Electronic Supplementary Information to accompany a manuscript submitted to *RSC Advances*]

A computational study to unravel the selectivity in an iron-catalysed [3+2] cycloaddition of aziridine and heterocumulenes

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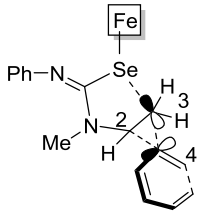
Table of Contents *Page number*

S1. Anchimeric assistance in TS-4'

In TS-4', the C^3 carbon, being incipient carbocationic (primary) in nature, is very electron deficient and the neighboring –Ph group from the C^2 carbon offers some stability by neighboring group participation or anchimeric assistance. The hybridization of the C^4 carbon in the phenyl ring is slightly changed from pure SP^2 toward SP^3 so that efficient overlap of the *p*-orbital of the C^4 can happen with the LUMO of C^3.



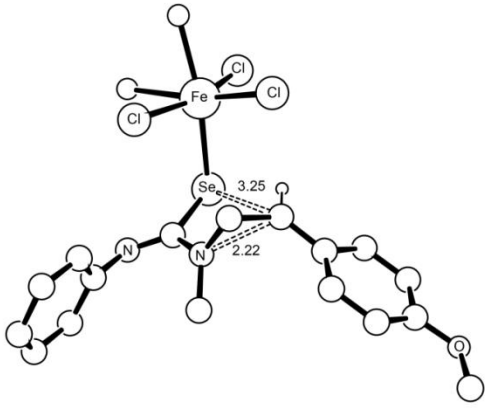


Figure S1. Computed transition state structure for major product formation where the substrate is *N*-methyl-2-(4-methoxyphenyl)aziridine. The transition state is concerted, asynchronous in nature and the cleaving and forming 'bonds' are provided in Å. All the hydrogens except for that on C^2 have been removed for clarity.

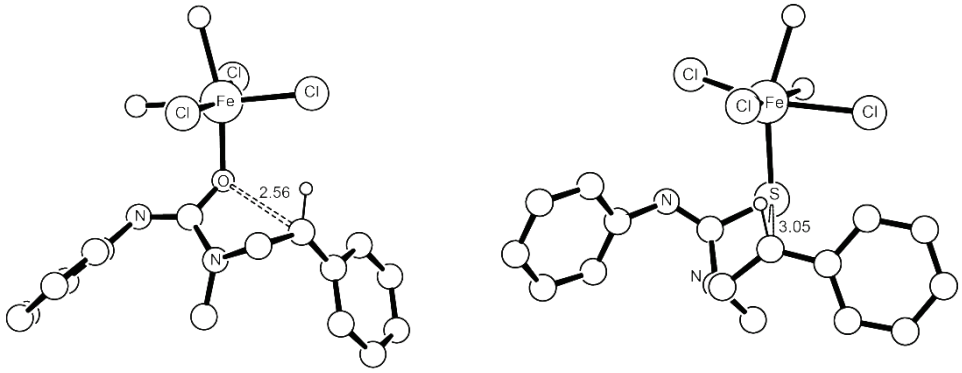


Figure S2. Computed transition state structures for major product formation where phenyl isocyanate (left) and phenyl isothiocyanate (right) are involved as heterocumulene substrates. Both transition states are concerted, asynchronous in nature which was observed for the heterocumulene phenyl isoselenocyanate. The length of the newly formed bond at the TS is represented in Å. All the hydrogens except for that on C^2 have been removed for clarity.

