
0.4959909362024035	0.8425045182798101	0.3049363778379472
0.3708955170506130	0.8423143996598839	0.3050739622118002
0.8685736452550543	0.3428479493200385	0.3053632975861404
0.7485621486613994	0.3429483169855416	0.3051899755278029
0.9344214689369394	0.0837119778168258	0.3058372828868912
0.9965263584733890	0.8456728278498176	0.3057676236787756
0.6829174156261431	0.0847865936723053	0.3051894249897416
0.6225121505331330	0.8445104822512448	0.3051746672822304
0.5580893832436473	0.5913924576774718	0.3050384421087529
0.4965902064908860	0.3419407439604143	0.3046613040479400
0.6211000040588459	0.3409064959155543	0.3051500439342973
0.1246454807859720	0.8436460666792271	0.3064101995485657

0.2448764347098376	0.8438342953973006	0.3050372694772889
0.0600921431551455	0.5848490720528048	0.3068489176991207
0.9962908170066029	0.3428062832686081	0.3069592488152963
0.6829701229366449	0.4313943870517818	0.3051999539878167
0.6225459113112422	0.6716964073979099	0.3051778747609788
0.5580575152907272	0.9249233025681391	0.3050630131205239
0.4965577877437326	0.1744783051284173	0.3046790933004146
0.6210720085146377	0.1753588785429088	0.3051398996058552
0.1247266110215079	0.6713393018812965	0.3062259222814205
0.2449608405604096	0.6723374258943693	0.3046390987470176
0.0600061050946721	0.9300733547209461	0.3069689170380272
0.9962711887267446	0.1722603035585735	0.3070153597706309
0.3092775301832873	0.0935748932276397	0.3028564113517760
0.4334799868938575	0.5915560060598395	0.3045605640915525
0.8084984138395015	0.0943742275748249	0.3052585592341899
0.9359718041379210	0.5907697783791193	0.3054734099634544
0.3095269334171249	0.4233908257536712	0.3010813311066585
0.4334272772510985	0.9249774856271387	0.3048604654450600
0.8085896692427141	0.4213686593216011	0.3052510163113737
0.9358863115812710	0.9243291557748137	0.3055166891360130
0.6823014270626615	0.9264689080807926	0.3052870008017265
0.5589211295869774	0.4251296473289869	0.3051422383712321
0.1847462902438153	0.9235860090191395	0.3061750896578204
0.0586587145509441	0.4217337858336734	0.3087795958507513
0.6823568253590224	0.5897245374012385	0.3053130137643478
0.5588974255046750	0.0911880485442467	0.3051501715256251
0.1849764400475635	0.5918884797023622	0.3055832762666242
0.0586240685752415	0.0932265646232651	0.3088961101154197
0.1276228415134995	0.2572718459758363	0.3311999671812771
0.2332746787697744	0.2591282285948395	0.2994076756278474
0.2493478067586850	0.2761680097945742	0.3904458123478136
0.3032503161504465	0.2095236438612815	0.4548697772083372
0.2276949759923639	0.2750510594063229	0.4796744788773921
0.1436828556040268	0.1648602119591445	0.5089022872716669
0.1787583957824168	0.2539394978791805	0.5696768788835342
0.2344639095222618	0.1866308796402265	0.6608750156650203
0.1569337274094664	0.2038142931215958	0.6741356789824096
0.2699566742603139	0.2931468475440013	0.4469831934134518
0.1679450125083122	0.2611650862002577	0.5202841688239417
0.1949167228974602	0.2506805310903246	0.6499294997990503

Transition state ai (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3088245180150801 0.9305098574150090 0.3045403798206150
0.3714835949653749 0.1738161513563585 0.3033938942783190
0.4344262556798618 0.4255874274607793 0.3041072329062711
0.4960469426477745 0.6739976591566719 0.3048871297756638
0.3710313822086349 0.6743421765372642 0.3048372448048801
0.8685636338865560 0.1726019894303254 0.3053808553750098
0.7486094922055692 0.1730630048119327 0.3052067105022174
0.9345547666684432 0.4314342118460296 0.3057858334618979
0.9966370244846262 0.6693337528580402 0.3057000993971523
0.3089822751027769 0.5861998953050278 0.3037957911352090
0.3715703952547391 0.3428862877356789 0.3029589597938407
0.4343613179923064 0.0910331371130419 0.3043402825883854
0.4960150990677263 0.8425199938606863 0.3049659928308512
0.3709641747844530 0.8424237163494915 0.3050730218396016
0.8686011736483930 0.3427752987923981 0.3053663095182773
0.7486474380174057 0.3429286120316100 0.3052049042761599
0.9345035956945740 0.0837143398451960 0.3058268782358954
0.9965866751875108 0.8457502450803110 0.3057281474697760
0.6829198555547906 0.0848076021194554 0.3052063251596691
0.6225386967754417 0.8445614167273213 0.3051838574249588
0.5581186849446966 0.5913758666249619 0.3050764126675431
0.4966513012152975 0.3419846879479459 0.3046757716763040
0.6211163497160263 0.3409340679017485 0.3051851015850202
0.1247633147290363 0.8436596283227358 0.3065016686586612
0.2449188305294419 0.8438367884266778 0.3050944432423314
0.0601485086823193 0.5848518884559456 0.3069120093337256
0.9963986360833147 0.3428915661253757 0.3070754900627970
0.6829695301362498 0.4314206386430184 0.3052149270366931
0.6225704665484977 0.6717224174425681 0.3051913747728510
0.5580847760155985 0.9250248996222207 0.3051023271184954
0.4966108011949170 0.1745138472488746 0.3047050595619364
0.6210872284436618 0.1753859125868960 0.3051808380220291
0.1248390506425745 0.6714164223095049 0.3062884968568483
0.2450011813297150 0.6723871038997096 0.3046900035620412
0.0600690716406064 0.9301281330944251 0.3070367363599306
0.9963713565913807 0.1722004715145745 0.3071257605874256

0.3093451674680440	0.0935940441619984	0.3026660681784716
0.4335193930154348	0.5915588722041748	0.3044810532905160
0.8085351815027151	0.0943865313207105	0.3052379686599790
0.9360726067406605	0.5907061946859840	0.3054106074114380
0.3095993735190524	0.4234533719675917	0.3011020041318292
0.4334632444329001	0.9250613579274425	0.3048135230702826
0.8086370150462412	0.4212934523488563	0.3052185217086626
0.9359987932999806	0.9244101048510225	0.3054219866464598
0.6822852982633808	0.9265800303592484	0.3052423478343778
0.5589381432791459	0.4252220534489361	0.3051421577687881
0.1848396293688552	0.9235629119001312	0.3062557001794928
0.0586882727937138	0.4218755606296317	0.3089703254889069
0.6823412707940802	0.5896720147424823	0.3052562807582816
0.5589156343603588	0.0911802969234744	0.3051537944012297
0.1850630851181237	0.5919982098728981	0.3055992863186284
0.0586508868710166	0.0931502677936057	0.3090698173473622
0.1276616986644247	0.2573054103210274	0.3314122782812344
0.2333471480368270	0.2591699756800521	0.2993968922955658
0.2488649858224065	0.2756849569780813	0.3897382877153124
0.3027461660001679	0.2090767225179321	0.4547438590384156
0.2276495726568621	0.2751014222912130	0.4793564368454990
0.1431161960075154	0.1645640155220256	0.5090699323180939
0.1782871303971171	0.2537655368289078	0.5696719596140006
0.2343823833992166	0.1866503365751537	0.6607977249173812
0.1570243650445230	0.2039437638582146	0.6745523933816485
0.2697343575024385	0.2932791603191672	0.4467968948359584
0.1675699044768166	0.2606657680965853	0.5202855017657310
0.1947983484925497	0.2508032933337999	0.6500728566595941

Transition state ai (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3089138565386599	0.9306322034211617	0.3044910348819249
0.3715510876657624	0.1738587859795734	0.3033124487907854
0.4344798485516250	0.4256607865927234	0.3040739088662781
0.4960582054211567	0.6740729269756447	0.3048882132658191
0.3710856041989528	0.6743035407627296	0.3048093449461975

0.8685838237311716 0.1726294290248635 0.3053679778409598
0.7486758616136640 0.1730961837990478 0.3052048756406074
0.9346132277314345 0.4314892239218264 0.3057894084777751
0.9966623229553764 0.6693198962567442 0.3056818258933687
0.3090756563172694 0.5861676207049225 0.3037627784206689
0.3716399122353052 0.3429317275498053 0.3028899698938027
0.4344138170109101 0.0910470441909147 0.3043015784725827
0.4960261234563236 0.8425252424234447 0.3049684088911304
0.3710171317647885 0.8425535654310679 0.3050393001484401
0.8686227280136163 0.3427769961420724 0.3053566947350223
0.7487153705513417 0.3429437185267464 0.3052011413298848
0.9345620417905776 0.0836874564254215 0.3058228846623385
0.9966116773363206 0.8457898691579817 0.3057087104498721
0.6829283877385386 0.0847761364888115 0.3052134453606908
0.6225617745544467 0.8446082883844975 0.3051905906655396
0.5581675548083168 0.5913674556156647 0.3050855448587015
0.4967198136757104 0.3420532541644412 0.3046649295566790
0.6211311946465023 0.3409842376258451 0.3052032944911070
0.1248853330177128 0.8436780819429121 0.3065913024494403
0.2449797910054772 0.8438829518367391 0.3051024912750546
0.0602032058748878 0.5847764279698057 0.3069625746464984
0.9965184097695258 0.3430007768102636 0.3071827158586313
0.6829798065976620 0.4315152475593912 0.3052175772000360
0.6225948667736746 0.6717418743841448 0.3051949712669971
0.5581316582880818 0.9251064392312356 0.3051162810720378
0.4966779040489092 0.1745255899982616 0.3046955569977232
0.6211009761254186 0.1754038740025165 0.3052020321126787
0.1249639268153592 0.6714329212282616 0.3063681790612451
0.2450644072419803 0.6724166673573241 0.3046967780258621
0.0601214822860633 0.9302254135352531 0.3070961925340343
0.9964898360403547 0.1721201654555914 0.3072325199422078
0.3094329761965760 0.0936647588913290 0.3025477638204014
0.4335695980659994 0.5916111244658218 0.3044624037240551
0.8085700309124887 0.0944517962654860 0.3052303309633747
0.9361756489680236 0.5906348358723201 0.3053749416374948
0.3096921268774509 0.4234784940186880 0.3010192276255529
0.4335094021776777 0.9250940821772338 0.3047878811372287
0.8086747413790863 0.4212647317577795 0.3052107191271192
0.9361015946154754 0.9245088257682734 0.3053747652899950
0.6822958519245457 0.9266558252736131 0.3052378343815227
0.5589554097464278 0.4253039711825861 0.3051505038609434
0.1849345211591596 0.9234744123444653 0.3062757522228683
0.0586842974217520 0.4220112310060870 0.3090986934535461

0.6823546582737831	0.5896584464734325	0.3052474579595011
0.5589334261425195	0.0911735877375404	0.3051677842556124
0.1851634834428546	0.5921425741668078	0.3056018714748843
0.0586450861974573	0.0930392948154232	0.3092059454614711
0.1277382922085317	0.2572961189183705	0.3317052424830663
0.2334696000291620	0.2592468296221420	0.2994019297075560
0.2483126759476767	0.2752117208792139	0.3886950459453647
0.3023367993619854	0.2085229849010293	0.4546727530077427
0.2276853624183260	0.2751507779981882	0.4791261551215646
0.1425377546922467	0.1641147549473520	0.5092588834101329
0.1777453066200572	0.2534748520955606	0.5697236116893418
0.2343192166837214	0.1867180599873403	0.6607263951458671
0.1570764634888841	0.2041045895895637	0.6750062845714360
0.2696164307855201	0.2933480704599677	0.4468313219487111
0.1669265739304648	0.2603259770236157	0.5204001442831042
0.1946827175287746	0.2509218529174582	0.6502591126580874

Transition state ai (n = -0.75)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3089896102244046 0.9307494840934998 0.3044333823878716

0.3716150031917921 0.1738888236159012 0.3032468767837631

0.4345221069145432 0.4257361304006095 0.3040479004540476

0.4960561879232997 0.6741461882338990 0.3048851213738809

0.3711286273716222 0.6742767866766638 0.3047735197855457

0.8685890653980091 0.1726610597093584 0.3053603992880560

0.7487304438403062 0.1731330720253845 0.3052029891754108

0.9346567316561836 0.4315466706834816 0.3057887153136361

0.9966679566587090 0.6693107821869806 0.3056704989177544

0.3091565148046652 0.5861297085196254 0.3037062178540139

0.3717065377129424 0.3429747428834216 0.3028276206864666

0.4344541247384337 0.0910415624764592 0.3042715701040373

0.4960238953661978 0.8425182640316659 0.3049639627453001

0.3710582127659283 0.8426582683940781 0.3050019653756713

0.8686284445052089 0.3427805567271847 0.3053494145367064

0.7487707753847792 0.3429565897940254 0.3051985606165589

0.9346047655758192 0.0836584578653309 0.3058230647170050

0.9966157603876435 0.8458223476823753 0.3056993806444019
0.6829270137754401 0.0847373237030357 0.3052170091743301
0.6225778746434111 0.8446503522526770 0.3051957356214950
0.5582126431000812 0.5913523166646516 0.3050881590169199
0.4967855881240916 0.3421043635111238 0.3046527170376954
0.6211357128895484 0.3410314595370787 0.3052096389444928
0.1249908889223355 0.8436861897803700 0.3066377843688574
0.2450253469038688 0.8439238960742813 0.3050724022811281
0.0602364740466825 0.5846969629338752 0.3069896981519011
0.9966234964563774 0.3431080255632016 0.3072543552362010
0.6829793864311324 0.4316103919916282 0.3052196231625534
0.6226116637966240 0.6717584066155333 0.3051990071920637
0.5581759274179963 0.9251832855369222 0.3051190429695473
0.4967430597516840 0.1745401727023693 0.3046827920994914
0.6211050745897647 0.1754154258425449 0.3052091248041064
0.1250733405082327 0.6714476834568667 0.3064089698462263
0.2451137209618761 0.6724371312907489 0.3046630926118913
0.0601525443290180 0.9303186814344523 0.3071319047753514
0.9965938401900237 0.1720362374568007 0.3073084315451184
0.3095099270615297 0.0937296178691262 0.3024433532618576
0.4336189954221945 0.5916432985307194 0.3044474115017420
0.8085923895444136 0.0945194312347421 0.3052262458521584
0.9362569887129705 0.5905614101985314 0.3053565926906762
0.3097774934104430 0.4234980323302727 0.3009236656807464
0.4335560933833306 0.9251328247459345 0.3047642368516448
0.8086993811286345 0.4212394452821355 0.3052062941931869
0.9361813209820051 0.9246075004665069 0.3053559707124798
0.6823019590678695 0.9267265024187118 0.3052395644757956
0.5589632844311674 0.4253943422333777 0.3051501930391430
0.1850118033988681 0.9233784922691747 0.3062577708921369
0.0586654842655650 0.4221512362487840 0.3091796202633841
0.6823616250459794 0.5896439117318156 0.3052472504028638
0.5589408273968259 0.0911460966952511 0.3051678228070725
0.1852465525534424 0.5922788124245729 0.3055740603394245
0.0586244545098837 0.0929167805487005 0.3093005693853348
0.1278040029127847 0.2572798139505402 0.3320232690083447
0.2336126058833597 0.2593217163872364 0.2993935763602321
0.2478751669141013 0.2748066682553994 0.3877716424719941
0.3020272195422857 0.2080097843184127 0.4547206027505724
0.2277277196358516 0.2751239753385200 0.4790461234018927
0.1421031508637131 0.1636923228948604 0.5094374775313579
0.1772883663354639 0.2532067227294844 0.5698185562564205
0.2342735151416829 0.1868065677049862 0.6606554494713321

0.1571179419251713 0.2043060354336049 0.6753366368008931
0.2695564261944038 0.2933662807986371 0.4469925087838263
0.1663402509392114 0.2601059005351696 0.5205537422004268
0.1945987745961883 0.2510682156768263 0.6503904983569888

Transition state ai (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3087459816444686 0.9303477007857385 0.3044744548245119

