Supporting Information for

Can a Three-Carbon Olefin Close a Five-Membered Ring on Reaction with the Silicon Nitride Radical (SiN, $X^2\Sigma^+$)? A Crossed Molecular Beams and Ab Initio Study

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Beam	v_p (m s^{-1})	S	E_c (kJ mol^{-1})	Θ_{CM} (degree)
Silicon nitride Radical (SiN)	1216 ± 9	4.0 ± 0.1		
Propene (C_3H_6)	833 ± 12	11 ± 0.1	22.8 ± 0.3	35.25 ± 0.5

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) for all reactants, products, and intermediates involved in the reactions between silicon nitride radical (SiN) and propene at the B2PLYP-D3(BJ)/ Def2-TZVPP level of theory. S6-S15

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Table S1. Peak velocities (vp) and speed ratios (S) of the Silicon Nitride radical (SiN) and propene (C_3H_6) beams along with the corresponding collision energies (EC) and center-of-mass angles (Θ_{CM})

Rice–Ramsperger–Kassel–Marcus (RRKM) Calculations

Rice–Ramsperger–Kassel–Marcus (RRKM) theory[1, 2] was applied to calculate microcanonical, energy-dependent rate constants for all unimolecular reaction steps on the potential energy surface of the reaction between Silicon nitride radical (SiN) and propene (C_3H_6). The calculations were performed using our in-house program *Unimol*,[3] which evaluates RRKM rate constants as functions of internal energy within the harmonic approximation. *Unimol* is an enhanced implementation of our earlier code developed for treating multiwell, multichannel unimolecular reaction systems under single-collision conditions and includes numerical solutions of the corresponding first-order kinetic equations.In the present study, the internal energy of each intermediate was defined as the sum of the experimental collision energy and the chemical activation energy, equivalent to the negative of the relative energy of the species with respect to the separated reactants. Because the calculations are intended to model crossed molecular beam experiments conducted under zero-pressure conditions, only a single internal energy level was considered. After determining all RRKM rate constants, product branching ratios were obtained by solving the kinetic equations under the steady-state approximation.