S2. Coordinates and vibrational frequencies of investigated structures

Table S1. Cartesian coordinates

1			
Fe	0.524316593	2.192434259	-0.098924610
Cl	1.866338546	1.216523642	1.584279935
Cl	2.085138027	2.518531125	-1.637850768
Cl	-1.286987365	3.201523572	-1.065852418
O	-0.062121533	0.229598232	-0.678963170
H	0.492672650	-0.369129445	-0.157084906
H	-0.968970915	0.115664633	-0.362508445
O	0.930494112	4.054669721	0.938631710
O	-1.014951668	1.780809632	1.505330491
H	-0.500251712	1.755924602	2.324838662
H	-1.601809996	2.547769890	1.537320975
H	0.889442778	4.756579027	0.274157269
H	1.852100630	3.985111555	1.228032007
N-Me-phenyl aziridine			
H	-0.281985441	1.729327849	-0.498787953
C	-0.078758011	0.839507750	0.108648636
C	-0.854061986	0.769423135	1.378707840
N	-1.176277852	-0.092196837	0.267018595
H	-1.529444730	1.600722287	1.598036787
H	-0.409645101	0.283935745	2.247957876
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H	-2.311309921	-0.145610137	-1.484372739
H	-2.590453917	1.316409324	-0.500868844
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C	3.915703182	-0.664316722	-0.204486570
C	1.586669210	-1.022207225	0.314454194
C	2.332527418	1.135461198	-0.443223094
C	3.634098555	0.656458051	-0.537167055
C	2.887432523	-1.501170068	0.219470111
H	0.769142878	-1.669192376	0.627509789
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H	4.430563780	1.316139081	-0.875081591
H	3.100283003	-2.537675536	0.473182144
H	4.932990696	-1.041967849	-0.279838748
H	-3.243142464	-0.258270980	0.022672857

Ph-isoselenocyanate			
N	-0.421790060	-0.408667167	-0.904078868
Se	-2.176992661	-2.700334919	-1.437525394
C	0.344990789	0.729432357	-0.860964529
C	0.993844914	1.081206892	0.325915936
C	0.471590327	1.527477128	-2.002858484
C	1.766147192	2.233489036	0.364012538
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C	1.247325355	2.676134626	-1.946992308
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Fe	0.508999034	1.973947971	-0.204607913
Cl	1.756117390	2.097738476	1.624672870
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H	0.273268068	3.898054528	-2.089658328
C	2.727003136	4.903852045	0.045576117
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4

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4-TS

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Cl	2.047964187	-0.663196728	1.579666968
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Se	0.121277077	-1.245589576	-1.483937794
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C	1.718448564	2.845444426	0.502863882
C	1.758918533	3.622371308	-1.786411026
C	2.071203325	4.119411585	0.930756641
H	1.608261839	2.024541072	1.210711896
C	2.089635648	4.896904075	-1.344926215
H	1.651808450	3.400702244	-2.846320099
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H	2.215022357	4.304065190	1.993498602
H	2.238366689	5.694390704	-2.069980073
C	0.264458799	0.620040934	-0.914509265
C	-1.233991193	0.514432524	1.111376146
C	-2.200167853	-0.418312139	0.505615649
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C	-4.261988363	0.979076374	0.584270953
C	-5.490288008	-0.896990236	-1.096597682
H	-3.607764332	-1.945842267	-1.056931892
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H	-3.794746596	1.685640425	1.266137008
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H	-5.977113214	-1.616176787	-1.749101815

H	-6.140847257	2.014277270	0.555337658
H	-7.221461575	0.370708843	-0.944789581
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4-TS'