0.3714791878738274 0.1737705436729711 0.3034175122825962

0.4344193834644337 0.4254602591899350 0.3041731298520374

0.4960736663749895 0.6739339236463289 0.3049127906617135

0.3709775619830538 0.6744609873277226 0.3048640392759237

0.8686020997601297 0.1725426561571878 0.3054088081741231

0.7485398330842212 0.1730069540581746 0.3052224407521564

0.9345041607797597 0.4314236306760146 0.3058267974451666

0.9966117492570716 0.6695451473932987 0.3057329484730037

0.3088916767164157 0.5863063826327672 0.3037972744639066

0.3715592854539988 0.3428727253682910 0.3030139312566436

0.4343547150394466 0.0911009099359734 0.3043842537329746

0.4960415237824002 0.8425279893835143 0.3049896172918750

0.3709142035159285 0.8422370706318731 0.3050739803487532

0.8686336555276462 0.3428574898155223 0.3053977838827541

0.7485725952451403 0.3429652995623337 0.3052196934889084

0.9344567760461673 0.0837856742239797 0.3058575443638719

0.9965662770689054 0.8456109347988963 0.3057549238373314

0.6829941508485499 0.0848604827547616 0.3052260081683060

0.6225695419677382 0.8445035576907223 0.3052014680911319

0.5581208273643543 0.5914606982018188 0.3051044625144394

0.4966277797962286 0.3419509313830505 0.3047312062544054

0.6211503777142519 0.3409161820932645 0.3052156251936928

0.1246849183476998 0.8437757526684387 0.3064536616183637

0.2449415432231281 0.8438667351247870 0.3050253309005086

0.0601639046729934 0.5850076319602522 0.3069592764980351

0.9963537688488091 0.3427817334032222 0.3071408517590647

0.6830428268562535 0.4313312283680262 0.3052295289899646

0.6226001661485685 0.6717474525942915 0.3052057213738386

0.5580928410762497	0.9248971245476506	0.3051332679646558
0.4965933393356829	0.1744980203576697	0.3047579008733980
0.6211250179428754	0.1753676257630697	0.3052148706269237
0.1247555637097491	0.6713756599640797	0.3062527160461596
0.2450198966488705	0.6723284908203114	0.3046549466076133
0.0600964500184982	0.9300573765423996	0.3070767554321842
0.9963300972775331	0.1723797285264894	0.3071870170229454
0.3092909621313183	0.0936094333621393	0.3025562105502577
0.4335081419551248	0.5916141922497056	0.3045035745144424
0.8085461261161944	0.0943163310029276	0.3052559011595623
0.9359868243455306	0.5907990285812782	0.3054153133919482
0.3095407218247178	0.4233641415781638	0.3010642627141988
0.4334629759400530	0.9249468604747948	0.3048232753172060
0.8086423130367172	0.4213621516448122	0.3052388463734064
0.9359222434785830	0.9243726245402523	0.3054149121837939
0.6823663018060885	0.9264325553506859	0.3052510087402114
0.5589905898493918	0.4251215950098888	0.3051776703153560
0.1848018844854549	0.9237690209655709	0.3061462476899651
0.0587291232327695	0.4218105547158222	0.3090324195328079
0.6824147367504297	0.5897859683985609	0.3052592091235007
0.5589615182716942	0.0912374168274710	0.3051942354297280
0.1850023591233035	0.5918227008161511	0.3055377784959581
0.0586983796494202	0.0933055479454581	0.3091344475029598
0.1278024554931235	0.2573833779240463	0.3308613174171510
0.2332165686596637	0.2591259379717397	0.2991333816094079
0.2492005059866567	0.2763417306513031	0.3910470988315163
0.3025679386622730	0.2087967789789006	0.4548221830643898
0.2267702211192826	0.2741009770711265	0.4799255934663298
0.1432935804393754	0.1648257499153553	0.5089156555159867
0.1789179554367803	0.2533967132257902	0.5697466271128000
0.2344097782456886	0.1871041400554619	0.6602452379005380
0.1569976889698527	0.2049888278465872	0.6738551270403560
0.2693398765083739	0.2925698828875556	0.4470161325956725
0.1681591166202700	0.2603256221899663	0.5202429343429503
0.1949007524803116	0.2513125794715986	0.6493611013133269

Final state ai (n = 0)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3086891713086337	0.9286442055138482	0.3017660187738085
0.3714194312840414	0.1721297318960573	0.3017984852666975
0.4340550224342034	0.4238005817150370	0.3038059382327583
0.4955228883982426	0.6723690780871425	0.3044971197609250
0.3704431490213004	0.6720081560499681	0.3033730103216044
0.8681332288177113	0.1723567238331172	0.3055361561083033
0.7483280503450180	0.1720345847122518	0.3054765001352552
0.9339771939947700	0.4317400982593710	0.3058637858604955
0.9961764070916718	0.6694423821775086	0.3054759536006509
0.3084712846765356	0.5842531956761058	0.3018020397400952
0.3712741441155835	0.3409902532133071	0.3018242259524045
0.4341509483730561	0.0893119500911263	0.3037507802417081
0.4955687145182512	0.8407781090651258	0.3044880333721794
0.3705315818613335	0.8408213224422780	0.3033473874368579
0.8680596527932402	0.3425614719104632	0.3055335651453043
0.7482616219919608	0.3418234302497099	0.3054678143656649
0.9340952977549551	0.0836050606293162	0.3058671796445617
0.9962693886253026	0.8460104992025635	0.3054950712726950
0.6825644332506732	0.0832550525096885	0.3054787511302747
0.6221971651072551	0.8430795176655637	0.3053459198011846
0.5577508357224807	0.5896946690002156	0.3050813214591469
0.4963140727236320	0.3403560972652994	0.3047327059571288
0.6206303068612570	0.3395049663254585	0.3054206511530660
0.1246245273882105	0.8439023723902302	0.3052510969480512
0.2447793161071616	0.8427070350194863	0.3027311953159594
0.0596497940896092	0.5849134811124364	0.3064905736282487
0.9958169200482909	0.3431717520809299	0.3070645003826322
0.6824841514216432	0.4302670801012646	0.3054592308784072
0.6221524428540626	0.6703347629779369	0.3053348949630949
0.5577898716819047	0.9235687779026970	0.3050801865754084
0.4963686619939954	0.1728274182274948	0.3047118317687555
0.6206713232889675	0.1738820766557959	0.3054282671474438
0.1245249986464780	0.6715188968621627	0.3052478918257095
0.2446374180530052	0.6709573614796865	0.3027750453659924
0.0598000403821222	0.9306460160698743	0.3065493701809381
0.9958860011052536	0.1722829489523889	0.3070928580968529
0.3094113873907858	0.0921533616717780	0.2986815707513888
0.4331099285508598	0.5898632858034231	0.3037618668198221
0.8082416115773906	0.0938162628693683	0.3054354220337774
0.9356126406179668	0.5908293151495092	0.3054189038038767
0.3091285294054802	0.4206219281104389	0.2985875649999096
0.4331718499422252	0.9231712086719258	0.3037323909204028

0.8080573048974204	0.4205680599985295	0.3054245543974048
0.9357395695478807	0.9245437106828454	0.3054370877112756
0.6819659203114711	0.9253921565450974	0.3054770581156131
0.5585623281475453	0.4239056563051022	0.3052622573482945
0.1848468811790920	0.9227322908939859	0.3037822546908586
0.0579871104757466	0.4222091880302340	0.3088721214596117
0.6818957693162709	0.5880754238417722	0.3054528467626469
0.5586105824877573	0.0893953422225510	0.3052619862893735
0.1845051145058553	0.5920155389416117	0.3038445602445209
0.0581177971544073	0.0934472165681108	0.3090086591513458
0.1255373757406595	0.2584063929270665	0.3345358343893280
0.2330351423984385	0.2555539462286754	0.3012040745201554
0.2180601940769444	0.2585275773225888	0.3802036191162720
0.3124655222373410	0.2250082490421787	0.4489031329701066
0.2524806369872615	0.2821465797235416	0.4933201671984681
0.1482022684276030	0.1632622192908097	0.5042058022455493
0.1732202089003355	0.2545565664609404	0.5677950940375266
0.2324687253957827	0.1928384542652005	0.6594827238857685
0.1557829806196913	0.2025955040634454	0.6770613068440622
0.3021006744751831	0.2961893935797097	0.4855468145990229
0.1667204228078192	0.2639656371958368	0.5183531491718338
0.1914400982930427	0.2539369542707877	0.6512780037115574

Final state ai (n = -0.25)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3087283287347926	0.9287502119386623	0.3018233906928336
0.3714441640039754	0.1721349621068236	0.3018421542293717
0.4340438835203022	0.4238562544873689	0.3038146799393214
0.4954807440997295	0.6724331749436213	0.3045074600018595
0.3704430805305427	0.6719878116703220	0.3033821459674013
0.8680917289152671	0.1723180617415860	0.3056068021679209
0.7483259727778053	0.1720424358728385	0.3054738243012244
0.9339696065953436	0.4317208129751646	0.3059452096507662
0.9961308016524687	0.6693609118264350	0.3055318573564625
0.3085146226884763	0.5841652775831011	0.3018044395026379
0.3712987819753890	0.3410326543307736	0.3018356157677168
0.4341406689179846	0.0893139908068173	0.3037831644487207

0.4955256575783265 0.8407817964927757 0.3045063650649680
0.3705325646765339 0.8408734105050769 0.3033801010845942
0.8680244164431945 0.3425371057400575 0.3056092459499596
0.7482673309576522 0.3418592713550621 0.3054770213183473
0.9340792630039728 0.0835261973384303 0.3059522810695269
0.9962200010404285 0.8459908793874290 0.3055568725945306
0.6825354038717680 0.0832419577979130 0.3054484747314023
0.6221853952922580 0.8431546751044687 0.3053173483955392
0.5577619684135291 0.5896901586641458 0.3050747154746531
0.4963534750935415 0.3403975396569516 0.3047420668383453
0.6206021341899746 0.3395661778395196 0.3054021668462070
0.1246761752751570 0.8438704258568539 0.3053032221615121
0.2447833154413891 0.8426981096892648 0.3027599112837548
0.0596413530688103 0.5848113569780923 0.3065228524564254
0.9958678859203123 0.3432184369691290 0.3071714406137367
0.6824616760171811 0.4303560714227467 0.3054503144107473
0.6221438206051696 0.6703448509263925 0.3053170279355610
0.5578017703869005 0.9236541833335818 0.3050682302785199
0.4964082002558802 0.1728693672766029 0.3047249645897868
0.6206405726206183 0.1739058443818807 0.3054026980509908
0.1245806292407282 0.6714865393893448 0.3052841367837162
0.2446430010001040 0.6709719464987609 0.3027741931924494
0.0597837333877933 0.9306548159827895 0.3065980308800794
0.9959306072710492 0.1721320387194064 0.3072058547921945
0.3094425492249562 0.0921336167671870 0.2988058913519730
0.4331329501664832 0.5898906657949506 0.3037816468399488
0.8082176594809317 0.0938454420367052 0.3054661574721367
0.9356448119173978 0.5907147376945977 0.3055102181370002
0.3091621279458395 0.4206723581670671 0.2986187018026880
0.4331969329815071 0.9232010602498494 0.3037830879764005
0.8080504295359972 0.4205294208386168 0.3054712412180686
0.9357644426367597 0.9245552442427717 0.3055331447334358
0.6819319750848318 0.9254488552522787 0.3054421398367632
0.5585366793367339 0.4240079555822131 0.3052530717847975
0.1848736142575264 0.9226143157577665 0.3038204797645502
0.0579174413122099 0.4222731040235749 0.3089411213773817
0.6818665306961358 0.5880999208192127 0.3054439640993230
0.5585827977058945 0.0893726473749983 0.3052475401152478
0.1845438103288455 0.5921005865323842 0.3038404148820886
0.0580385642988903 0.0932722045206916 0.3090992420996764
0.1256118160577215 0.2583414651280566 0.3344988015814434
0.2330538253854730 0.2555644762547428 0.3008218004602703
0.2188165170101386 0.2587935987843556 0.3797968437337119

0.3123760689769413	0.2229420103304258	0.4493929037462530
0.2520341392392128	0.2829469007203240	0.4926891990439128
0.1477658722149758	0.1633177555535312	0.5044888807373407
0.1733998974812216	0.2546999133507411	0.5677981353679394
0.2327256404203014	0.1921068201909747	0.6596314321443676
0.1559968181166689	0.2022818444514976	0.6768607723971856
0.3015116162172817	0.2979770674481644	0.4844606676752164
0.1664264398547462	0.2640174656109507	0.5184164074410993
0.1918633306500718	0.2538473669311407	0.6514619973560214

Final state ai (n = -0.5)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5216999054000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	N	Fe	Ru	H	O
36	16	1	1	7	3

Direct

0.3087204170712970	0.9288212905764915	0.3019254444339055
0.3714253316248692	0.1720840263085240	0.3019732090539608
0.4339977331643846	0.4238488626564941	0.3038315314391722
0.4954001612594730	0.6724452620447755	0.3044775732068228
0.3703985327123927	0.6719370532987381	0.3033905285751612
0.8680171422276352	0.1723148690523010	0.3055179928518375
0.7482842200061856	0.1720179563115390	0.3054374189382033
0.9339164652790389	0.4317649047619349	0.3058311341408917
0.9960415370066988	0.6693524219847475	0.3053942188671083
0.3085024290740676	0.5840496258749268	0.3019183512418778
0.3712802287165246	0.3410322396826838	0.3019711857386237
0.4340966852985601	0.0892652970127169	0.3037925569189982
0.4954456445646904	0.8407091368063223	0.3044753713660836
0.3704891231339814	0.8408686480170950	0.3033814724352415
0.8679466894307035	0.3425557661397072	0.3055210296730069
0.7482254357828998	0.3418494840906565	0.3054407592624078
0.9340302490242209	0.0835146828810426	0.3058370575745300
0.9961322327397562	0.8460364283775297	0.3054188458861042
0.6824728196526193	0.0831622194306290	0.3054270528957517
0.6221331986998992	0.8431519373291967	0.3052969859990158
0.5577345647036456	0.5896318130602981	0.3050447381019943
0.4963453669463882	0.3403886287664209	0.3047104487697408
0.6205282255707878	0.3395562923655796	0.3053767021539339
0.1246961752394885	0.8438879593206613	0.3052933806806855
0.2447501480532308	0.8426813630762245	0.3028021395120823

0.0595949703768532	0.5847626683273377	0.3064601488610171
0.9958926029727466	0.3433584399233530	0.3071423992915484
0.6823979723320620	0.4303823237522769	0.3054294062074762
0.6220919048797293	0.6702902038885803	0.3052960982396109
0.5577731645574038	0.9236515820340884	0.3050362697408429
0.4963983738930625	0.1728169173283722	0.3046890151977420
0.6205653871109100	0.1738552320859872	0.3053764391624988
0.1245947026742132	0.6714882767218060	0.3052810069133123
0.2446044366030113	0.6709604962013475	0.3028263439677895
0.0597393957498356	0.9307399446908644	0.3065319542115673
0.9959571941515349	0.1720279421369676	0.3071765785149050
0.3094421808963960	0.0920754063656373	0.2990851409233026
0.4331105977880748	0.5898823121861946	0.3037763874827253
0.8081650435823349	0.0938710540578226	0.3054121094859986
0.9356441680526414	0.5906762468519930	0.3053854276670757
0.3091564764443375	0.4206858604920526	0.2989007258293372
0.4331740716357143	0.9231507728173173	0.3037705417991178
0.8079897931485287	0.4204953892071324	0.3054157673838202
0.9357651339195380	0.9246309850423624	0.3054096935529250
0.6818609144564609	0.9254303047566679	0.3054274800571268
0.5584639176356627	0.4240271153283882	0.3052167200667118
0.1848738841424591	0.9225195003731370	0.3038424964116016
0.0577992710286024	0.4224203038283008	0.3089782801689731
0.6817961721231820	0.5880643502570736	0.3054263490930652
0.5585120729636744	0.0892896662979050	0.3052053160837281
0.1845371841364438	0.5921901675981126	0.3038821954987764
0.0579226307200451	0.0931554999309921	0.3091363319234249
0.1255850366310660	0.2583671135403033	0.3347051785409001
0.2330326821280984	0.2555442268348392	0.3005640613823503
0.2200237652679733	0.2585985353087550	0.3795240627822953
0.3126797817674272	0.2238906459487847	0.4494064902345169
0.2523912539979135	0.2825033205196725	0.4931797699842027
0.1480521058382649	0.1632331788228684	0.5043818648094729
0.1733439180001621	0.2547225253017795	0.5677942851711539
0.2325592640419685	0.1924826799649344	0.6595549013470180
0.1558722877637569	0.2023296330591970	0.6770123825281608
0.3018362016742254	0.2979621963720431	0.4848449388475342
0.1667330546466584	0.2638727595557163	0.5183536565174846
0.1916043072836680	0.2539445910617540	0.6514508404017678

Final state ai (n = -0.75)

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 16 1 1 7 3

Direct

0.3085633629508804 0.9287957331834933 0.3023896337409022
0.3712350722214443 0.1719606352927129 0.3023109656450694
0.4338998122359897 0.4238898701369045 0.3038428166825018
0.4952687328426184 0.6725105822005495 0.3044419553926940
0.3702928159437934 0.6720917504283106 0.3035849464780224
0.8678374749711281 0.1723033711326442 0.3053188201145586
0.7481359654823782 0.1719958360333480 0.3053053846536410
0.9337604849077332 0.4317817828894502 0.3056227566934975
0.9958137089562700 0.6693772136766214 0.3052017248062194
0.3083404750579059 0.5840016199472913 0.3023551438057877
0.3710923810695196 0.3410662232858691 0.3022874909895652
0.4340022376714135 0.0891259735730312 0.3038072837075493
0.4953139027684245 0.8405366856664580 0.3044389002875513
0.3703845240660346 0.8406224837893903 0.3035833833613101
0.8677651832102525 0.3425653151645242 0.3053205786845469
0.7480742769673732 0.3418021286417969 0.3053039502762933
0.9338779926741985 0.0835202840547820 0.3056300929289630
0.9959102854781106 0.8460481743851663 0.3052256029615260
0.6823057784768987 0.0830578387074993 0.3053282025410914
0.6219929462326107 0.8430979550248595 0.3052044722260931
0.5576210383542956 0.5895954586093980 0.3049505483414149
0.4961714096775710 0.3404719323918295 0.3046032769313705
0.6203373952699015 0.3395197583949834 0.3052729298844379
0.1245169814849032 0.8438846410255771 0.3053426103258300
0.2445366502125679 0.8426571689559077 0.3031197805657719
0.0593971862142562 0.5847952074923640 0.3063535696031430
0.9957878112708624 0.3434540891493089 0.3069975653123559
0.6822260637286420 0.4303808289318013 0.3053264042002816
0.6219506310947125 0.6702267009905640 0.3052016999857527
0.5576633182216258 0.9235711566738657 0.3049420245477852
0.4962242296468931 0.1726211633676319 0.3045785797261613
0.6203757757169328 0.1737783001433093 0.3052691912061853
0.1244060842674885 0.6714997963589153 0.3053409468774729
0.2443820228111953 0.6709288741990360 0.3031445022335875
0.0595483101750230 0.9307467588273951 0.3064206114865022
0.9958557475341739 0.1719698608219569 0.3070310610012948
0.3094543952576743 0.0916849277274450 0.3000165891263931
0.4329714213811113 0.5898664111678370 0.3038382802952718