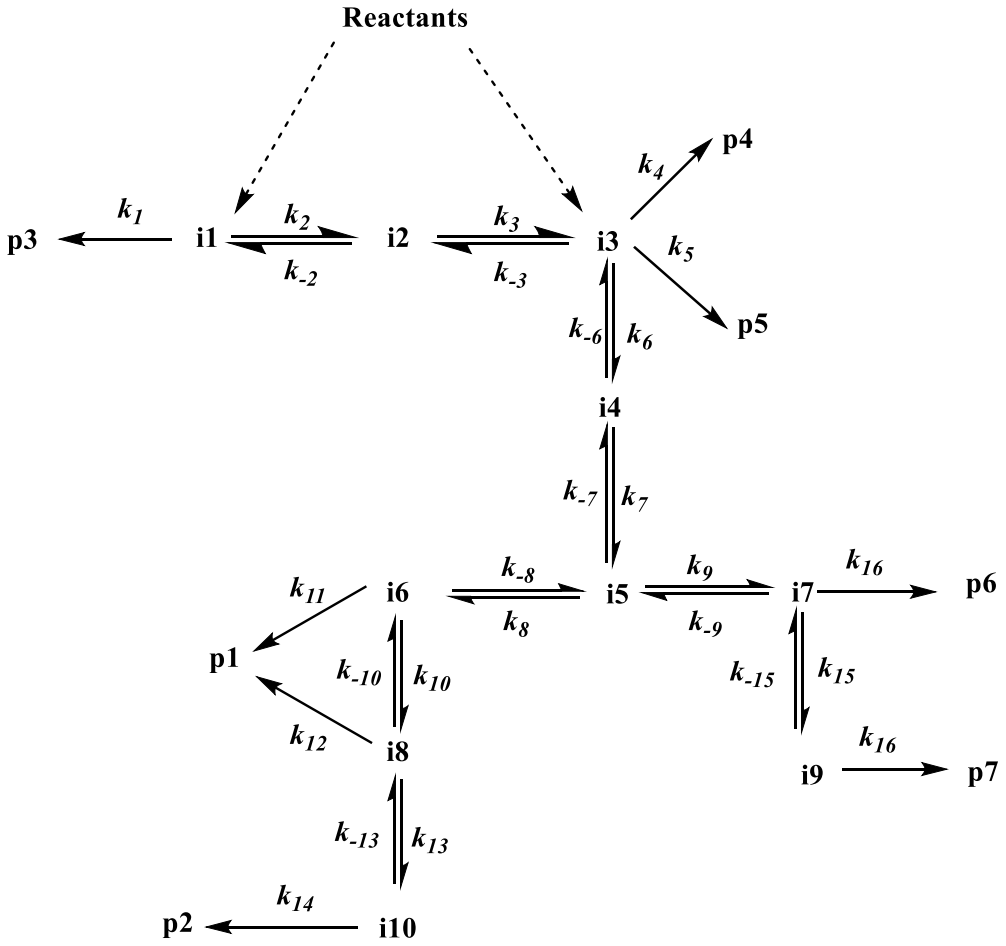

Table S2. RRKM rate constants (s^{-1}) for the reaction of silicon nitride radicals (SiN) with propene (C_3H_6) computed with B2PLYP-D3(BJ)/Def2-TZVPP zero-point energy corrected CCSD(T)-F12/cc-pVTZ-F12 energies, and B2PLYP-D3(BJ)/Def2-TZVPP harmonic frequencies at collision energies of 0.0 kJ mol^{-1} and 22.8 kJ mol^{-1} relative to the entrance channel.

Rate Constant	At 0.0 kJ mol^{-1}	At 22.8 kJ mol^{-1}
k_1	2.00×10^{6}	1.48×10^{7}
k_2	2.42×10^{9}	4.54×10^{9}
k_{-2}	1.67×10^{11}	2.78×10^{11}
k_3	3.90×10^{11}	6.56×10^{11}
k_{-3}	3.06×10^{9}	5.89×10^{9}
k_4	6.36×10^{6}	4.67×10^{7}
k_5	4.91×10^{4}	1.18×10^{6}
k_6	1.03×10^{3}	7.33×10^{4}
k_{-6}	3.00×10^{3}	2.06×10^{5}
k_7	4.86×10^{10}	5.98×10^{10}
k_{-7}	4.13×10^{12}	4.86×10^{12}
k_8	2.92×10^{5}	5.50×10^{6}
k_{-8}	4.61×10^{2}	1.29×10^{4}
k_9	0.00×10^{0}	2.38×10^{3}
k_{-9}	0.00×10^{0}	1.59×10^{3}
k_{10}	7.55×10^{5}	4.33×10^{6}
k_{-10}	5.56×10^{5}	2.85×10^{6}
k_{11}	2.55×10^{8}	8.62×10^{8}
k_{12}	3.47×10^{7}	1.22×10^{8}
k_{13}	1.56×10^{9}	2.92×10^{9}
k_{-13}	3.46×10^{8}	7.93×10^{8}
k_{14}	2.67×10^{8}	7.71×10^{8}
k_{15}	0.00×10^{0}	2.07×10^{3}
k_{-15}	0.00×10^{0}	1.05×10^{4}
k_{16}	0.00×10^{0}	9.38×10^{3}
k_{17}	0.00×10^{0}	1.65×10^{4}

Table S3. Statistical branching ratios (%) for the products of the reaction between Silicon nitride radical and propene at the collision energy of 0.00 kJ mol^{-1} and 24.0 kJ mol^{-1} for the starting intermediate i1 and i3.

Branching ratio (%)				
	At 0.0 kJ mol^{-1}		**At 22.8 kJ mol^{-1}**	
Products	**i1**	**i3**	**i1**	**i3**
p1	0.007	0.007	0.032	0.032
p2	0	0	0	0
p3	14.525	14.424	14.863	14.467
p4	84.813	84.913	83.015	83.401
p5	0.655	0.656	2.09	2.1
p6	0	0	0	0
p7	0	0	0	0

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) for all reactants, products, and intermediates involved in the reactions between silicon nitride radical (SiN) and propene at the B2PLYP-D3(BJ)/ Def2-TZVPP level of theory.