0.8080126139266798	0.0938729404280382	0.3052612675258049
0.9354858989676719	0.5906405583769762	0.3051710839871776
0.3091659295139970	0.4210108583646456	0.2997550540800681
0.4330363525459062	0.9230637187283863	0.3038392988281257
0.8078278613941231	0.4204599658128108	0.3052546714986298
0.9356120446749734	0.9246992340174712	0.3052005976027227
0.6817209642056685	0.9254076645892598	0.3053409622507674
0.5582822907514718	0.4239876823968535	0.3050977644231004
0.1846909909190926	0.9224777622546472	0.3040933815125382
0.0575931525365995	0.4225882482115415	0.3088672863343732
0.6816531577282881	0.5879802073496159	0.3053388588604060
0.5583346358878876	0.0892124886109988	0.3050808059493405
0.1843444356390198	0.5922042235055947	0.3041588134264422
0.0577226232975075	0.0930295380154535	0.3090284085547575
0.1255390808354193	0.2584113168082951	0.3345178977802162
0.2329623665373053	0.2555363522649057	0.2992917619093208
0.2247617838835544	0.2584284209841548	0.3781345942951758
0.3139243763440654	0.2245148682557981	0.4502249997250486
0.2532049472590298	0.2819863243741326	0.4938805358907558
0.1489165672167533	0.1630103537054952	0.5042134833006446
0.1735324852510054	0.2546423050727974	0.5678549051754780
0.2321357728544532	0.1932487484656864	0.6596070271451281
0.1554592492011693	0.2022929771388952	0.6772156084156570
0.3025202444519126	0.2991790347658731	0.4852485971105023
0.1677620898211153	0.2633900087532278	0.5182966612998837
0.1910522318505951	0.2541982443045643	0.6515475814895721

Final state ai (n = +0.25)

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
---------------------	--------------------	--------------------

0.0000000000000000	8.5216999054000002	0.0000000000000000
--------------------	--------------------	--------------------

0.0000000000000000	0.0000000000000000	20.0000000000000000
--------------------	--------------------	---------------------

C N Fe Ru H O

36 16 1 1 7 3

Direct

0.3087283287347926	0.9287502119386623	0.3018233906928336
0.3714441640039754	0.1721349621068236	0.3018421542293717
0.4340438835203022	0.4238562544873689	0.3038146799393214
0.4954807440997295	0.6724331749436213	0.3045074600018595
0.3704430805305427	0.6719878116703220	0.3033821459674013
0.8680917289152671	0.1723180617415860	0.3056068021679209
0.7483259727778053	0.1720424358728385	0.3054738243012244
0.9339696065953436	0.4317208129751646	0.3059452096507662

0.9961308016524687	0.6693609118264350	0.3055318573564625
0.3085146226884763	0.5841652775831011	0.3018044395026379
0.3712987819753890	0.3410326543307736	0.3018356157677168
0.4341406689179846	0.0893139908068173	0.3037831644487207
0.4955256575783265	0.8407817964927757	0.3045063650649680
0.3705325646765339	0.8408734105050769	0.3033801010845942
0.8680244164431945	0.3425371057400575	0.3056092459499596
0.7482673309576522	0.3418592713550621	0.3054770213183473
0.9340792630039728	0.0835261973384303	0.3059522810695269
0.9962200010404285	0.8459908793874290	0.3055568725945306
0.6825354038717680	0.0832419577979130	0.3054484747314023
0.6221853952922580	0.8431546751044687	0.3053173483955392
0.5577619684135291	0.5896901586641458	0.3050747154746531
0.4963534750935415	0.3403975396569516	0.3047420668383453
0.6206021341899746	0.3395661778395196	0.3054021668462070
0.1246761752751570	0.8438704258568539	0.3053032221615121
0.2447833154413891	0.8426981096892648	0.3027599112837548
0.0596413530688103	0.5848113569780923	0.3065228524564254
0.9958678859203123	0.3432184369691290	0.3071714406137367
0.6824616760171811	0.4303560714227467	0.3054503144107473
0.6221438206051696	0.6703448509263925	0.3053170279355610
0.5578017703869005	0.9236541833335818	0.3050682302785199
0.4964082002558802	0.1728693672766029	0.3047249645897868
0.6206405726206183	0.1739058443818807	0.3054026980509908
0.1245806292407282	0.6714865393893448	0.3052841367837162
0.2446430010001040	0.6709719464987609	0.3027741931924494
0.0597837333877933	0.9306548159827895	0.3065980308800794
0.9959306072710492	0.1721320387194064	0.3072058547921945
0.3094425492249562	0.0921336167671870	0.2988058913519730
0.4331329501664832	0.5898906657949506	0.3037816468399488
0.8082176594809317	0.0938454420367052	0.3054661574721367
0.9356448119173978	0.5907147376945977	0.3055102181370002
0.3091621279458395	0.4206723581670671	0.2986187018026880
0.4331969329815071	0.9232010602498494	0.3037830879764005
0.8080504295359972	0.4205294208386168	0.3054712412180686
0.9357644426367597	0.9245552442427717	0.3055331447334358
0.6819319750848318	0.9254488552522787	0.3054421398367632
0.5585366793367339	0.4240079555822131	0.3052530717847975
0.1848736142575264	0.9226143157577665	0.3038204797645502
0.0579174413122099	0.4222731040235749	0.3089411213773817
0.6818665306961358	0.5880999208192127	0.3054439640993230
0.5585827977058945	0.0893726473749983	0.3052475401152478
0.1845438103288455	0.5921005865323842	0.3038404148820886

0.0580385642988903	0.0932722045206916	0.3090992420996764
0.1256118160577215	0.2583414651280566	0.3344988015814434
0.2330538253854730	0.2555644762547428	0.3008218004602703
0.2188165170101386	0.2587935987843556	0.3797968437337119
0.3123760689769413	0.2229420103304258	0.4493929037462530
0.2520341392392128	0.2829469007203240	0.4926891990439128
0.1477658722149758	0.1633177555535312	0.5044888807373407
0.1733998974812216	0.2546999133507411	0.5677981353679394
0.2327256404203014	0.1921068201909747	0.6596314321443676
0.1559968181166689	0.2022818444514976	0.6768607723971856
0.3015116162172817	0.2979770674481644	0.4844606676752164
0.1664264398547462	0.2640174656109507	0.5184164074410993
0.1918633306500718	0.2538473669311407	0.6514619973560214

3.2: Step ij ($H \rightarrow 2H$)

Initial state ij ($n = 0$)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3132765835329323	0.9227383323368556	0.3076066046643646
0.3758923123671423	0.1671964880280967	0.3075728769456703
0.4368206342723653	0.4192244859185976	0.3091726369685261
0.4985235236002623	0.6682750338365082	0.3082813821583557
0.3728697483161199	0.6659329162709327	0.3095460681569264
0.8713452254265874	0.1822380741859675	0.3078481549872762
0.7515518027112478	0.1733753495557622	0.3074871458044015
0.9352423803773462	0.4450173826928960	0.3079518822506984
0.9974522084307083	0.6843030826674195	0.3085318498330878
0.3097745373676801	0.5780997475672223	0.3117554912788876
0.3739074380696223	0.3362925578755949	0.3102109178674084
0.4382601789201743	0.0844529587301750	0.3072821111599779
0.4993033309460344	0.8366149564568275	0.3076192064557901
0.3743607228949486	0.8338122294272168	0.3077202796851424
0.8700153895987626	0.3528969336394212	0.3077384614184098
0.7503987495406932	0.3435062501204555	0.3074565523782624
0.9372376810503127	0.0971174207169909	0.3086382784844872
0.9991012948023794	0.8599435401027549	0.3094117933582794
0.6863538500370936	0.0821378799735797	0.3074497035812485

0.6257795542951783 0.8410188723529046 0.3075606500279662
0.5606059223770217 0.5867813991723736 0.3078720903213679
0.4991296580226958 0.3364284676343843 0.3081146118352081
0.6235176125312236 0.3371797741185887 0.3075064927027995
0.1278950554095388 0.8579296465095183 0.3124879881735509
0.2487122357183082 0.8426523362503886 0.3109234301364125
0.0607178412878326 0.6008590712342397 0.3083233364910569
0.9973618919173646 0.3575683520728461 0.3083805262527122
0.6849395331029626 0.4288723584050942 0.3074374638273838
0.6250504259466751 0.6684118826459624 0.3075606378920099
0.5612562119741469 0.9201302109962057 0.3075367153334696
0.4999893406447100 0.1687675123327779 0.3076904672756342
0.6242149224861606 0.1714585830687554 0.3074417636727915
0.1261115284973755 0.6856113496247929 0.3098140504202789
0.2462344944782018 0.6708212580942288 0.3109880680147583
0.0634083195602173 0.9450508487061953 0.3118393859079447
0.9986545180659903 0.1864729108672094 0.3099473419526575
0.3149376196534348 0.0854213808383051 0.3065567437793177
0.4358953389036131 0.5851244371067494 0.3094308659849716
0.8123695290590618 0.0994279469355916 0.3076116639823496
0.9367603776096018 0.6048775392874148 0.3079498207386635
0.3104737304852137 0.4126385230828475 0.3142972943553985
0.4367544585568410 0.9178415405048028 0.3070153176353756
0.8092360791195929 0.4264758195043612 0.3074750273266531
0.9389698431249300 0.9378193940313011 0.3085200880438705
0.6857087695803301 0.9233889680054546 0.3075190918484054
0.5614405466326033 0.4206361974332111 0.3077928154468452
0.1902826452689581 0.9315985932487294 0.3132921192470448
0.0589139484639958 0.4387178726638297 0.3080588652654868
0.6845182310864075 0.5868866231909351 0.3074413638794056
0.5623002999582241 0.0864513074522648 0.3074877623006316
0.1842866464060009 0.5999759268937694 0.3091298003205196
0.0612353860668264 0.1087866481617326 0.3133751533721778
0.1295762738984081 0.2818361664515550 0.3261002240417454
0.2389202459831239 0.2308937042530772 0.3303733770641770
0.1907776343586889 0.3225116428995563 0.3910484018006315
0.2379605505899463 0.1365220573524226 0.4416954737905314
0.2801636194889525 0.1551511357644486 0.5082214837153884
0.1844450115593830 0.0973333972083950 0.5257552041743949
0.1110432291414725 0.1893827024191523 0.5411212505648990
0.1477919564645518 0.1029402720297128 0.6069438247625172
0.2045570757562487 0.1398627240074575 0.6879817958849657
0.1270360475718348 0.1694131067206044 0.7005106025496488

0.2451048681253027 0.0900605656568345 0.4874042353223587
0.1380901362078362 0.0977311655410986 0.5541482809762641
0.1591276793005889 0.1015957751646184 0.6769836531501241

Initial state ij (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3133029439935591 0.9227614428031237 0.3076318616094278

0.3759037077740565 0.1671325402984014 0.3075855895359594

0.4368334786719132 0.4192531612126178 0.3091891180063845

0.4984993377447563 0.6682571237453209 0.3082865153741446

0.3728650708918195 0.6658848399085384 0.3095650671071322

0.8713212421867459 0.1822674637834827 0.3078466050012241

0.7515896798158228 0.1734322162557929 0.3074861200832235

0.9352537740493908 0.4451073749648842 0.3079489884707229

0.9974395460660659 0.6843196618999546 0.3085289812571744

0.3097949931679263 0.5780342771985639 0.3117604567961164

0.3739201568501491 0.3363052686687986 0.3102217048651837

0.4382753677108924 0.0843846826323609 0.3072917980878282

0.4992870706984761 0.8365562935578962 0.3076116542490079

0.3743672447714728 0.8337986423106444 0.3077352742460174

0.8699766438648284 0.3528689778901166 0.3077314654137707

0.7504339388485164 0.3434790649097965 0.3074514563443191

0.9372643322524813 0.0970949959866988 0.3086463155621351

0.9991190314287960 0.8599885000052830 0.3094174130219721

0.6863228485770069 0.0820757240561747 0.3074491367953086

0.6257830651781301 0.8410505742493652 0.3075595558737552

0.5606069844781144 0.5866970489382995 0.3078715076127057

0.4991420071391424 0.3364341615002464 0.3081213232682092

0.6234867200287775 0.3371758520339113 0.3075074991876528

0.1279234472027355 0.8579299632774895 0.3124950685188947

0.2486912990922085 0.8426567125991585 0.3109301157888648

0.0606757214238032 0.6007898245065553 0.3083325605988373

0.9973682906253832 0.3576821740322559 0.3083855488816731

0.6849267876616020 0.4288706999885303 0.3074348991268113

0.6250513800620787 0.6683451156719276 0.3075564220865221

0.5612717212152175 0.9201753533584983 0.3075386533524458

0.5000011837396033	0.1687374318009590	0.3076888745629052
0.6241811666347451	0.1714434130207274	0.3074465223428742
0.1261319826216858	0.6856333971778255	0.3098232758631129
0.2461938344839919	0.6708604802453467	0.3109858407607805
0.0633840943681341	0.9451662626968326	0.3118602069905531
0.9986741386402953	0.1864739786594301	0.3099509401378439
0.3149721956792641	0.0853864054165833	0.3065794739604955
0.4358915677032614	0.5850750877689844	0.3094286957040460
0.8123786257571670	0.0994877310826038	0.3076236188717154
0.9367791656283496	0.6048340084876193	0.3079655970236336
0.3104969103664892	0.4126326182411571	0.3143213893198323
0.4367736093416018	0.9178457115960982	0.3070102134884052
0.8092366642974683	0.4264444021094383	0.3074811535984349
0.9389979775172255	0.9379248846248445	0.3085387811447337
0.6856852106332344	0.9234422039662399	0.3075151133392310
0.5614250778128685	0.4206841030038605	0.3077977048896463
0.1902919224067526	0.9315538762235427	0.3133241950612020
0.0588161460944768	0.4388965086119040	0.3080863954075049
0.6845053116911566	0.5867937469524838	0.3074385154202496
0.5622686688123819	0.0863746861965288	0.3074927599968562
0.1842845873989619	0.6000587835938632	0.3091730469465740
0.0611793870612418	0.1087207188769153	0.3133408875610659
0.1296394015501680	0.2818601466214133	0.3260778870464134
0.2389424316601223	0.2308215207790268	0.3303766202528182
0.1907903671883416	0.3224117497014482	0.3910454820880406
0.2379719875734172	0.1366868000670187	0.4416903693016117
0.2802058672602302	0.1549795773482859	0.5081897308735172
0.1843950576727183	0.0974200012561967	0.5257351946883767
0.1109752353204166	0.1892825136880022	0.5410968189579951
0.1478082467609165	0.1029977623216404	0.6069105182879788
0.2045514537317595	0.1398287736316527	0.6879969291018766
0.1270345283574692	0.1693332304967415	0.7004905992602276
0.2451355121729697	0.0901781131413728	0.4873120550090037
0.1381160946283414	0.0977583448559122	0.5541069935078590
0.1591309909608943	0.1016548814927859	0.6769269421091270

Initial state ij (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3132642286958431	0.9226493404707632	0.3076459520344684
0.3758785269448708	0.1671664002902468	0.3076225229885063
0.4368314832247540	0.4191848180241742	0.3091972959661983
0.4985498324753387	0.6682351428256610	0.3082863689187040
0.3728793605718363	0.6659869231062244	0.3095898970860778
0.8713806306259159	0.1822025442870391	0.3078512532712131
0.7515226384044263	0.1733310315730383	0.3074846572262430
0.9352336053199464	0.4450426450931660	0.3079617834593110
0.9974515423943325	0.6843605675871816	0.3085496372090833
0.3097547790581663	0.5781710998338710	0.3117749048418657
0.3739030434788249	0.3362569696307035	0.3102417426338721
0.4382609379731734	0.0844633479434646	0.3072845506355590
0.4993345576834093	0.8366203450556904	0.3076090626906458
0.3743836434371920	0.8337704524113307	0.3077374611082082
0.8700449121752311	0.3529235760259780	0.3077272982528610
0.7503692993503984	0.3435134648644981	0.3074506570352368
0.9372158275891497	0.0972032555763969	0.3086513638605378
0.9991151898920816	0.8599437265327707	0.3094211719155346
0.6863781458078299	0.0821335956103485	0.3074507366656185
0.6257785094591343	0.8409148787145408	0.3075618808095498
0.5606006795367209	0.5867985583388976	0.3078712277175354
0.4991304699332531	0.3363953730226928	0.3081204071566444
0.6235639164313028	0.3371114806911466	0.3075095253103477
0.1278539807501234	0.8580346568928230	0.3125026670052335
0.2487162441958740	0.8426274938053006	0.3109450185366160
0.0607328271621498	0.6009546066800511	0.3083450931189758
0.9973364704063683	0.3575973313885347	0.3084065379503100
0.6849672131968549	0.4287846361051065	0.3074313473016884
0.6250463270034770	0.6684166181519177	0.3075530146612520
0.5612554723774043	0.9200682871286513	0.3075409701526073
0.4999795846832555	0.1687435288200297	0.3076821582733328
0.6242493370097167	0.1714507729194578	0.3074539687167177
0.1260585432728717	0.6856116747969956	0.3098448450120991
0.2462339989362299	0.6708276878012728	0.3110063360837604
0.0634405427992938	0.9450826132827749	0.3118406599635726
0.9986165239765862	0.1866057527426205	0.3099559641673410
0.3149063487597716	0.0853460415173802	0.3066509455655742
0.4358955008356020	0.5850883696695014	0.3094563629224295
0.8123682070788045	0.0993935865778810	0.3076291393316063
0.9367098644603502	0.6050144283475735	0.3079722647300479
0.3104921023231878	0.4126780099230903	0.3142881610929129

0.4367574952272855	0.9178200247372031	0.3069824533071113
0.8092416160542554	0.4264888942317569	0.3074803550873299
0.9389668442409540	0.9377793443003050	0.3085517620606898
0.6857339433883309	0.9232815342247749	0.3075112044445287
0.5614362654972548	0.4205637076819573	0.3078028860929047
0.1902800229407419	0.9317248502201422	0.3132730010104957
0.0589919529167564	0.4386373521243693	0.3081074718944958
0.6845641277159679	0.5869035856943888	0.3074345556363930
0.5623099454426670	0.0864398208211785	0.3074934248152315
0.1842454248794379	0.5998844673693887	0.3091585041334307
0.0612437843935446	0.1089694713117507	0.3134036445668395
0.1295212284286017	0.2817418621469717	0.3260173520793675
0.2389284711061471	0.2308649409517630	0.3305119571701099
0.1907076348729753	0.3224127351630934	0.3911057772472183
0.2379897925998228	0.1368403718258627	0.4415116244776312
0.2802576141893644	0.1548732621603870	0.5081708398837335
0.1844627061581243	0.0975087177878908	0.5256493738316422
0.1109069197630084	0.1891891894219052	0.5410677670598231
0.1478153833985803	0.1030596568185350	0.6068571519194016
0.2045509006834649	0.1397993036615506	0.6880091989687789
0.1270270920892646	0.1692690045397346	0.7004738285168073
0.2450730041596398	0.0902554464044173	0.4872829684810232
0.1381056991985639	0.0977808447773128	0.5540799638359738
0.1591417179641840	0.1016995655625476	0.6769041390991066

Initial state ij (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3132442526414154 0.9225798605469064 0.3076802671094302

0.3758612833876162 0.1671538312253991 0.3076749539746397

0.4368316326808013 0.4191434629242617 0.3092149643669231

0.4985743344795893 0.6682014907741293 0.3082904718183817

0.3728931881623554 0.6660582498114138 0.3096228033803585

0.8714126956405356 0.1821583672718987 0.3078562594681974

0.7514932244494562 0.1732797680862848 0.3074852733647385

0.9352242499557613 0.4450545169961742 0.3079754922999889

0.9974461923017290 0.6844593497988942 0.3085740879594617

0.3097310698804965 0.5782538444382600 0.3118022177049247
0.3738849766253017 0.3362501680224551 0.3102697098327634
0.4382557231415717 0.0844772083541740 0.3072811836751264
0.4993619375169936 0.8366216707825558 0.3076023226449159
0.3744037115313307 0.8337149588040442 0.3077468362073189
0.8700642505444821 0.3529680222002488 0.3077247943671920
0.7503313449587243 0.3435134141742067 0.3074477623526219
0.9371820957317768 0.0972624038092609 0.3086635926029483
0.9990955305452585 0.8598898362756553 0.3094373664490773
0.6864113798210491 0.0821354664147369 0.3074524324284937
0.6257871149083647 0.8408390180075791 0.3075619211811703
0.5606032907492626 0.5867969923219944 0.3078731252689832
0.4991311763590097 0.3363304152932896 0.3081254484327499
0.6236063503673928 0.3370404517875815 0.3075131917686265
0.1278106192165989 0.8581250143675371 0.3125059582943732
0.2487304765263370 0.8425999166990836 0.3109690819984808
0.0607560557250463 0.6010583751918566 0.3083699845926605
0.9973284695268426 0.3575747116289256 0.3084408246441210
0.6850066754218939 0.4287118910183112 0.3074273113362830
0.6250594925672117 0.6684121762292218 0.3075487230087997
0.5612599609374416 0.9200016593604325 0.3075412591987891
0.4999778077844636 0.1687506905360148 0.3076756271967368
0.6242927491948846 0.1714391826899149 0.3074610731148583
0.1260256140443853 0.6856238843982599 0.3098681263789611
0.2462555054551235 0.6708392144398572 0.3110344740048930
0.0634706587192569 0.9450498475943486 0.3118409814298084
0.9986004241106907 0.1867050665838685 0.3099787959108113
0.3148662247806950 0.0853156270091040 0.3067761001540767
0.4359007343637373 0.5850557620936689 0.3094898534575738
0.8123663640796912 0.0993412289298747 0.3076372243724427
0.9366677651307459 0.6050974753818904 0.3079868037533253
0.3104794806361645 0.4126830009549908 0.3142845350730807
0.4367593734123069 0.9178290440957545 0.3069597361271134
0.8092570851038295 0.4265096498010316 0.3074779955114305
0.9389446900126356 0.9377411753678105 0.3085755346819062
0.6857699443108942 0.9231706339533862 0.3075067133599583
0.5614495922443428 0.4205217380454350 0.3078122962836796
0.1902875536988572 0.9318886036616139 0.3132432077003659
0.0590648529024713 0.4385804263509837 0.3081480429746396
0.6846028628467652 0.5869540563478698 0.3074252089697299
0.5623347596951266 0.0864084919477465 0.3074933223087630
0.1842139458787077 0.5997831711167476 0.3091680495720259
0.0612527394975739 0.1090814539082974 0.3134362621381808

0.1294849950609883	0.2817084289286551	0.3259653624030444
0.2389023200205206	0.2308114848531731	0.3306254512016194
0.1905881840404847	0.3223812636415089	0.3911804890257030
0.2380305866112119	0.1371186215464200	0.4413259597263753
0.2803256936187979	0.1546192983302769	0.5080951949858288
0.1845141673580688	0.0977154169326184	0.5255111731001858
0.1107866785243336	0.1889994131738224	0.5410014989621467
0.1478369485621230	0.1031688826160979	0.6067573261274600
0.2045597555257617	0.1397650470978955	0.6880342875565112
0.1270097223391672	0.1691643829227758	0.7004460877470212
0.2450109227719436	0.0904479439518991	0.4871915449813253
0.1381204785038985	0.0978169834854108	0.5540082638042052
0.1591504998576674	0.1017404826941708	0.6768457931716394

Transition state ij (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001	0.0000000000000000	0.0000000000000000
---------------------	--------------------	--------------------

0.0000000000000000	8.5216999054000002	0.0000000000000000
--------------------	--------------------	--------------------

0.0000000000000000	0.0000000000000000	20.0000000000000000
--------------------	--------------------	---------------------

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3137606735212949	0.9190849514446049	0.3121800518946657
0.3748216407666353	0.1651140238411265	0.3120530214460348
0.4359321674507990	0.4162518292085340	0.3121689291034012
0.4978358361452900	0.6658185968150568	0.3104444421178369
0.3723561797909791	0.6622695934472315	0.3135005467772933
0.8719616582200924	0.1845778525571532	0.3098370333314528
0.7519984973361141	0.1728779509471018	0.3084684555804945
0.9358204171728711	0.4493644180061782	0.3098121473803396
0.9986797748198802	0.6872058486671946	0.3097092312580021
0.3091769251047841	0.5752016392980339	0.3153880198029739
0.3722480877855237	0.3336966122642520	0.3140952326125912
0.4375303509877717	0.0821462154110635	0.3109946280309513
0.4989142008862452	0.8340619986232702	0.3099928262643357
0.3744513180762768	0.8312316613519437	0.3121527816993945
0.8702330923410259	0.3551949338253408	0.3094550171388373
0.7504764564660886	0.3425697762446140	0.3082500515741130
0.9383115930195077	0.1001828711640488	0.3108133192223291
1.0008094270546335	0.8650434376153109	0.3107678764176481
0.6862460208395595	0.0801584328591319	0.3081926270372122
0.6253879303016122	0.8389662487324109	0.3082399664270374

0.5600889691726533 0.5842552496947336 0.3091344620952317
0.4982679254815254 0.3339597957393148 0.3102930094760310
0.6229403375959507 0.3349492259398568 0.3084569236891023
0.1289945446340055 0.8628466088335458 0.3135253501094071
0.2494555215703249 0.8410363271317414 0.3143587587380143
0.0617638305012711 0.6040376166350991 0.3094847686470589
0.9975765267213516 0.3613296338279151 0.3100967463081980
0.6844195824426527 0.4272876493108287 0.3079694691272590
0.6243882281750206 0.6665092737476143 0.3081514427261096
0.5609577584489739 0.9181064551724558 0.3089871900027583
0.4993454716379266 0.1662025456289145 0.3100910895209281
0.6238344565847690 0.1694110015754028 0.3084900747549267
0.1266733357645908 0.6887603684980944 0.3116048927187744
0.2461965415769262 0.6694873796097209 0.3143636241616857
0.0653618014646716 0.9504946557601668 0.3121983404383634
0.9990678977296252 0.1914728878794176 0.3112064306331409
0.3141637868781772 0.0823038499809620 0.3107932873492494
0.4353059945684609 0.5823162244112365 0.3124417342011858
0.8131661986862371 0.1005809544382871 0.3091313555083032
0.9375750744262600 0.6092724769498501 0.3092584162991672
0.3089057924829525 0.4082107851187637 0.3176525014757581
0.4363903766984304 0.9153757275733889 0.3107469585232529
0.8090215924441646 0.4268433481237226 0.3085609244258021
0.9405589891990986 0.9412482156374452 0.3103283026131818
0.6855415771990089 0.9220207687844606 0.3079543879485607
0.5608070776877389 0.4184121326374975 0.3090645028282477
0.1921654471445979 0.9355930915976350 0.3153446653911349
0.0604582402985747 0.4393170872203651 0.3094429599438180
0.6839677371828525 0.5844622028927616 0.3076462882620441
0.5618380312370442 0.0840448142186417 0.3089791003725399
0.1838920847450140 0.5998030600395783 0.3120288107257685
0.0631066271670113 0.1174163266637725 0.3121235911793581
0.1263634231067176 0.2817798670615481 0.3232673632131891
0.2305664488299037 0.2090521157406820 0.3267863001901629
0.1706683286541294 0.2854902210960596 0.3913591640624438
0.2373909698922666 0.1594690348150861 0.4123601580882733
0.2826367042510703 0.1720415029577911 0.4924746956344046
0.2051583469325573 0.1086517901065536 0.5004733017745527
0.1103451269883717 0.1927631818427516 0.5319827881414166
0.1484159193024797 0.1091202866847008 0.5919551068672469
0.2049962088823250 0.1439798863089494 0.6883948465401357
0.1272900210584037 0.1635266598370901 0.6991414925693036
0.2493781806967199 0.1012796854596556 0.4721166847587216

0.1402898549778690 0.1049465931847790 0.5423330652763928
0.1610079619918749 0.1025366720279307 0.6746595167915915

Transition state ij (n = -0.25)

C N Fe Ru H O

1.000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3137301987878527 0.9190272078027163 0.3121109403586447
0.3747849878889021 0.1649770310647662 0.3121277956826541
0.4358567157022227 0.4162256351635810 0.3124048437622324
0.4977049643808893 0.6658262654467633 0.3107882608154564
0.3722594360649839 0.6620667107937102 0.3136351624944405
0.8718834995709426 0.1846196295996941 0.3102045799109477
0.7519771999330608 0.1729119686884786 0.3089122023545945
0.9357987478327029 0.4493159031056290 0.3100363858313372
0.9986592428923700 0.6869901634842948 0.3097900880383113
0.3091527908772299 0.5749997669390144 0.3154068866992655
0.3721992449572752 0.3336115112980086 0.3141823236604364
0.4374662986286184 0.0820243459861028 0.3113164595034312
0.4987799805366724 0.8339224109213172 0.3103886853183898
0.3743519712026633 0.8312180200310232 0.3123119423408456
0.8701822964838286 0.3551878625135715 0.3097912179696941
0.7504738668957216 0.3425478496265231 0.3086771594826792
0.9383232911123440 0.1001194008456880 0.3110670562183299
1.0008077961827297 0.8651059717758911 0.3108512123901014
0.6861519994252601 0.0800691494365153 0.3086585982767060
0.6253027376440381 0.8389642335359321 0.3087357962360391
0.5600270239935122 0.5841405618206794 0.3095368341389095
0.4982246924205300 0.3339414234631546 0.3106552678516568
0.6228257276502130 0.3349443888073427 0.3088511351143710
0.1289949763318665 0.8626417806885894 0.3133735845032330
0.2493793621471406 0.8408713973524973 0.3142160069600657
0.0617340922797118 0.6038508176985273 0.3094649952425106
0.9975349309087645 0.3613297599854587 0.3101963732643815
0.6843237137224890 0.4273506714232598 0.3084297522997161
0.6242967083939771 0.6664722728895859 0.3086413470506397
0.5609140676780540 0.9181355699801486 0.3094284154260213
0.4993122925173041 0.1661367997402546 0.3105010475438813

0.6237225149737853	0.1693845349539583	0.3088927064155857
0.1266399094800528	0.6885778708293472	0.3115410791032935
0.2461070967049631	0.6693923651715370	0.3143366526908375
0.0652829074921358	0.9504775854551087	0.3121496369108425
0.9990211026991633	0.1913250278906665	0.3113006888838181
0.3141515837419975	0.0822294085705113	0.3105513087287909
0.4352287840261450	0.5822100056617021	0.3126182880458214
0.8131439256026332	0.1006554084898050	0.3095556875153876
0.9376015045680521	0.6092602416699736	0.3094648668727860
0.3088631903343117	0.4080705173410841	0.3175541364315387
0.4363636844791821	0.9153151402122274	0.3110966419165394
0.8089688303794940	0.4268157912347876	0.3089297359667507
0.9405556387095035	0.9412145547212661	0.3105640736394535
0.6854446616808068	0.9220623325484806	0.3084948841389738
0.5607101182118243	0.4185374934610368	0.3094448211857083
0.1920735871804916	0.9352518547861389	0.3150806041964745
0.0603870106488909	0.4391874014235287	0.3094204131679165
0.6838528785012689	0.5843657340100845	0.3081905959010070
0.5617224617943202	0.0838892007707479	0.3094208563012161
0.1838729694552290	0.5997355455609101	0.3120727546101014
0.0630533037130429	0.1172340866084131	0.3120883119958883
0.1262738853728073	0.2816191355751543	0.3232066003576294
0.2304866730356158	0.2089951224175301	0.3262474241892705
0.1699247276554650	0.2837638208231885	0.3913265202972306
0.2377025227780421	0.1614361726100519	0.4102728538909488
0.2830901617418399	0.1744773638911248	0.4920761847779974
0.2063228247805582	0.1087916997619469	0.4998046344541142
0.1107286386790573	0.1937863716209005	0.5308698131753613
0.1483057910373830	0.1092980148617519	0.5908686706226183
0.2050896881851221	0.1450451835949105	0.6872830178800290
0.1273007515969097	0.1620952260147436	0.6981926959575783
0.2506239539820636	0.1013447369737040	0.4720690197382116
0.1401775114311868	0.1051332747180257	0.5412803483784981
0.1613277787029742	0.1020955191761056	0.6736817006835415

Transition state ij (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3137136298303722	0.9190989643682969	0.3122388266870040
0.3748107746426055	0.1652671868464570	0.3119966024021445
0.4359689570422184	0.4162115698198715	0.3119691646441753
0.4979644921329456	0.6657457684905649	0.3102216217782448
0.3724068394637233	0.6625684843435441	0.3133813549541201
0.8719995211169825	0.1843647925807610	0.3095989177389631
0.7519216797091965	0.1726975681739825	0.3082049574016497
0.9357424147292642	0.4493413030539385	0.3097453171411166
0.9985992295735117	0.6874933937114017	0.3097868557021028
0.3091137152867033	0.5755293995942431	0.3152873902232664
0.3722415474712836	0.3338098770872208	0.3139782499784767
0.4375538937698127	0.0822842861570370	0.3107422571454749
0.4990475561412516	0.8342351920744933	0.3097328464130800
0.3745153273745662	0.8311656816962801	0.3120399793504171
0.8702294123233879	0.3551381791615379	0.3092600159298785
0.7503676694582493	0.3425762836134232	0.3079811381627060
0.9381501930254378	0.1002174502873322	0.3106524810595020
1.0006918568281531	0.8648625910557992	0.3107900621078341
0.6863337118688539	0.0802284012016784	0.3079129449672351
0.6254384704277994	0.8388909917012336	0.3079615785635552
0.5601077910815857	0.5844132233030656	0.3088948826258416
0.4982466952000632	0.3339045082721344	0.3100207741906776
0.6230539768260220	0.3349032645880267	0.3081996156211413
0.1288759825063762	0.8631791145063317	0.3136721541448899
0.2494842141604257	0.8412699373408453	0.3144523918980631
0.0617037603023997	0.6043144814410251	0.3096518205338422
0.9975380456171832	0.3612644038011057	0.3101652003996986
0.6845176489325394	0.4271097667181533	0.3076924777574970
0.6244490676287283	0.6665045124661994	0.3078773048314876
0.5609404876144480	0.9179963348258752	0.3087092357201039
0.4993157374581610	0.1662336962698148	0.3097683463168188
0.6239425480219030	0.1693800274256650	0.3082106800042758
0.1266129164477241	0.6890136983880019	0.3116974421544954
0.2462460492428530	0.6696347241735519	0.3143080657180144
0.0653894999040828	0.9504476085058365	0.3122890066823419
0.9990338941417355	0.1916369954061573	0.3112267894246204
0.3141186704514936	0.0823411547777570	0.3110295238101612
0.4353582155360868	0.5824575154460181	0.3123120478348495
0.8130879606321254	0.1003341527337026	0.3088745197697911
0.9374129117645777	0.6092399135973506	0.3092261428902375
0.3088671320282390	0.4083787203053957	0.3176012030843072
0.4363414827335408	0.9153822348027458	0.3104930294917871