REACTANTS

C3H6 (Cs , ^{1}A')

C	-8.658275	1.147272	-0.815633
C	-7.253023	1.124622	-0.303914
C	-6.323147	0.248752	-0.672647
H	-8.882655	2.099658	-1.298172
H	-9.372768	1.031831	0.000696
H	-8.829353	0.349449	-1.536053
H	-6.993044	1.887818	0.421352
H	-6.537960	-0.529414	-1.393113
H	-5.322725	0.282559	-0.267252

Frequencies:

231.88
431.72
608.44
929.10
942.73
958.12
1039.71
1086.74
1197.80
1331.92
1420.22
1471.66
1499.08
1517.82
1711.19
3034.90
3100.36
3129.55
3146.46
3160.68
3245.36

SiN ($C_{\infty v}$, $^2\Sigma^+$)

Si	0.000000	0.000000	-0.522865
N	0.000000	0.000000	1.047191

Frequency:

1224.48

PRODUCTS

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p1 (Cs, ^{1}A')

C	-8.529753	1.113916	-1.072508
C	-7.276752	1.135843	-0.261754
C	-6.315773	0.273328	-0.631906
H	-9.391264	0.884715	-0.435918
H	-8.717883	2.100026	-1.510790
H	-9.103957	-0.038992	-2.732080
H	-5.377929	0.228530	-0.093795
H	-7.206200	1.831314	0.566937
N	-8.337600	0.102319	-2.095486
Si	-6.845304	-0.761904	-2.132269

Frequencies:

274.54
352.96
516.68
529.16
641.40
678.82
771.71
804.06
919.65
978.40
1019.68
1068.65
1121.10
1189.75
1266.85
1332.45
1409.45
1470.42
1584.93
2999.15
3034.86
3165.65
3190.35
3629.83

p2 (Cs, ^{1}A')

C	-8.425070	1.111538	-1.042441
C	-7.336130	1.209589	-0.271240
C	-6.265561	0.219759	-0.613808
H	-9.171598	0.002612	-2.626483
H	-6.013436	-0.432018	0.231191
H	-5.320461	0.703712	-0.887257
H	-9.311839	1.723692	-0.968996
H	-7.250380	1.938262	0.520287
N	-8.369770	0.106705	-2.027112
Si	-6.913481	-0.842064	-2.090410

Frequencies:

202.53
436.75
514.87
557.12
611.50
631.66
734.98
764.15
809.15
938.23
951.75
1049.26
1075.49
1125.76
1182.49
1331.69
1377.11
1407.52
1652.79
3008.77
3050.52
3204.93
3226.10
3633.47

p3 (Cs, ^{1}A')

C	-8.536498	1.221222	-0.725430
C	-7.087938	1.014842	-0.376870
C	-6.355416	0.006281	-0.871097
H	-8.675590	2.200766	-1.182505
H	-9.146390	1.193943	0.177364
H	-8.887352	0.456230	-1.413368
H	-6.794029	-0.706769	-1.551406
H	-5.317960	-0.111705	-0.599450
N	-6.561271	1.939216	0.490527
Si	-6.023122	3.026715	1.484391

Frequencies:

141.70
160.02
216.95
367.31
517.11
530.99
676.39
734.78
876.05
935.43
1029.83
1071.79
1213.71
1405.29
1429.95
1479.79
1494.36
1510.42
1666.69
3040.00
3112.96
3146.36
3173.09
3275.84

p4 (Cs, ^{1}A')

C	-8.417989	-0.284794	-0.028043
C	-7.200915	0.565445	0.132539
C	-5.957720	0.074071	0.225870
H	-8.952753	-0.039561	-0.947407
H	-9.119018	-0.130739	0.794197
H	-8.160059	-1.342152	-0.058776
H	-7.332849	1.639900	0.175866
H	-5.802590	-1.000376	0.184597
N	-4.828593	0.830989	0.373355
Si	-3.509469	1.664354	0.539173

Frequencies:

137.63
145.06
221.33

347.31
369.71
484.74
828.28
862.81
964.83
968.95
1064.84
1140.50
1308.49
1343.95
1425.31
1485.84
1491.50
1510.36
1683.18
3026.96
3088.71
3125.90
3137.15
3171.15

p5 (Cs, ^{1}A')