0.8090306277830320	0.4268269920344976	0.3083183927875490
0.9404478782331437	0.9411808853546041	0.3101951947217206
0.6856175685176955	0.9218111223246630	0.3076604331577237
0.5608917878208990	0.4181401130576601	0.3088400696527763
0.1922163545398914	0.9361709672126935	0.3155440929018127
0.0604655076034310	0.4394613712256371	0.3096638609223890
0.6840770068252718	0.5846356422821265	0.3073547738669996
0.5619551923070966	0.0842264278424377	0.3086650064360834
0.1838085832352128	0.5998668555817922	0.3118915903609457
0.0630603259019445	0.1176896479080264	0.3122048110644136
0.1264388026233737	0.2819960770961512	0.3233376788674882
0.2305911719261867	0.2090330908651783	0.3272806994168015
0.1716846486357658	0.2874352037585384	0.3913738106438556
0.2372280850054209	0.1565677901671947	0.4150902934677101
0.2824604989091897	0.1702193324084680	0.4926721050622270
0.2040303675917842	0.1088912898464874	0.5012711165425391
0.1104612899526082	0.1915729070334148	0.5322369191401871
0.1490223984353028	0.1093205742517060	0.5924513615103344
0.2050402376131603	0.1433657878545530	0.6889255715428657
0.1273132836065276	0.1641373586657796	0.6992792485471268
0.2484019711882953	0.1015052046724465	0.4722565332828694
0.1409421686649832	0.1048450885214542	0.5427643503089733
0.1609852090487962	0.1029539217742989	0.6748301400415679

Transition state ij (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3137136298303722	0.9190989643682969	0.3122388266870040
0.3748107746426055	0.1652671868464570	0.3119966024021445
0.4359689570422184	0.4162115698198715	0.3119691646441753
0.4979644921329456	0.6657457684905649	0.3102216217782448
0.3724068394637233	0.6625684843435441	0.3133813549541201
0.8719995211169825	0.1843647925807610	0.3095989177389631
0.7519216797091965	0.1726975681739825	0.3082049574016497
0.9357424147292642	0.4493413030539385	0.3097453171411166
0.9985992295735117	0.6874933937114017	0.3097868557021028
0.3091137152867033	0.5755293995942431	0.3152873902232664

0.3722415474712836 0.3338098770872208 0.3139782499784767
0.4375538937698127 0.0822842861570370 0.3107422571454749
0.4990475561412516 0.8342351920744933 0.3097328464130800
0.3745153273745662 0.8311656816962801 0.3120399793504171
0.8702294123233879 0.3551381791615379 0.3092600159298785
0.7503676694582493 0.3425762836134232 0.3079811381627060
0.9381501930254378 0.1002174502873322 0.3106524810595020
1.0006918568281531 0.8648625910557992 0.3107900621078341
0.6863337118688539 0.0802284012016784 0.3079129449672351
0.6254384704277994 0.8388909917012336 0.3079615785635552
0.5601077910815857 0.5844132233030656 0.3088948826258416
0.4982466952000632 0.3339045082721344 0.3100207741906776
0.6230539768260220 0.3349032645880267 0.3081996156211413
0.1288759825063762 0.8631791145063317 0.3136721541448899
0.2494842141604257 0.8412699373408453 0.3144523918980631
0.0617037603023997 0.6043144814410251 0.3096518205338422
0.9975380456171832 0.3612644038011057 0.3101652003996986
0.6845176489325394 0.4271097667181533 0.3076924777574970
0.6244490676287283 0.6665045124661994 0.3078773048314876
0.5609404876144480 0.9179963348258752 0.3087092357201039
0.4993157374581610 0.1662336962698148 0.3097683463168188
0.6239425480219030 0.1693800274256650 0.3082106800042758
0.1266129164477241 0.6890136983880019 0.3116974421544954
0.2462460492428530 0.6696347241735519 0.3143080657180144
0.0653894999040828 0.9504476085058365 0.3122890066823419
0.9990338941417355 0.1916369954061573 0.3112267894246204
0.3141186704514936 0.0823411547777570 0.3110295238101612
0.4353582155360868 0.5824575154460181 0.3123120478348495
0.8130879606321254 0.1003341527337026 0.3088745197697911
0.9374129117645777 0.6092399135973506 0.3092261428902375
0.3088671320282390 0.4083787203053957 0.3176012030843072
0.4363414827335408 0.9153822348027458 0.3104930294917871
0.8090306277830320 0.4268269920344976 0.3083183927875490
0.9404478782331437 0.9411808853546041 0.3101951947217206
0.6856175685176955 0.9218111223246630 0.3076604331577237
0.5608917878208990 0.4181401130576601 0.3088400696527763
0.1922163545398914 0.9361709672126935 0.3155440929018127
0.0604655076034310 0.4394613712256371 0.3096638609223890
0.6840770068252718 0.5846356422821265 0.3073547738669996
0.5619551923070966 0.0842264278424377 0.3086650064360834
0.1838085832352128 0.5998668555817922 0.3118915903609457
0.0630603259019445 0.1176896479080264 0.3122048110644136
0.1264388026233737 0.2819960770961512 0.3233376788674882

0.2305911719261867	0.2090330908651783	0.3272806994168015
0.1716846486357658	0.2874352037585384	0.3913738106438556
0.2372280850054209	0.1565677901671947	0.4150902934677101
0.2824604989091897	0.1702193324084680	0.4926721050622270
0.2040303675917842	0.1088912898464874	0.5012711165425391
0.1104612899526082	0.1915729070334148	0.5322369191401871
0.1490223984353028	0.1093205742517060	0.5924513615103344
0.2050402376131603	0.1433657878545530	0.6889255715428657
0.1273132836065276	0.1641373586657796	0.6992792485471268
0.2484019711882953	0.1015052046724465	0.4722565332828694
0.1409421686649832	0.1048450885214542	0.5427643503089733
0.1609852090487962	0.1029539217742989	0.6748301400415679

Final state ij (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3123570580099994	0.9295601591971284	0.3063561988914236
0.3749090986379688	0.1721744772382072	0.3069892691032652
0.4372445993986391	0.4247479061006072	0.3073890990227361
0.4985614294338988	0.6736277477858305	0.3070916769910392
0.3733295243114993	0.6727036608347731	0.3073306547089392
0.8711022812563490	0.1775852705410186	0.3070804388605848
0.7514566443443512	0.1747774201164535	0.3068050930831213
0.9362474496156229	0.4382429860045934	0.3072046838889068
0.9984004205805346	0.6759576639407365	0.3070326337831963
0.3112026887121440	0.5844780831675652	0.3080760910789271
0.3742668449531932	0.3422282621074452	0.3079837725949500
0.4378755525249095	0.0895649554434332	0.3064208436665534
0.4988518739234740	0.8410392568477018	0.3067610705670755
0.3738585606527933	0.8406019168670247	0.3063139656202385
0.8705648006719200	0.3481613133933361	0.3069529462877467
0.7509952158918992	0.3444709089166524	0.3067387037125136
0.9370356061977937	0.0898267689001264	0.3077447259720943
0.9990069936838447	0.8528395126983729	0.3076304621017892
0.6857869519708937	0.0847681504891608	0.3067776314115147
0.6254359653531654	0.8444490037745830	0.3068310196784467
0.5609333719321561	0.5908082699106146	0.3069646134278669

0.4993203397376278 0.3414658011674385 0.3068560971585846
0.6234911622606027 0.3409117168100642 0.3067794486671405
0.1274448789919030 0.8495030249158243 0.3080651061887130
0.2478010866561865 0.8446104286520748 0.3067080819749600
0.0619407723367904 0.5911873452748778 0.3071908571533975
0.9980726539943127 0.3499860730856030 0.3082732126276508
0.6852909723764298 0.4321743878730489 0.3067350874783679
0.6252083692729903 0.6718627559972244 0.3068313626565974
0.5612299137319258 0.9245858641947483 0.3067777545245949
0.4996002190544487 0.1733803590504824 0.3065998509996404
0.6237362549501581 0.1751507816438137 0.3067456819943459
0.1269053821062578 0.6778375834563782 0.3068124697734887
0.2470620337425178 0.6733417174138698 0.3067330818105802
0.0629164323479528 0.9374688768329843 0.3092936713858210
0.9985895928717613 0.1785825228262168 0.3093591170188531
0.3137891225428452 0.0923799882643161 0.3078707341872750
0.4362660708442235 0.5907026899753928 0.3075520713372075
0.8115572919988544 0.0979530738698332 0.3068832252048538
0.9380317951953728 0.5976391198016232 0.3069239014083698
0.3119724739228301 0.4203518795166336 0.3099836277269458
0.4365857833735879 0.9235196508055562 0.3063685382858011
0.8104096521602951 0.4245376485745780 0.3066934449722760
0.9387111842349068 0.9305775243960789 0.3075006429322286
0.6853065724111130 0.9271873713401013 0.3068141989708188
0.5615302768211878 0.4253597245148161 0.3069045455778646
0.1882142525539272 0.9253898587112728 0.3060896385707300
0.0599391927463062 0.4289079751000311 0.3088238999928389
0.6848550649177637 0.5896311297219403 0.3067508990126933
0.5619212687289620 0.0900421255179043 0.3066968068469452
0.1863659796155290 0.5979679042041949 0.3046501902627721
0.0610029280966303 0.1008263975796718 0.3125488145685420
0.1292007152064483 0.2671619085978541 0.3304471839947649
0.2388030121755028 0.2487132852323345 0.3384063246763181
0.1888810510923053 0.3588526892499631 0.3899843668056344
0.2220176962072531 0.1320715529183326 0.3996452442108978
0.2679262645312410 0.1416720500532162 0.4721272111464251
0.2176948158043770 0.0983613990619908 0.5286578100217327
0.1107782917111883 0.1898690940859540 0.5387095671456593
0.1381234762019407 0.0997133536989051 0.6017065675918277
0.2038680775995685 0.1426340123286470 0.6904946199903359
0.1284046729104896 0.1732687273273779 0.7086788202792328
0.2672410088499046 0.1030661299847684 0.5183300506848170
0.1316007838020016 0.0911857447209877 0.5522468313595217

0.1581162972545373 0.1008499773757431 0.6848715873690009

Final state ij (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3123802400354545 0.9295252689867909 0.3063748235591865
0.3749068483879653 0.1720899802874511 0.3070296459410625
0.4372484573061841 0.4247857337122727 0.3074055311320663
0.4985063137476953 0.6737069913114782 0.3070833972032486
0.3733119251682041 0.6725981213208414 0.3073393860843786
0.8710869037003082 0.1776118796324738 0.3070790020175640
0.7514992524002709 0.1747909825715862 0.3067975057429450
0.9362477523164066 0.4382080392203928 0.3072109203606464
0.9983723958775780 0.6757659382894481 0.3070416642577749
0.3112274363665952 0.5844800626005420 0.3081002124136728
0.3742634796088216 0.3423038515913407 0.3080294224401079
0.4378811620821173 0.0895210370914441 0.3064275360635662
0.4987961570969746 0.8409660709304451 0.3067453561558162
0.3738495242991131 0.8406914533017182 0.3063178670852920
0.8705499573265443 0.3481690322035346 0.3069525979222612
0.7510383221742234 0.3444409341953668 0.3067283422316815
0.9370507592793411 0.0899071492742841 0.3077460262586622
0.9989931165218309 0.8530858540874841 0.3076413585832997
0.6857651217559346 0.0847002649814576 0.3067663568385663
0.6254296780766460 0.8444954977106683 0.3068178588842147
0.5609522125561850 0.5907311180959751 0.3069511911943980
0.4993307510513547 0.3414809348151485 0.3068541753025592
0.6234470597239973 0.3409279858936826 0.3067576187667474
0.1274685187938792 0.8495215304349776 0.3080539677696749
0.2477864109367246 0.8445833242880558 0.3067155034680979
0.0619291571634939 0.5911817716517146 0.3071953483063218
0.9980752710853432 0.3502002393686204 0.3082901613081324
0.6852635092981023 0.4322368084031881 0.3067198018815092
0.6251963937166058 0.6718225199860972 0.3068198441256851
0.5612485198590239 0.9246703722295657 0.3067583138749530
0.4996084137415241 0.1733699459931742 0.3065940761731767
0.6236960129704915 0.1751380895093873 0.3067256350022587

0.1269187276992805	0.6778450705567644	0.3068113000702860
0.2470357266377132	0.6733452186639365	0.3067479115626796
0.0629017750160093	0.9375273213430170	0.3092890005909273
0.9986024854713279	0.1784166510476935	0.3093617468591354
0.3138220723356481	0.0924635263315960	0.3079368932500950
0.4362672038429167	0.5907163819704339	0.3075458902025004
0.8115727214795069	0.0979675387736065	0.3068835448247165
0.9380929374411093	0.5977298375107274	0.3069212888633264
0.3120016608386335	0.4202398334011233	0.3100397942752355
0.4365841692122527	0.9235091344619747	0.3063581880021137
0.8104088286729823	0.4245285252498596	0.3066899783115518
0.9387668021050599	0.9305544479198310	0.3075097209381773
0.6852765127336489	0.9272510752987090	0.3068075197464585
0.5615125686651451	0.4254746172127394	0.3068863184894570
0.1882158590521698	0.9253704674152647	0.3061525899026431
0.0598687360307412	0.4288485102772839	0.3088047067553976
0.6848270810824720	0.5895488527901314	0.3067415356587546
0.5619013282288128	0.0899405251136836	0.3066768221079556
0.1863680990521764	0.5979902592448760	0.3047230383413658
0.0609507591499273	0.1009484519636669	0.3125049074128890
0.1292381287071338	0.2672464741834439	0.3303163329018959
0.2387984952289590	0.2485776360935973	0.3382976629688334
0.1889097956171312	0.3585412060929782	0.3899794265410338
0.2220041479848997	0.1321595986092612	0.3996296829112463
0.2679770308667553	0.1415255213931365	0.4721110199492660
0.2177605506995385	0.0985111033775983	0.5287205996355651
0.1108004315179787	0.1896678042232632	0.5386398236828849
0.1381119102487416	0.0997146584371844	0.6017020418367736
0.2038172807763279	0.1426085203251154	0.6905041996784839
0.1283791229709493	0.1732554076213781	0.7087725711843993
0.2673001643740203	0.1033079617974862	0.5183589610572690
0.1316969183727856	0.0911076736858722	0.5522241364877412
0.1580510034623120	0.1009083236422063	0.6848782376493956

Final state ij (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3123342650691885 0.9295403132873421 0.3063648842851731
0.3749086127338810 0.1722437068553765 0.3070064421418923
0.4372373358964513 0.4247080169480741 0.3073982634243017
0.4986149210199280 0.6735588196981300 0.3070819346315374
0.3733397179627125 0.6727607994486944 0.3073367026481075
0.8711179388251865 0.1775767777083937 0.3070856131684666
0.7514135148972064 0.1747584518741209 0.3067989453812202
0.9362343565028313 0.4383228700196165 0.3072055336059343
0.9984145856718226 0.6762083308880880 0.3070410320323105
0.3111617595552761 0.5844745847401868 0.3080838623033449
0.3742547141134328 0.3421616360981215 0.3079949964772996
0.4378755558592657 0.0896218836946474 0.3064231604153312
0.4989116081195017 0.8411208151453456 0.3067467362360375
0.3738714517827150 0.8405354020732446 0.3063138873466318
0.8705715205791422 0.3481676982068148 0.3069501840737835
0.7509468892939920 0.3444846539977474 0.3067302438294603
0.9370245685299580 0.0897955821567982 0.3077563908194521
0.9990186106685034 0.8526335608992551 0.3076365569959713
0.6858064171322520 0.0848467512905591 0.3067679025456849
0.6254321195812189 0.8444109537966753 0.3068186182841425
0.5609061270370428 0.5908861357878054 0.3069480809498173
0.4992973928944463 0.3414621702153926 0.3068476227001743
0.6235323908930623 0.3409100063207247 0.3067592014242750
0.1274211070748184 0.8495408617084986 0.3080690876667775
0.2478216148976321 0.8446289717943939 0.3067181093834525
0.0619321840443046 0.5912553625646756 0.3072100843899244
0.9980577277045327 0.3498166402388848 0.3082692480899139
0.6853094907315322 0.4320971199625138 0.3067224903661835
0.6252069820952064 0.6719014091583049 0.3068184232259972
0.5612003112146177 0.9244998395303196 0.3067595675431415
0.4995796207464014 0.1733901941755252 0.3065876224932584
0.6237745557900046 0.1751568824866220 0.3067271804373599
0.1268798531127617 0.6778675677867509 0.3068342907145315
0.2470797517005812 0.6733071302759761 0.3067493532522700
0.0629376254088704 0.9374723779777255 0.3092870559444958
0.9985819737883075 0.1787980518054408 0.3093560768900154
0.3137783263886080 0.0922916900353006 0.3078822550480154
0.4362512080720245 0.5907152979205715 0.3075642451062989
0.8115418489617892 0.0979353655639189 0.3068815506505314
0.9379549641058436 0.5975939385219170 0.3069165131493645
0.3119312245951800 0.4204120692337636 0.3099831513473023
0.4365667126014454 0.9235132875986953 0.3063592012185685
0.8103980358258086 0.4245480799513201 0.3066838609209825