C	0.000190	0.037400	-0.003712
C	1.506479	0.024561	-0.002403
C	2.297421	1.090104	0.000965
H	1.941102	-0.968699	-0.004524
H	1.890043	2.090361	0.003088
H	3.371902	0.985309	0.001662
N	-0.586065	1.325508	-0.001063
Si	-1.198316	2.762281	0.003827
H	-0.345375	-0.524364	-0.878257
H	-0.346984	-0.528563	0.867480

Frequencies:
125.81
160.84
272.42
337.17
567.13
574.86
791.83
923.73
945.90
997.24
1032.49
1085.13
1269.35
1324.51
1369.14
1448.85
1480.53
1491.44
1706.72
3007.00
3028.68
3160.40
3175.60
3259.43

p6 (Cs, ^{1}A')

C	-8.516895	1.284460	-0.884063
C	-7.356732	1.207458	-0.196797
C	-6.344092	0.194370	-0.682631
H	-9.163758	-0.407741	-3.257631
H	-6.106917	-0.487645	0.142702
H	-5.405670	0.715890	-0.906025
H	-9.314795	1.965305	-0.635721
H	-7.125160	1.823354	0.664946
Si	-8.266900	0.013939	-2.174896
N	-6.776808	-0.567604	-1.846153

Frequencies:
327.11
385.09
458.76
526.42
670.22
699.99
739.92
852.81
887.91
936.66
959.86
988.21
1057.37
1148.43
1186.86
1278.26
1322.21
1424.54
1544.39

2316.80
2998.30
3028.73
3171.33
3242.10

p7 (Cs, ^{1}A')

C	-8.592606	1.278274	-0.898747
C	-7.233337	1.245400	-0.245276
C	-6.352642	0.368602	-0.786049
H	-9.401562	1.008334	-0.215004
H	-8.843395	2.256596	-1.316229
H	-6.995435	1.880856	0.594127
H	-5.346247	0.255268	-0.402777
H	-9.132401	-0.564465	-3.248620
Si	-8.263543	-0.022245	-2.198809
N	-6.710343	-0.443610	-1.883088

Frequencies:
121.85
382.87
460.67
491.97
627.31
670.18
707.78
733.10
837.14
937.55
956.15
966.07
1050.30
1067.57
1155.65
1209.34
1374.01
1395.91
1549.16
2323.11
3044.70
3090.99
3185.59
3224.89

p8 (Cs, ^{1}A')

C	-8.652814	1.161953	-0.801592
C	-7.241051	1.146052	-0.282226
C	-6.318669	0.255708	-0.665404
H	-8.879910	2.107408	-1.293043
H	-9.370650	1.039034	0.008681
H	-8.798590	0.355218	-1.518609
H	-6.564117	-0.512776	-1.389376
H	-5.308459	0.258318	-0.282121
Si	-6.732219	2.434396	0.968056
N	-6.389877	3.565225	2.025903

Frequencies:
93.56
98.53
188.13
280.45
344.59
377.71
567.43
703.77
941.98
979.81
1031.20
1079.70
1162.02
1229.16
1421.77
1459.61
1495.10
1509.16
1646.48
3035.60
3117.01
3136.48
3140.44
3238.39

p9 (Cs, ^{1}A')

C	-8.350219	-0.159128	0.007368
C	-7.011352	0.489037	0.113163
C	-5.846821	-0.174172	0.160028
H	-8.867660	0.185488	-0.889061
H	-8.974051	0.121635	0.857160
H	-8.270405	-1.242908	-0.027210
H	-7.008970	1.573065	0.153499
H	-5.837625	-1.257529	0.120421
Si	-4.228161	0.695899	0.294686

N	-2.825449	1.425263	0.410115

Frequencies:

57.32
100.38
140.53
226.51
232.92
370.91
707.78
727.59
951.40
1003.16
1077.10
1099.05
1178.69
1256.51
1357.99
1419.00
1484.17
1490.25
1642.61
3039.69
3105.99
3139.06
3159.76
3167.38

p10 (Cs, ¹A')

C	-8.625957	1.205736	-0.849995
C	-7.212291	1.182900	-0.357109
C	-6.346790	0.210119	-0.627747
H	-8.903213	2.175535	-1.264714
H	-8.805330	0.443106	-1.607527
H	-6.907314	2.015178	0.264697
H	-6.620974	-0.639328	-1.238450
H	-5.338172	0.239310	-0.245009
Si	-9.857065	0.872205	0.565134
N	-10.828920	0.628307	1.792703