0.9386569488998154	0.9306462112656542	0.3075134527847027
0.6853290400368856	0.9271238019113390	0.3068068981019844
0.5615401003030165	0.4252290570359177	0.3068838375031669
0.1882190954030993	0.9254319378240835	0.3060288101451001
0.0599972599561309	0.4290357807195654	0.3088175816676338
0.6848798740140396	0.5896999576743314	0.3067411701886927
0.5619486697953829	0.0901690256143313	0.3066741490825935
0.1863434940338123	0.5979570748473113	0.3046333482774141
0.0610661254827763	0.1007785878573421	0.3125472413477184
0.1292689013596924	0.2672101360708348	0.3302407680336721
0.2388542644312970	0.2486690560974751	0.3386183571009173
0.1888013376698099	0.3588396932310582	0.3900089043337524
0.2219476965221791	0.1317386969471219	0.3997293540679189
0.2679055365431043	0.1414437620303013	0.4720682801886176
0.2177895212589951	0.0985037416330572	0.5287067438956463
0.1108022620354993	0.1896601566501027	0.5386307799642447
0.1381058307629030	0.0997227044991554	0.6017032072814679
0.2038197335496166	0.1426100710380759	0.6905038058650409
0.1283781831630141	0.1732583955293360	0.7087717567649393
0.2673308357341261	0.1033862553375491	0.5183697847532951
0.1316772473292692	0.0911012861346823	0.5522356518955008
0.1580546182362484	0.1009094706091482	0.6848877941972271

Final state ij (n = +0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 8 3

Direct

0.3123120780113989	0.9295317897747475	0.3063700452820736
0.3748928293812928	0.1722794941677633	0.3070135443412418
0.4372368661461312	0.4246690226345373	0.3073985884139569
0.4986721750031987	0.6734820737557285	0.3070710522949601
0.3733501810371213	0.6728201595974697	0.3073405092166231
0.8711352253824973	0.1775690453918946	0.3070904373624461
0.7513822631460845	0.1747381215094814	0.3067922866922596
0.9362224528783450	0.4383561749633975	0.3072010112911058
0.9984176068730872	0.6763898531087325	0.3070510285664973
0.3111272679626902	0.5844843162058820	0.3080756207666930
0.3742284160354629	0.3421644538432171	0.3079887984009643

0.4378877712127122	0.0897020981330411	0.3064149845094136
0.4989814401168302	0.8412042770694277	0.3067340940544089
0.3738913811573812	0.8404934256795139	0.3063133884234576
0.8705854873776518	0.3481641827601737	0.3069468469576076
0.7509172707287668	0.3445074204951640	0.3067210803764875
0.9370085469567436	0.0897938473223360	0.3077631195731072
0.9990173361915060	0.8524890068662406	0.3076446943268540
0.6858277684465351	0.0849110759583172	0.3067568464887783
0.6254388613756273	0.8443900319321644	0.3068049272423515
0.5608854831945275	0.5909379088697775	0.3069284966028989
0.4992658816195966	0.3414519849007638	0.3068343107457995
0.6235855247173994	0.3408778390886931	0.3067410246618975
0.1273941962523938	0.8495882714908840	0.3080598400239255
0.2478256293279410	0.8446558749444655	0.3067112690316416
0.0619297334703876	0.5913015237999216	0.3072271321810972
0.9980506464810761	0.3496978218924232	0.3082631026649514
0.6853295486448235	0.4320487330357891	0.3067096634817866
0.6252144435922925	0.6719034347476037	0.3068026604354733
0.5611708216087543	0.9244101446166191	0.3067406252530716
0.4995435566623491	0.1734000139855479	0.3065699574852255
0.6238225080985182	0.1751709292395281	0.3067104075692342
0.1268539852202999	0.6778995012033190	0.3068527225044598
0.2470856502989219	0.6732752283807319	0.3067502439377269
0.0629615913997408	0.9374896979610501	0.3092733253038197
0.9985762592199078	0.1789611695524464	0.3093523975251147
0.3137637000764650	0.0922659787468987	0.3079098198382909
0.4362368010811092	0.5907546224243184	0.3075781186844915
0.8115327923869968	0.0979047654330737	0.3068805690930747
0.9378898322057435	0.5975545960306909	0.3069133019771981
0.3118840917711870	0.4204431461139483	0.3099692357834055
0.4365309096233642	0.9234994015427445	0.3063522618952543
0.8103917170955001	0.4245690665500723	0.3066723071890449
0.9386159625471350	0.9306906807560260	0.3075302869253583
0.6853500195215741	0.9270507515896311	0.3067976998444308
0.5615575833794103	0.4250828058313401	0.3068634429049005
0.1882192953753988	0.9254911225238170	0.3059345457641198
0.0600510609750516	0.4290969275632595	0.3088240162265393
0.6849120224851637	0.5897615952888182	0.3067296957154567
0.5619895401821742	0.0903039992160102	0.3066514596978404
0.1863192510389253	0.5979404625285897	0.3046027367341315
0.0611155511580453	0.1007830091972017	0.3125674983379906
0.1293408635674912	0.2672283658162871	0.3300429022197628
0.2389042901906782	0.2486616431525314	0.3389253313453809

0.1887033031567646	0.3589572961855451	0.3900854716471559
0.2218524708612243	0.1312460287208526	0.3998375042887843
0.2678600843865074	0.1411963791861092	0.4719885893561265
0.2178982176496227	0.0986381882728515	0.5287604135866578
0.1108250622823784	0.1894684221049656	0.5385463187950971
0.1380880799528411	0.0997399726968663	0.6016977372564188
0.2037742039680751	0.1425911732942788	0.6905137184124338
0.1283491156489082	0.1732543392563117	0.7088585538584543
0.2674236592236200	0.1037072739543534	0.5184049755239797
0.1317443364322720	0.0910010226988766	0.5522316524621681
0.1579955665463727	0.1009639344449909	0.6849075916466431

3.3: Step jk (2H→ 3H)

Initial state jk (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3116735728160892 0.9423675916157938 0.3202083983119534

0.3758250567705082 0.1844556080261729 0.3183181644652224

0.4401431712155517 0.4364366284389429 0.3152837160665831

0.5009633259539086 0.6844172004989901 0.3160872510754669

0.3760544305271791 0.6865340092885849 0.3160064316015989

0.8716143677186935 0.1706554654626768 0.3161691876755549

0.7520395364144384 0.1785060096259498 0.3160879840001509

0.9383571173948705 0.4270639418829095 0.3171112225335231

0.0004972791594199 0.6643611823984028 0.3176029933680669

0.3148741491204026 0.5974815065103685 0.3162060083674529

0.3776273235182083 0.3535632464957155 0.3157817011501031

0.4387434218971775 0.1015047248485761 0.3173719794934111

0.5002561572313988 0.8526286202456472 0.3167947749011422

0.3746738912721655 0.8545840069314324 0.3181195528647350

0.8727138789891862 0.3414423770083138 0.3163461466630257

0.7530210279249032 0.3486147134528663 0.3161109409362104

0.9368388912845484 0.0789140779500236 0.3161416615287900

-0.0008621320614643 0.8397939066764935 0.3164779526142480

0.6866906325000890 0.0926414468585761 0.3160650405224577

0.6267864148283685 0.8529907015764349 0.3161637168311379

0.5629628431061250 0.6010349403695586 0.3160748569341865

0.5016731665497722	0.3523755104393446	0.3158019550602972
0.6257904748235896	0.3499190436957780	0.3160364497816255
0.1278181201184906	0.8379311295219392	0.3170417500057977
0.2481629284277716	0.8505615169894556	0.3186404136121535
0.0647757724086444	0.5790211286110759	0.3200454303758484
-0.0000558264501203	0.3375393594783984	0.3182679842070516
0.6878518930232784	0.4395116815683529	0.3160702706148705
0.6273766636617372	0.6804901115457348	0.3161705782083858
0.5623331698359334	0.9344532617153187	0.3164137371148890
0.5009287568643563	0.1844073679817534	0.3163205403467235
0.6252135868061669	0.1841851689725633	0.3160861224807299
0.1292801059677187	0.6656723431392074	0.3203399928378169
0.2502159385834695	0.6785217269654837	0.3190368673397920
0.0625061413216682	0.9231356057750534	0.3156895933933075
-0.0010988599693366	0.1666236282600782	0.3161860451507216
0.3127453344083723	0.1080559439969926	0.3224913901282305
0.4384015045934770	0.6029316189122907	0.3153240919764839
0.8110444573401111	0.0962681351058793	0.3160466700417127
0.9403673943892208	0.5861330173425739	0.3169930486390887
0.3168596256282766	0.4349631184359923	0.3158913413863479
0.4376180491559160	0.9355357051344070	0.3179774807156927
0.8135596571048009	0.4234613433467527	0.3162103253359228
0.9383930304171320	0.9192767402132569	0.3162034420550945
0.6863102001115514	0.9346318355828446	0.3160865966622017
0.5640399773629907	0.4348572509602869	0.3159737375229574
0.1863262415816448	0.9220303769917733	0.3158401246360089
0.0621155505580145	0.4157118829835046	0.3217995048923923
0.6873035003718573	0.5979828759650244	0.3161365246248328
0.5631635257266399	0.1005460935531670	0.3162928684627253
0.1915625297445658	0.5914771425194777	0.3211729933639418
0.0605530342007165	0.0856537842937818	0.3152874011337296
0.1287732334550353	0.2421511481711278	0.3387014707015050
0.2414866175415818	0.2890417564144015	0.3430424382786802
0.2602341545887883	0.3278121360738970	0.4183074198017048
0.1884883675191742	0.1765157011061504	0.3947482168422058
0.1934750168356422	0.2364373420570095	0.4757205500065287
0.2196702649829100	0.1390689203924999	0.5373951904026446
0.1290916817031981	0.2359076570426125	0.5554277984347435
0.0508572306792842	0.1618290415293203	0.5668476268127558
0.0895732761603401	0.2391857174950058	0.6340879667111655
0.1444338873042206	0.1866631541731372	0.7150012556831855
0.0662334339433079	0.1911620988309772	0.7295046537979757
0.1939056832490827	0.2328724154465534	0.5252454477497791

0.0814316882252604 0.2461538658086201 0.5811229736387384
0.1024001845619809 0.2415279522987177 0.7038732101260370

Initial state jk (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3124233259500505 0.9421795195149489 0.3200783864548667
0.3766745214337419 0.1843067038082004 0.3178887344267890
0.4409645261752865 0.4363274644407285 0.3151159662744584
0.5017227649117085 0.6842559361244961 0.3159991652121140
0.3768662229297901 0.6863446112940482 0.3160092636961968
0.8721979568058768 0.1699165678335189 0.3181727741880203
0.7527207727165791 0.1781518754339991 0.3170072984864443
0.9390451964116012 0.4262073427082878 0.3193575057594898
0.0011745134551615 0.6633827883364303 0.3199123727253111
0.3157467252525946 0.5972709069668822 0.3161512365783967
0.3785171863062727 0.3533738223608180 0.3153654686618673
0.4395490230128256 0.1013034022901812 0.3171169842513439
0.5009959984925274 0.8524124046869845 0.3166980293820508
0.3754374018847218 0.8545168100145484 0.3180621013830647
0.8733273698709753 0.3405248663408704 0.3183432711241351
0.7537478708493985 0.3481186530461924 0.3170454848209242
0.9374504773166543 0.0779146661634437 0.3185408726300317
-0.0002539662923145 0.8387908549636094 0.3189045323765957
0.6873437776044209 0.0923423608476309 0.3164424571613251
0.6275314328060529 0.8527385272878314 0.3161995734310868
0.5637479029762624 0.6007606260493937 0.3160355845841514
0.5024970033261598 0.3522199018342685 0.3157091196599197
0.6265170059119408 0.3496971736822808 0.3162057389342319
0.1285127343937270 0.8367870459849275 0.3183579619482866
0.2488644278673589 0.8500224061088231 0.3189164945344548
0.0653999328070668 0.5779590201047584 0.3218486109494066
0.0005568726948623 0.3366104443634527 0.3202738648652158
0.6885727851403248 0.4392651964592104 0.3164705836244502
0.6281523437424830 0.6802098823090100 0.3162076538630020
0.5630808705278100 0.9342548733629961 0.3163669697355876
0.5017256645253930 0.1841866500670594 0.3161855376976864

0.6259098834743518	0.1839261790522530	0.3162439171743086
0.1301006349230314	0.6647292883586529	0.3216664155982494
0.2510212380982799	0.6780365529957245	0.3193757719799050
0.0630730605697024	0.9220510630831489	0.3176769697844404
-0.0005211453754903	0.1655499834735932	0.3184270302434367
0.3135838448306355	0.1078791380871432	0.3219855190115908
0.4392124740636547	0.6027766408298011	0.3152137003588146
0.8116333630951812	0.0956613344987818	0.3175262614350857
0.9410296859521839	0.5850537258918970	0.3194373600754650
0.3177719338554066	0.4349236313400768	0.3152630555075968
0.4383608317170427	0.9353843474523261	0.3178023538173251
0.8142985233646771	0.4227819954937606	0.3177190318804348
0.9389966041753262	0.9183549666042347	0.3188753432476805
0.6870047942529467	0.9344260005519840	0.3163093019047668
0.5647930444639481	0.4346870730413729	0.3159543594905531
0.1869564188406716	0.9209656232610768	0.3164367566091177
0.0627036231608486	0.4149682249362543	0.3232534808805864
0.6880664444611332	0.5976336958435831	0.3163816951034364
0.5639053426633867	0.1002886770491600	0.3162462078215528
0.1924085315699414	0.5907873549855568	0.3219380864090755
0.0610487784734890	0.0843644201878328	0.3174747900099818
0.1293117437439582	0.2416672774044235	0.3399555072643123
0.2422875907741090	0.2888732566459034	0.3412272926012100
0.2602946548384874	0.3258757707133450	0.4165545091508389
0.1911343154266390	0.1697929987465835	0.3919456560444887
0.1827390835480266	0.2352354466466709	0.4686323150601052
0.2151305517678509	0.1520057939726524	0.5311768371958755
0.1235231841369719	0.2379766061297735	0.5515797110940810
0.0462800337688123	0.1606128791227567	0.5670617147182619
0.0872640958768277	0.2408466017174934	0.6320604453762309
0.1440794620245520	0.1896408725267535	0.7129366013125580
0.0662583043863049	0.1978469806010897	0.7287949827732964
0.1855095179946609	0.2388403909315107	0.5181763810298685
0.0768316139600289	0.2463603237187672	0.5797314980467917
0.1022334963841334	0.2456553015078796	0.7020740480861669

Initial state jk (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3131289193782610	0.9387609125462846	0.3194618908295335
0.3766861428831666	0.1813493054159565	0.3179962079348418
0.4408472104598229	0.4337176012309896	0.3153199194782835
0.5017044845761470	0.6820656959337696	0.3157906999931708
0.3767264817219358	0.6831738269077239	0.3162292572312293
0.8729483884303271	0.1699070534369944	0.3176551971227309
0.7533777062833641	0.1768395483285693	0.3164991454670606
0.9399157390686242	0.4268838546766541	0.3189222918316741
0.0017279302745082	0.6639172793310233	0.3193556408091448
0.3154360467679805	0.5939801018933413	0.3170913416947447
0.3779370070370516	0.3510385100170860	0.3165990767823246
0.4396488550756920	0.0987034258562528	0.3169564692817716
0.5011304987265248	0.8497238625155429	0.3163466808008374
0.3756551950657571	0.8510992124750638	0.3178334577334119
0.8739301860882657	0.3403480715926821	0.3178154548154474
0.7542553872404167	0.3464644883522279	0.3165191108968282
0.9384717049220207	0.0785417768475573	0.3181544173973052
0.0005940674484842	0.8401084970835363	0.3184178426009879
0.6876766745891562	0.0902691375273988	0.3160562988666034
0.6277114403891508	0.8506979114736677	0.3159036111130299
0.5639437197857281	0.5985101306151943	0.3156775267936976
0.5023566464892621	0.3498220995154371	0.3153933934756125
0.6265755955172703	0.3475542588631217	0.3157686915945295
0.1290032813270243	0.8388909912855322	0.3176015269801122
0.2492554153906462	0.8484464164488937	0.3181233074745322
0.0658435755694274	0.5787191307790657	0.3209209580578278
0.0013198208387591	0.3375119170632213	0.3200539709830140
0.6887192563062174	0.4375333840911094	0.3160264724296866
0.6281841647968853	0.6782591061422535	0.3158578982772368
0.5633907070394850	0.9320645704667465	0.3160428879148286
0.5018220049690733	0.1817516419384980	0.3159092086929662
0.6261114661848148	0.1819373438461933	0.3158659955177236
0.1302224712606970	0.6670922896142027	0.3200400793515332
0.2507294093962899	0.6768743663169350	0.3185198979116601
0.0639313017458765	0.9246778181998107	0.3174092795530897
0.0004169737521402	0.1666504118720107	0.3184171856703624
0.3138409606221083	0.1039900331870568	0.3211485578367348
0.4392745696616682	0.5999965582727195	0.3154348014691652
0.8124408885337131	0.0950469215076688	0.3169650942192550
0.9414828592752760	0.5859150606685585	0.3191645769863335
0.3172599155301183	0.4315580230153017	0.3186102325201816