Frequencies:

65.00
85.33
145.61
259.22
371.87
545.80
694.53
754.64
934.31
961.30
1024.16
1052.16
1163.69
1174.33
1205.54
1337.28
1435.39
1468.23
1693.05
3055.50
3126.32
3155.03
3174.76
3262.30

INTERMEDIATES

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i1 (C1, ²A)

C	-8.584824	1.313481	-1.101239
C	-7.513927	0.954826	-0.071077
C	-6.309456	0.338283	-0.706806
H	-7.211956	1.867578	0.450332
H	-6.440706	-0.356586	-1.523188
H	-5.359095	0.357613	-0.196624
H	-8.192606	2.030007	-1.821589
H	-8.900161	0.417678	-1.634636
H	-9.454245	1.745179	-0.609947
N	-8.045917	0.047652	0.907497
Si	-8.608035	-0.986567	1.938862

Frequencies:

127.57
139.65
184.46
261.01
336.64
441.16

480.34
600.06
715.94
899.81
931.38
1036.98
1150.53
1181.09
1331.60
1357.27
1406.93
1435.48
1471.95
1500.65
1508.15
3027.50
3055.48
3131.92
3139.32
3163.28
3275.51

i3 (C_1, ^2A)

C	-8.558188	1.262490	-1.099621
C	-7.248861	1.177621	-0.405501
C	-6.304516	0.060655	-0.715030
H	-7.107731	1.713604	0.522684
H	-6.201543	-0.049130	-1.799240
H	-5.312256	0.280803	-0.316983
H	-9.039953	2.225015	-0.939373
H	-8.446415	1.105374	-2.174229
H	-9.250869	0.489778	-0.743555
N	-6.764712	-1.183890	-0.169005
Si	-7.323312	-2.508924	0.445988

Frequencies:
62.84
108.00
166.25
249.87
328.18
427.32
534.54
759.80
890.96
924.20
1005.61
1137.16
1154.77
1272.53
1341.95
1390.41
1418.89
1443.52
1486.29
1495.03
1498.98
2991.40
3015.75
3063.94
3065.25
3123.59
3194.75

i4 (C_1, ^2A)

C	-8.434191	1.316547	-1.204400
C	-7.111674	1.358428	-0.534207
C	-6.248456	0.117295	-0.800941
H	-7.234024	1.446064	0.553991
H	-6.082427	0.020717	-1.876956
H	-5.270055	0.259540	-0.336048
H	-8.973555	2.225305	-1.418233
H	-8.937160	0.375010	-1.357150
H	-6.554191	2.244311	-0.847291
N	-6.843503	-1.072318	-0.301891
Si	-7.524319	-2.365057	0.252491

Frequencies:
107.88
133.62

172.67
272.35
334.73
469.64
519.94
704.56
833.57
899.89
1022.84
1057.62
1123.68
1211.02
1291.88
1357.53
1381.71
1462.44
1477.00
1479.36
1505.16
2973.36
3027.06
3060.78
3063.07
3178.63
3284.03

i5 (C_1, ^2A)

C	-8.355595	1.244700	-1.317814
C	-7.421263	0.990704	-0.092479
C	-6.197684	0.161574	-0.517513
H	-5.764920	-0.436654	0.277946
H	-5.416973	0.756410	-0.992246
H	-9.365278	1.459852	-0.965585
H	-7.118229	1.936989	0.356380
H	-7.981403	0.428062	0.655297
H	-8.004778	2.131469	-1.855930
N	-8.374850	0.131847	-2.276761
Si	-7.141854	-0.859539	-1.855661

Frequencies:

165.02
247.27
417.84
535.53
584.16
714.72
807.94
844.99
884.55
930.24
1000.64
1022.70
1081.95
1134.61
1235.51
1246.45
1334.36
1337.71
1460.43
1487.91
1496.09
3009.45
3052.30
3069.39
3074.85
3104.56
3156.19

i6 (C_1, ^2A)

C	-8.509218	1.062742	-1.101662
C	-7.485556	0.966585	-0.022877
C	-6.302010	0.155230	-0.585161
H	-5.758575	-0.377520	0.193315
H	-5.577663	0.823188	-1.066345
H	-9.385779	1.691027	-1.074832
H	-7.199471	1.949939	0.351337
H	-7.920490	0.426696	0.831273
H	-9.125615	0.000870	-2.714265
N	-8.388658	0.076278	-2.028369
Si	-6.976675	-0.986666	-2.000754

Frequencies:
161.62
321.64
434.03
488.54
569.89
604.14
707.79
754.66
782.24
882.15
910.16
1000.12
1093.31
1139.30
1141.49
1252.21
1278.07
1354.20
1433.21
1456.88
1484.06
2952.36
3011.07
3076.41
3109.89
3222.95
3593.88

i7 (Cs - ²A'')

C	-8.693685	1.070490	-0.841450
C	-7.445978	1.054250	-0.004514
C	-6.376088	0.105730	-0.656417
H	-6.117835	-0.690599	0.047060
H	-5.450969	0.661194	-0.831188
H	-9.548904	1.658498	-0.548532
H	-7.044992	2.068707	0.092231
H	-7.675979	0.729009	1.015172
H	-9.149381	-0.369803	-3.366380
Si	-8.328597	0.007293	-2.210481
N	-6.797303	-0.506400	-1.913841

Frequencies:
94.60
298.12
499.36
533.46
598.42
629.48
721.89
776.87
839.68
841.63
894.72
992.62
1002.49
1075.16
1164.50
1171.72
1233.05
1305.53
1333.56
1455.07
1484.83
2314.82
3007.57
3022.34
3029.89
3052.25
3234.21

i8 (Cs - ²A'')

C	-8.522510	1.159344	-1.081262
C	-7.398314	0.963604	-0.123604
C	-6.328489	0.015656	-0.538672
H	-6.142530	-0.768315	0.206250
H	-5.352088	0.507224	-0.662109
H	-9.492392	0.941295	-0.615987
H	-7.386508	1.505610	0.811172

H	-8.961051	0.258341	-2.933040
H	-8.582453	2.198620	-1.432105
N	-8.267982	0.249806	-2.201346
Si	-6.871345	-0.743864	-2.229181

Frequencies:

38.34
228.89
350.35
506.90
542.67
606.51
666.99
720.90
798.73
903.72
950.00
1017.87
1053.44
1107.53
1171.08
1188.13
1260.84
1357.88
1415.36
1430.91
1504.84
2964.85
2965.71
2979.17
3001.59
3198.92
3611.96

i9 (Cs , ^{2}A'')

C	-8.441075	1.474726	-1.126388
C	-7.175555	1.285721	-0.337381
C	-6.316944	0.079637	-0.654142
H	-6.183933	-0.535962	0.244733
H	-5.304609	0.396460	-0.935358
H	-9.342873	1.478036	-0.505431
H	-6.895827	1.977571	0.444982
H	-9.161553	-0.542793	-3.251977
Si	-8.260594	-0.055506	-2.198150
N	-6.873819	-0.754980	-1.728917
H	-8.462272	2.410937	-1.694141

Frequencies:

132.50
273.65
345.03
463.50
476.45
641.66
669.64
715.22
819.48
851.96
924.75
926.41
1033.88
1039.66
1124.52
1163.75
1191.16
1306.63
1342.45
1440.14
1474.79
2299.58
2978.19
2987.63
3008.27
3027.47
3193.38

i10 (C_1, ^{2}A)

C	0.004604	-0.000772	-0.000323
C	1.506469	-0.019869	-0.006192
C	2.146511	1.158697	0.016473

H	-0.377386	-0.482013	-0.908196
H	2.006253	-0.981135	-0.021678
H	-1.390832	1.574136	-0.023324
H	-0.368618	-0.589676	0.846131
N	-0.411655	1.391101	0.099678
Si	0.887345	2.525673	-0.042519
H	3.224749	1.217088	0.003186
H	0.943268	3.517363	1.074882

Frequencies:

192.31
341.36
369.91
516.98
610.75
666.39
682.44
729.94
792.71
833.75
916.92
987.64
1019.01
1069.58
1137.07
1212.02
1268.60
1339.15
1414.15
1500.68
1605.91
2115.61
2993.61
3011.24
3172.58
3216.04
3663.81

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