0.4386800300437317	0.9326747718706457	0.3173612826083384
0.8147254357560297	0.4217695887931296	0.3171289506445326
0.9399734512236020	0.9190761369295705	0.3182597048240612
0.6873348729066852	0.9327747590536118	0.3160215822441214
0.5648371339839552	0.4326936444350552	0.3155216844171330
0.1878495739944531	0.9212708677783245	0.3157678486860749
0.0639524623502541	0.4152307633412467	0.3233490532448217
0.6882174743154283	0.5953124129858282	0.3160251086262120
0.5640074128980933	0.0979108172655969	0.3159446340840957
0.1916893143093513	0.5930083180204541	0.3192262950320026
0.0622905406337151	0.0869971334491187	0.3172597384304298
0.1335058277438161	0.2468155523374717	0.3336889941965159
0.2430391244990874	0.2788925052976616	0.3507931612786380
0.2383811674960051	0.3851287476412469	0.4172912515182353
0.1911160090417070	0.1595720219886775	0.3964687512565824
0.1952370801291790	0.2496225637788605	0.4759951197374922
0.2155218616834285	0.1476996825705937	0.5385273162010015
0.1231073356276156	0.2390240411861569	0.5518955908649797
0.0461359676699396	0.1578792583605653	0.5637705160826262
0.0839917797124111	0.2411129766665536	0.6301888435941471
0.1398136107957796	0.1878284292311790	0.7105437426813809
0.0622522496284435	0.2031931319484169	0.7270826324862045
0.1898292760033477	0.2406320391681362	0.5252720559643747
0.0752246717107435	0.2457472750197490	0.5772529037386492
0.0986989364766252	0.2465481543603241	0.6995949268618056

Initial state jk (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3121679301531244 0.9414071826704797 0.3199959948270783

0.3762592959163040 0.1836446887897031 0.3180233493140265

0.4404911771326460 0.4356561149161647 0.3153056675829926

0.5013838784197854 0.6837055903940176 0.3161077016249638

0.3764231524133328 0.6857489975816081 0.3160652886357316

0.8721439128036127 0.1710950392177178 0.3174088752728296

0.7524932161538265 0.1782806006428450 0.3164539203409959

0.9386504686974673 0.4277683467537654 0.3188309740308535

0.0008574965350177	0.6651412862613826	0.3194602458688676
0.3151767705234423	0.5967064857986611	0.3162863786150786
0.3779650179922291	0.3527911794504094	0.3156859854686102
0.4391792605322627	0.1007958108645289	0.3172691161994002
0.5007226492538115	0.8519726420719511	0.3167906972271542
0.3751340763329296	0.8536236179614795	0.3180749367801632
0.8731511941807174	0.3420702785139469	0.3175626319641877
0.7533925194699800	0.3485170519057293	0.3164492240984221
0.9373116888295354	0.0796700539626211	0.3178762894676017
-0.0003571346861813	0.8406445787505392	0.3183353078022213
0.6872100704349901	0.0922453632021011	0.3161713620349990
0.6272360141555531	0.8524773726219101	0.3161529715746861
0.5633540204286849	0.6004926170063605	0.3160648478960730
0.5020449413475400	0.3516575531627188	0.3158195664066383
0.6262276461344701	0.3493833173080348	0.3160550634491676
0.1282527544437500	0.8384395374222224	0.3181170664628744
0.2486519746670763	0.8498454321252272	0.3187789125758272
0.0651481649147375	0.5798190672872225	0.3218078771680024
0.0002366609672043	0.3382597727893879	0.3202789087417152
0.6882549506559413	0.4390583069375508	0.3161370401099549
0.6277690942549743	0.6800378616356719	0.3161386641651558
0.5627828500292421	0.9338074839587717	0.3164135156590108
0.5013511771383636	0.1837863769825817	0.3163166540298971
0.6256997359994281	0.1836737557647783	0.3161248938922799
0.1295823718205462	0.6660207314885442	0.3214855847237329
0.2505767882279804	0.6779290001067477	0.3192937029113255
0.0630880156630615	0.9238995414182021	0.3173086522249826
-0.0006601132373878	0.1674431493352191	0.3181169530754479
0.3132036625204389	0.1069974843941079	0.3218671792978829
0.4388059599615374	0.6021686996618303	0.3153844172013671
0.8116101727103396	0.0964320433267544	0.3168007588273857
0.9407064915288198	0.5871127117725625	0.3188370442902063
0.3171136953383365	0.4341209033749692	0.3158558879511743
0.4380893147164222	0.9347928959754688	0.3179171034582803
0.8138609513147599	0.4236940134142449	0.3169228780364403
0.9388977107674317	0.9198805509567705	0.3180030921129393
0.6868082346879251	0.9340993193558708	0.3161295129610934
0.5644466957733498	0.4342448343283386	0.3159677589322796
0.1869145123450202	0.9218491211661246	0.3162043129038558
0.0624377434418035	0.4163012330601472	0.3240538553859568
0.6877023787219796	0.5976211773199597	0.3161323818658189
0.5636319561439055	0.0999691521353810	0.3163031879797965
0.1917849194462756	0.5913105265622493	0.3216273915628717

0.0611591167950344	0.0868179154513621	0.3169712500043887
0.1290235498171125	0.2437913408426691	0.3400988461799163
0.2417906464705694	0.2872966102453917	0.3425523313987500
0.2605122604809552	0.3258855693065591	0.4177420119336169
0.1896611381636123	0.1706476913063876	0.3934836040781157
0.1861225236946229	0.2318982233626389	0.4702980007510122
0.2172398220833719	0.1471907915834638	0.5334052544904312
0.1265353258021931	0.2360724235310529	0.5519424692823328
0.0481753926897058	0.1613620400009056	0.5659656011900547
0.0883626005950339	0.2398431053247986	0.6316192054081148
0.1444501904444401	0.1885286095594698	0.7133728098098865
0.0665076826120812	0.1958343798669804	0.7285759787115325
0.1885156026957486	0.2352432326631557	0.5199724042319777
0.0790065677681750	0.2459903348388580	0.5792841654842114
0.1026115791130741	0.2443166203558931	0.7022413268319340

Transition state jk (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3125136334748930	0.9435186045968820	0.3196678365346202
0.3758970616982964	0.1857490909446540	0.3180877652792304
0.4404457291862798	0.4374852894587136	0.3166500775205847
0.5016187148651952	0.6856551713281718	0.3168329030250163
0.3768456461379799	0.6877528813911269	0.3173401059333116
0.8732620124116579	0.1722403292630688	0.3168745221030349
0.7534043321450099	0.1799182822786136	0.3162728263117742
0.9404232812533522	0.4286817153554523	0.3180205975697987
0.0024058547213102	0.6659681840123426	0.3192607756337082
0.3156125243997465	0.5988215857631545	0.3169086066441906
0.3777183397055666	0.3546286555906235	0.3164448485829325
0.4391723421122578	0.1029074106140513	0.3178681899694595
0.5009684802081651	0.8539266083671180	0.3172664185908260
0.3755294376041363	0.8557516426329954	0.3185597219435579
0.8743113221683956	0.3427513458192593	0.3168452044884305
0.7543461151368192	0.3498654801865371	0.3162429812877008
0.9388919752691578	0.0806678177841107	0.3179493205871964
0.0011116095394996	0.8419771031662648	0.3188414375659221

0.6876599260288287 0.0939455522042181 0.3162970821897346
0.6275531586253109 0.8543690958996706 0.3165046457287062
0.5636830926124503 0.6022443239791571 0.3166305876147604
0.5021727824719520 0.3536022998905892 0.3168154388421485
0.6265608793708211 0.3512050485203417 0.3164073340280424
0.1294609044129302 0.8402942654067331 0.3211686385457142
0.2494024967222046 0.8518502090062867 0.3201719482416010
0.0665123734074129 0.5802396159818954 0.3225181230842651
0.0022766703444717 0.3392635348188264 0.3208893870055576
0.6887760780823271 0.4408332746687122 0.3162612461400869
0.6281209906359280 0.6817118492649641 0.3164847572477214
0.5631096216901241 0.9358270203734520 0.3168622612411482
0.5014562511238125 0.1856524695086677 0.3171162370851448
0.6260201557668026 0.1854641607090812 0.3164711675082827
0.1308889423470703 0.6675569056613000 0.3223131973809288
0.2513182653690578 0.6797082551834635 0.3196154548709274
0.0645012285691209 0.9260789058800754 0.3206522258947899
0.0013125563418015 0.1685172239531241 0.3202096006055157
0.3128262077506605 0.1089851104074384 0.3194680497594007
0.4391056689895692 0.6040671274636864 0.3165638096823997
0.8125363023767491 0.0978376291532967 0.3164602760517283
0.9422938439801101 0.5873181673557255 0.3176287603826680
0.3169007793519683 0.4365025175711850 0.3147983683722799
0.4382799876458350 0.9370065138074324 0.3181327824780240
0.8150510572538323 0.4246010682849359 0.3164190324336786
0.9404917067652221 0.9214149278452339 0.3174912718171115
0.6871469597671265 0.9361596450932623 0.3162957940220181
0.5646387550058947 0.4359745856850381 0.3165872359556019
0.1879611652191784 0.9245304719757428 0.3202169071339540
0.0644530495465574 0.4169198511144501 0.3253700612357520
0.6881070857356804 0.5991287029203676 0.3163052060464082
0.5638886684681168 0.1018924063558160 0.3168222401709571
0.1927535778896825 0.5924933760322304 0.3212977305086113
0.0630183602104424 0.0887944274425507 0.3226725001365693
0.1304753041158904 0.2455183828149288 0.3550556342129880
0.2377757557948570 0.2898301552831626 0.3288709876629738
0.2537948060391528 0.3049107755873379 0.4053237893888877
0.1568047962764538 0.1243410716153548 0.4139200571912127
0.1691972418246408 0.1914253153471890 0.4481399257578076
0.2186835130081803 0.1550237361125539 0.5304036197370152
0.1465259650977018 0.2410373759868136 0.5410805050921965
0.0484300973665270 0.1614301997112690 0.5647211825705867
0.0840621306881388 0.2432892596338405 0.6266177676349969

0.1454861522215367	0.1853673591580929	0.7154595394563756
0.0688925349549478	0.1899414491581055	0.7341166837359268
0.1906515687992325	0.2412524752844476	0.5137103202138604
0.0760362028430279	0.2518154808513984	0.5771202017851280
0.1035138910256208	0.2433664133655071	0.7077139996360060

Transition state jk (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3121085958118698 0.9437402307324155 0.3213031448395289

0.3758800952968914 0.1855491759928105 0.3197179468360151

0.4402591191843723 0.4377407669208756 0.3172636619543585

0.5011405241506435 0.6858181061424766 0.3172470922280442

0.3763825557429053 0.6878349547621322 0.3177567263589312

0.8722080338520669 0.1703818489209544 0.3175168081176406

0.7527350725633798 0.1793763898766883 0.3166689469238451

0.9395537593969410 0.4263284251311053 0.3186318041935017

0.0014504716927658 0.6627040721060454 0.3196655738004273

0.3153660676548738 0.5991201891832533 0.3179872997863497

0.3777714868258400 0.3547822087138110 0.3178825105801340

0.4388918564426243 0.1026145632498965 0.3190183019675394

0.5003975486264537 0.8536492121782099 0.3178651434423898

0.3749709518907335 0.8560512890968710 0.3194664578974267

0.8735212202276215 0.3409177134016017 0.3175142057658447

0.7538513659854574 0.3491522705995225 0.3166555546742348

0.9376091539468330 0.0782862173219859 0.3181265058911247

0.9998342809146148 0.8400998132539259 0.3189574114561353

0.6869456737865860 0.0934322212425373 0.3165510564204410

0.6270888092552570 0.8540740793773419 0.3167114146666938

0.5633927615253063 0.6019432223426512 0.3169105500025947

0.5020133468242085 0.3534678874806320 0.3173325530628634

0.6260927076381921 0.3510305816604050 0.3166813543837643

0.1283887341610101 0.8384643807199487 0.3212533554173888

0.2484370646197527 0.8515753576230876 0.3213611994780340

0.0656773367974115 0.5779103721812983 0.3224297715642273

0.0008490848949822 0.3374643411315962 0.3206079368709976

0.6882634189779069 0.4406779726841717 0.3165169674236336

0.6277625353586419	0.6814528812368605	0.3166773130794910
0.5627572471691110	0.9358148643190929	0.3172815540993245
0.5012437566487318	0.1856024853920103	0.3178502536189051
0.6254481317093299	0.1852336423260173	0.3167727016335762
0.1300423294908526	0.6657431795905276	0.3226720546229808
0.2505807491102460	0.6800158940940689	0.3207049171085282
0.0630722139316090	0.9232315426120922	0.3195840311432454
0.9994856310181812	0.1656974296494005	0.3189595698849815
0.3127619579102988	0.1090380641661924	0.3220092036045302
0.4388509465265769	0.6039350751947629	0.3170248927923318
0.8115106214669842	0.0966782512599475	0.3169478107630782
0.9414534937863707	0.5858499620303910	0.3187359671561348
0.3170794035682888	0.4368134501873016	0.3176890840622781
0.4380407481314831	0.9370732154410800	0.3191167492148776
0.8145111222855960	0.4233529174114223	0.3169522064890223
0.9392866161858497	0.9182462805947313	0.3178874164620845
0.6865581769038197	0.9360303089085755	0.3164473643508273
0.5642200060461673	0.4363607661253091	0.3168659702502589
0.1866764946618790	0.9236852193165952	0.3211379658275851
0.0634379182016584	0.4137065407708055	0.3254569088809786
0.6876629843517247	0.5987410128331093	0.3164618619005902
0.5633961437877411	0.1011676042867378	0.3172632168550293
0.1922373172882839	0.5918594579413303	0.3221459261269028
0.0612697633232182	0.0862170956969086	0.3191071560177365
0.1296508324926377	0.2380019840953772	0.3420950798860548
0.2395467402108916	0.2906705637065702	0.3357561143038581
0.2529251996113732	0.3071569124981389	0.4133652490304435
0.1388983609096720	0.1675041962629888	0.4164847085037212
0.1816818639432477	0.2085178054332851	0.4089911993174585
0.2219977702102435	0.1371606955786971	0.5284730877077288
0.1599027554633705	0.2418317772127667	0.5480430021509904
0.0491819817314964	0.1620934390748694	0.5599257886380063
0.0822229570077941	0.2439129440860338	0.6225251588935116
0.1473836812744251	0.1849647497989488	0.7109384179526324
0.0719370755857763	0.1879225102052111	0.7333536913679103
0.2096560983979324	0.2450010359233799	0.5388354379644074
0.0750861289572742	0.2543413119116323	0.5732541815249713
0.1049429236537341	0.2424967797986080	0.7054468878089131

Transition state jk (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O
36 16 1 1 9 3

Direct

0.3131046765913569 0.9435181713386784 0.3192825976752555
0.3765640027876072 0.1855943024330312 0.3177410006475853
0.4411232267183926 0.4374501081981271 0.3163463972302294
0.5022084724365568 0.6855606060393920 0.3163959640513299
0.3775237764600630 0.6876796673082288 0.3170148200073448
0.8737507248180886 0.1705963955191891 0.3186335960031088
0.7540603840712501 0.1793388537620052 0.3172093804715516
0.9411866632156203 0.4266781754198409 0.3197071223457830
0.0031009328323237 0.6636625107783726 0.3206638011039258
0.3164286608446078 0.5985889735473630 0.3165900206320340
0.3784797034666003 0.3545026532406348 0.3161564030840682
0.4397962831437934 0.1026572755049356 0.3174859912841026
0.5015269334567138 0.8536090679019217 0.3167995238453538
0.3761336334463694 0.8557839735011666 0.3181775709443674
0.8749206354296408 0.3408935355461058 0.3186578589420910
0.7551227221019667 0.3490567932520418 0.3172348411185688
0.9394284197875921 0.0785115786462468 0.3195734728413659
0.0016328350011441 0.8399723333635016 0.3202439702173951
0.6881524310639950 0.0934489533923627 0.3165933837952042
0.6281481311879770 0.8540376121910238 0.3162713463470554
0.5644386530697378 0.6018346130079656 0.3162666848384191
0.5029403003868369 0.3533835925702616 0.3164732550325863
0.6271865030125080 0.3509190425699799 0.3164239850289585
0.1300642242305367 0.8383397828465414 0.3211598699172291
0.2499208510594758 0.8512741327234626 0.3198668537527233
0.0672094743799095 0.5780116638876187 0.3227831109843838
0.0029752027901511 0.3372332912120370 0.3214147759524619
0.6894460000991096 0.4405977627221906 0.3166207144354656
0.6288001880482939 0.6813340559933461 0.3162796611629388
0.5637842404233318 0.9356282884352628 0.3164678331521901
0.5021621876993327 0.1854454835572253 0.3167501534809897
0.6265695089705512 0.1851545377460833 0.3164559885536680
0.1317309115895659 0.6658167612375983 0.3222525176291862
0.2520246215057281 0.6791872472567391 0.3192703664303042
0.0649304916046444 0.9238224803652977 0.3208974926349824
0.0018423660819519 0.1662150999367817 0.3206994791588869
0.3134288592371656 0.1089552874190858 0.3190218534555502
0.4398918918853685 0.6038433010278208 0.3162095974808364

0.8129704960958151	0.0967133061803863	0.3178628466880539
0.9430483755160867	0.5850690561495013	0.3197539838470543
0.3177028313963902	0.4364267836665735	0.3143982116541564
0.4389496819586834	0.9369873927082546	0.3176651579630394
0.8158852468764880	0.4232666115387203	0.3179320537837211
0.9409940597735190	0.9193090184407510	0.3195821580195309
0.6876950589882187	0.9359818280563338	0.3163753140694722
0.5652531190797571	0.4359117556782403	0.3162517496591050
0.1883980805528106	0.9232627760577002	0.3200628013611788
0.0651802508580634	0.4149062705483560	0.3249203087967591
0.6888073994583479	0.5986119246694072	0.3164416313378637
0.5644723296668239	0.1014120235698443	0.3164487685590273
0.1936232529523493	0.5913333657248409	0.3209397051313948
0.0634547402481275	0.0864417972143306	0.3221590974718179
0.1312569547477813	0.2426255882329997	0.3531561044807913
0.2384650649638070	0.2897475769359695	0.3267336270667894
0.2517446557723053	0.3039840548871986	0.4036349957076716
0.1518542381197750	0.1204629727318108	0.4136194344005575
0.1646336844510475	0.1928762316873619	0.4453901841591460
0.2158581576359385	0.1724764320427368	0.5270726903038064
0.1421415144055210	0.2496607907145230	0.5388346108229006
0.0455725226340030	0.1631704503564820	0.5663421190017219
0.0823250965820899	0.2456154944248612	0.6273631706659338
0.1443160682534828	0.1874192196584609	0.7165372922534032
0.0678663671911496	0.1934423333187227	0.7355734513829844
0.1853129594929493	0.2537311669446006	0.5101437363821050
0.0731233591244979	0.2541045763324667	0.5780943149928287
0.1024033882054075	0.2457155460007451	0.7087263493383169

Transition state jk (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3125481254191211	0.9433710550250369	0.3193411397706630
0.3759801868517333	0.1856187662638474	0.3179005907243619
0.4405622487493931	0.4373244391854671	0.3164964277317852
0.5017666344151448	0.6855103738963195	0.3166873552118603
0.3769457701202449	0.6877105509313660	0.3171121458543651

0.8734003360338953 0.1721868919744108 0.3171410071229677
0.7534854675073327 0.1798352597565553 0.3162843013399972
0.9404725960790009 0.4286530394669047 0.3184766065762937
0.0024796964856476 0.6660098783906091 0.3197226947058662
0.3156987687605091 0.5988189135056683 0.3166762978453674
0.3778186367241290 0.3545105728728803 0.3162734140443637
0.4392777924594272 0.1028181870788952 0.3177601921540387
0.5011042949090481 0.8538664804084657 0.3171508822302459
0.3756356765274558 0.8556574087725479 0.3183550039990943
0.8744789277454990 0.3428606371321553 0.3171331221107917
0.7544367307060967 0.3499167803822685 0.3162689468274549
0.9389480899797187 0.0806811248083577 0.3182995294186269
0.0011794993859772 0.8418620791664102 0.3192387566825364
0.6878293585275278 0.0939535555269789 0.3162429935252857
0.6276807984075716 0.8542953489095340 0.3163871890257696
0.5637813112098451 0.6022011830506108 0.3164991794790725
0.5022758684345121 0.3534656390131043 0.3167000806968686
0.6267195952344854 0.3511295441264953 0.3163641054919290
0.1295195688427228 0.8403350901903068 0.3210627119119439
0.2495124722738464 0.8518024477805686 0.3198098753967680
0.0666938164477960 0.5802658931357619 0.3228498180261021
0.0023711524308858 0.3392036495050877 0.3212818818507168
0.6889279362485345 0.4407346711158149 0.3162136345307293
0.6282371077046177 0.6816725312625950 0.3163670170403691
0.5632045421392221 0.9357285777126357 0.3167732979717380
0.5015564790610115 0.1855703594898928 0.3170419789173475
0.6261702049415341 0.1854117541739721 0.3164352894264024
0.1309148721326388 0.6674028207551883 0.3223675584838264
0.2514087852157982 0.6796248236446057 0.3194047387773302
0.0646020012123893 0.9259769279979583 0.3207454373909193
0.0013591193562636 0.1686041374631205 0.3204290541931583
0.3128766167941431 0.1089655475629334 0.3191398623507389
0.4391928103249764 0.6039726799122196 0.3163467039905234
0.8126710568815313 0.0978151225607200 0.3165478926597400
0.9423741843577843 0.5874380615009775 0.3181812899663389
0.3170044891788219 0.4364182697847733 0.3145870212767856
0.4383784259399136 0.9368706433804881 0.3180185019634035
0.8151474455367197 0.4246661255138005 0.3165311286185861
0.9405449488650316 0.9213328423976962 0.3179727128246554
0.6872812398522474 0.9360168266417841 0.3161801613785210
0.5647927499710008 0.4358523745380891 0.3164403259744752
0.1880011496980135 0.9245930317599369 0.3197817922540356
0.0646090070424108 0.4166946912243696 0.3258288791638040

0.6882315709648296	0.5991757733168148	0.3161906983733572
0.5640279262787732	0.1018377586527639	0.3167553942446775
0.1928757209397949	0.5922782035156537	0.3211842343586838
0.0631069154963957	0.0887723152899058	0.3226931359011675
0.1306855971889500	0.2443862120345697	0.3545449902044134
0.2378470750400064	0.2898954430658251	0.3287680001460959
0.2536339136390977	0.3043330477612746	0.4053125255179214
0.1564781842149965	0.1241502095953155	0.4136251255521030
0.1686446283472104	0.1908930267708115	0.4487524631677487
0.2181141634074650	0.1573688008390479	0.5302403182306423
0.1451344190658288	0.2409212093302089	0.5408476545622647
0.0479746425892340	0.1621795665595644	0.5651586994803663
0.0841016541953591	0.2435925446707051	0.6269509460483547
0.1452701657764167	0.1858571733590524	0.7156898732775936
0.0686667692851479	0.1905021772292100	0.7341754951176893
0.1891071647946534	0.2412364679457737	0.5129605460292251
0.0759121040824387	0.2521022828117337	0.5774553074648668
0.1033763474522946	0.2440987545381854	0.7079510945775329

Final state jk (n = 0)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3120937699229295	0.9436936997244987	0.3212890176541300
0.3758726687064735	0.1855955987549973	0.3197097428142139
0.4402788636802292	0.4376932585134453	0.3172637758401701
0.5011977492402639	0.6857610748167178	0.3172515967702042
0.3763929930071094	0.6878881306646529	0.3177538246364288
0.8722324190284659	0.1703915030159352	0.3175128968452817
0.7527065758404110	0.1793806705706065	0.3166743787428082
0.9395551861893672	0.4263243756764671	0.3186255676859674
0.0014668437772194	0.6628085074410421	0.3196602600046400
0.3153357486721928	0.5991497233744845	0.3179848746761061
0.3777615127495729	0.3547469284440459	0.3178887147512824
0.4389154035870770	0.1026864400081283	0.3190160952006623
0.5004491640443703	0.8537059757101625	0.3178640128009320
0.3749811092382030	0.8559938063432629	0.3194605833161972
0.8735547800419223	0.3409375747306205	0.3175106266551816

0.7538253075472688 0.3491801974051886 0.3166591596716235
0.9376022778700051 0.0783049373882728 0.3181162487179515
-0.0001473814322503 0.8399884260008259 0.3189582314323846
0.6869717378706638 0.0934797652045039 0.3165609368941775
0.6270876414238733 0.8540337716983659 0.3167217531803384
0.5633794103427299 0.6020274900263506 0.3169187565887732
0.5019876022981311 0.3535147201823554 0.3173306217960504
0.6261304204795578 0.3510172222082856 0.3166926353237921
0.1283703644677619 0.8384944299666186 0.3212594135685341
0.2484669517897851 0.8516072059488907 0.3213563365700670
0.0657036493406233 0.5779751974924332 0.3224233927697170
0.0008478301094014 0.3373751007825866 0.3205986174091902
0.6882944892794167 0.4406537762929683 0.3165252690437453
0.6277594110567652 0.6815096024297411 0.3166883025872385
0.5627493799355271 0.9357406243301198 0.3172865495878111
0.5012135245564694 0.1855915372739548 0.3178480977595998
0.6254896359937346 0.1852638771493970 0.3167845607941547
0.1300180192770176 0.6657588326975343 0.3226638338857521
0.2506057523282910 0.6799936227494853 0.3206918488009867
0.0630873877626963 0.9231945912540706 0.3195869930463715
-0.0005229421487124 0.1658131954400048 0.3189353497003159
0.3127529454863056 0.1090078438136059 0.3219436929906839
0.4388279483634647 0.6039799811924463 0.3170218333658210
0.8115148348145594 0.0966710628801984 0.3169456260845826
0.9414183405343340 0.5858650994927752 0.3187285256919531
0.3170603113423915 0.4368338938988103 0.3176702766880148
0.4380329259352634 0.9370471127349582 0.3191195913023991
0.8145136873949012 0.4233931018324489 0.3169504880986925
0.9392558335658376 0.9182633241659809 0.3178840199618202
0.6866030037204848 0.9359910542126475 0.3164578639025015
0.5642563567244809 0.4362727141810598 0.3168713283230600
0.1866812724931373 0.9237552904432866 0.3211375080504367
0.0635055626683756 0.4137059521459578 0.3254985400027510
0.6877062492675974 0.5987889915086784 0.3164693957091195
0.5634196143564536 0.1012862312986024 0.3172696619063178
0.1922312343586595 0.5918364256918962 0.3220953877706368
0.0613048327070219 0.0861873317467578 0.3190731484698496
0.1295948376153898 0.2380386609362411 0.3421128499890694
0.2395036867641665 0.2905967513412910 0.3358162274586943
0.2529201990822272 0.3069616084588032 0.4134222279990191
0.1388391792467620 0.1672485211304419 0.4164310596088086
0.1816012499040356 0.2089271058354597 0.4090504804195074
0.2219349827983776 0.1370866551021791 0.5284792275079957

0.1598406114116905	0.2417987245485080	0.5479757295564213
0.0491515954784740	0.1620488429763876	0.5599810781636867
0.0822354000864828	0.2439080929554086	0.6225439893744543
0.1474205595483359	0.1848979379294149	0.7109431523053474
0.0719771268812824	0.1879135164947315	0.7333669440076626
0.2095859740226513	0.2449497187314009	0.5387691691122481
0.0750487758910906	0.2543274991819739	0.5732821225458913
0.1049873866612256	0.2424472724266459	0.7054573331097708

Final state jk (n = -0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3121085958118698	0.9437402307324155	0.3213031448395289
0.3758800952968914	0.1855491759928105	0.3197179468360151
0.4402591191843723	0.4377407669208756	0.3172636619543585
0.5011405241506435	0.6858181061424766	0.3172470922280442
0.3763825557429053	0.6878349547621322	0.3177567263589312
0.8722080338520669	0.1703818489209544	0.3175168081176406
0.7527350725633798	0.1793763898766883	0.3166689469238451
0.9395537593969410	0.4263284251311053	0.3186318041935017
0.0014504716927658	0.6627040721060454	0.3196655738004273
0.3153660676548738	0.5991201891832533	0.3179872997863497
0.3777714868258400	0.3547822087138110	0.3178825105801340
0.4388918564426243	0.1026145632498965	0.3190183019675394
0.5003975486264537	0.8536492121782099	0.3178651434423898
0.3749709518907335	0.8560512890968710	0.3194664578974267
0.8735212202276215	0.3409177134016017	0.3175142057658447
0.7538513659854574	0.3491522705995225	0.3166555546742348
0.9376091539468330	0.0782862173219859	0.3181265058911247
0.9998342809146148	0.8400998132539259	0.3189574114561353
0.6869456737865860	0.0934322212425373	0.3165510564204410
0.6270888092552570	0.8540740793773419	0.3167114146666938
0.5633927615253063	0.6019432223426512	0.3169105500025947
0.5020133468242085	0.3534678874806320	0.3173325530628634
0.6260927076381921	0.3510305816604050	0.3166813543837643
0.1283887341610101	0.8384643807199487	0.3212533554173888
0.2484370646197527	0.8515753576230876	0.3213611994780340

0.0656773367974115	0.5779103721812983	0.3224297715642273
0.0008490848949822	0.3374643411315962	0.3206079368709976
0.6882634189779069	0.4406779726841717	0.3165169674236336
0.6277625353586419	0.6814528812368605	0.3166773130794910
0.5627572471691110	0.9358148643190929	0.3172815540993245
0.5012437566487318	0.1856024853920103	0.3178502536189051
0.6254481317093299	0.1852336423260173	0.3167727016335762
0.1300423294908526	0.6657431795905276	0.3226720546229808
0.2505807491102460	0.6800158940940689	0.3207049171085282
0.0630722139316090	0.9232315426120922	0.3195840311432454
0.9994856310181812	0.1656974296494005	0.3189595698849815
0.3127619579102988	0.1090380641661924	0.3220092036045302
0.4388509465265769	0.6039350751947629	0.3170248927923318
0.8115106214669842	0.0966782512599475	0.3169478107630782
0.9414534937863707	0.5858499620303910	0.3187359671561348
0.3170794035682888	0.4368134501873016	0.3176890840622781
0.4380407481314831	0.9370732154410800	0.3191167492148776
0.8145111222855960	0.4233529174114223	0.3169522064890223
0.9392866161858497	0.9182462805947313	0.3178874164620845
0.6865581769038197	0.9360303089085755	0.3164473643508273
0.5642200060461673	0.4363607661253091	0.3168659702502589
0.1866764946618790	0.9236852193165952	0.3211379658275851
0.0634379182016584	0.4137065407708055	0.3254569088809786
0.6876629843517247	0.5987410128331093	0.3164618619005902
0.5633961437877411	0.1011676042867378	0.3172632168550293
0.1922373172882839	0.5918594579413303	0.3221459261269028
0.0612697633232182	0.0862170956969086	0.3191071560177365
0.1296508324926377	0.2380019840953772	0.3420950798860548
0.2395467402108916	0.2906705637065702	0.3357561143038581
0.2529251996113732	0.3071569124981389	0.4133652490304435
0.1388983609096720	0.1675041962629888	0.4164847085037212
0.1816818639432477	0.2085178054332851	0.4089911993174585
0.2219977702102435	0.1371606955786971	0.5284730877077288
0.1599027554633705	0.2418317772127667	0.5480430021509904
0.0491819817314964	0.1620934390748694	0.5599257886380063
0.0822229570077941	0.2439129440860338	0.6225251588935116
0.1473836812744251	0.1849647497989488	0.7109384179526324
0.0719370755857763	0.1879225102052111	0.7333536913679103
0.2096560983979324	0.2450010359233799	0.5388354379644074
0.0750861289572742	0.2543413119116323	0.5732541815249713
0.1049429236537341	0.2424967797986080	0.7054468878089131

Final state jk (n = -0.5)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

0.3121215830129632 0.9437666327125797 0.3213237606708151

0.3758904584004053 0.1855004227205220 0.3197450255496954

0.4402559900432229 0.4377820946565789 0.3172680516874164

0.5010990661118820 0.6858383439925051 0.3172439108320302

0.3763738595564463 0.6877105803623533 0.3177644313918338

0.8721737528656960 0.1703846081252076 0.3175172192468286

0.7527448275671160 0.1793916806689244 0.3166655717201705

0.9395403767354757 0.4263607295702756 0.3186555065076570

0.0014307753028581 0.6626848986155980 0.3196864077888874

0.3153909590402580 0.5991193717318987 0.3179792311383055

0.3777932704148834 0.3548288993035475 0.3178973863581346

0.4388872813039954 0.1025584269133107 0.3190250132431493

0.5003625071229735 0.8536109998727961 0.3178645941357421

0.3749650859660052 0.8561609299672246 0.3194801554796871

0.8734799705965477 0.3409000689397951 0.3175224757714837

0.7538624022763036 0.3491220328682630 0.3166508076383586

0.9376156845976140 0.0782428598146474 0.3181282256147741

0.9998145718102075 0.8401538665689582 0.3189424825111509

0.6869160290262105 0.0934456696357399 0.3165430938150554

0.6270791986844488 0.8541424632401126 0.3167032057656477

0.5633868662387372 0.6018584732826782 0.3169036005094600

0.5020275630653819 0.3534450289150949 0.3173339734781980

0.6260466895564447 0.3510656360384040 0.3166727419762096

0.1284207919018936 0.8384282581103526 0.3212388779930543

0.2484317349203604 0.8515744080116291 0.3213691566988025

0.0656552067557741 0.5778659654643383 0.3224483632422111

0.0008668103640042 0.3375431327706355 0.3206176298205609

0.6882337820711758 0.4406712155765558 0.3165093018563910

0.6277563609689358 0.6813686154101628 0.3166676957581929

0.5627442565337579 0.9358711698618550 0.3172775292903923

0.5012564396184629 0.1855931740719960 0.3178521713035954

0.6254007834785467 0.1851828097411085 0.3167630175715266

0.1300830879024901 0.6657334119945801 0.3226832880807093

0.2505812130452138 0.6800304686610608 0.3207167104450708

0.0630634484333907 0.9232626617988320 0.3195680457001356

0.9995140046259841	0.1656105165319998	0.3189886160783500
0.3127914777128492	0.1091574214896185	0.3220712558607719
0.4388533141288359	0.6039296870619452	0.3170321450185738
0.8115009205299448	0.0966801485860596	0.3169508633312918
0.9414836728237633	0.5857804013555964	0.3187325815765533
0.3171069013324965	0.4367306410104261	0.3177179836234146
0.4380213934019932	0.9370390427010905	0.3191093448893001
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0.0633550095796657	0.4138406075065687	0.3252897911940956
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0.5633774540450066	0.1011171467740091	0.3172564464867407
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0.1297310599752579	0.2379478002305233	0.3421268125516387
0.2395670624693760	0.2908339675180897	0.3356130486567626
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0.1599668254927023	0.2418667026409228	0.5481084452745913
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0.1048974214317323	0.2425407811556066	0.7054357996156863

Final state jk (n = +0.25)

C N Fe Ru H O

1.0000000000000000

19.6800003052000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.5216999054000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C N Fe Ru H O

36 16 1 1 9 3

Direct

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