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Fe	-3.027907778	-0.095369512	-0.619412182
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Se	-1.486207189	0.277950509	1.397566026
C	2.057416042	2.349368101	0.973909056
C	2.376983304	3.554120596	0.341507093
C	3.087005879	1.560253166	1.503187282
C	3.705257035	3.927135929	0.186872492
H	1.566451487	4.171210512	-0.040196462
C	4.412906708	1.950502016	1.358199435
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C	4.730499378	3.127947699	0.687315573
H	3.942802879	4.856873413	-0.326031584
H	5.204627490	1.332835033	1.778387088
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C	0.431738102	-1.218906334	-0.465200663
C	0.204536340	-1.987765317	0.709964515
C	1.556636988	0.711839737	-1.420964481
H	1.317586350	0.138605956	-2.323448849
H	1.184238415	1.729141434	-1.564720945
H	2.646071589	0.745923874	-1.281284008
H	-0.225362300	-1.413618499	-1.321442613
H	-0.556635823	-2.765600889	0.707468580
N	0.882389190	0.089116566	-0.284337337
O	-4.661640337	-0.788686564	-2.020598185
O	-4.308147465	-1.042560228	0.873525101
H	-4.770548540	-0.027018533	-2.605018998
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C	2.811063356	-2.125883944	0.092614153
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H	0.231549750	-3.774642481	-1.443857034
H	4.832541254	-2.829012466	0.206584264
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Se	-0.567296468	-0.917413788	-0.922581798
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C	2.232881487	2.717795635	0.269794218
C	1.576892746	3.746298543	-1.819293337
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C	2.348531636	4.858217844	-1.506056739
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C	3.065624728	4.908835008	-0.314152779
H	3.577935973	3.852094801	1.491943704
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H	3.673959731	5.778204323	-0.076618529
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C	-1.710737989	0.469157972	1.228371592
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C	-5.815764548	-0.820755509	-1.674498796
H	-5.813591737	-2.934432456	-1.262822994
H	-5.539526214	1.298752373	-1.934345887
H	-6.763501762	-0.843289677	-2.207071536
C	-0.957533607	2.808099093	0.906430276
H	-1.973160182	3.102415132	1.196648637
H	-0.290881570	2.912298281	1.774865564
H	-0.606057827	3.478913837	0.120448610
H	-1.104939799	0.181158440	2.100463132
H	-2.633167534	0.941474481	1.593164850
H	-1.960426992	-1.670104837	1.032704589
N	-0.992785379	1.441885299	0.418497386
O	2.902370376	-3.406821885	1.355489677
O	1.572420232	-3.643323390	-1.104358466
H	3.142416905	-3.940558248	0.584361295
H	2.359674569	-3.981128616	1.917146171
H	0.711498884	-4.085027259	-1.083350503
H	1.691175822	-3.219841596	-1.964366475

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Fe	-2.903432226	0.086802855	-0.648704827
Cl	-1.384697461	0.708105858	-2.185291503
Cl	-3.027201928	-2.193126626	-1.253307341
Cl	-3.423078142	2.139850216	0.205901759
N	0.546558398	1.711656180	1.056824304
Se	-1.261426913	-0.398434441	1.442838383
C	1.679342288	2.490409777	0.809019707
C	1.508616636	3.747974153	0.221396899
C	2.958508239	2.080946321	1.201164171
C	2.608771556	4.562480326	-0.006632237
H	0.502853433	4.052650140	-0.060163239
C	4.050187799	2.912715776	0.985032041
H	3.081030901	1.110216433	1.680753325
C	3.884186797	4.151935852	0.374411397
H	2.468125784	5.531859425	-0.480180911
H	5.041043080	2.587269520	1.295645948
H	4.742394613	4.796674551	0.200984974
C	0.371555246	0.511026412	0.726369785
C	0.488018925	-1.682850375	-0.321654157
C	-0.358506610	-2.069009228	0.880549413
C	1.888062429	0.184795360	-1.162713248
H	1.717186482	-0.409407536	-2.066789272
H	1.616468748	1.221038010	-1.378559184
H	2.952891117	0.142467777	-0.903718733
H	-0.167710264	-1.637361934	-1.209974376
H	-1.107096990	-2.819914260	0.614665682
N	1.048975817	-0.350365627	-0.092712243
O	-4.576894230	0.308418311	-2.071578677

O	-4.445576109	-0.600522629	0.781933471
H	-4.473103799	1.192382517	-2.450193336
H	-4.355511149	-0.325006677	-2.769762588
H	-4.892208753	-1.343843383	0.354711105
H	-5.080779903	0.119687886	0.892077476
C	1.544240165	-2.732143875	-0.543147871
C	2.740878711	-2.719272470	0.173830930
C	1.283387732	-3.776737564	-1.427422117
C	3.670969995	-3.735744495	-0.003166331
C	2.211033059	-4.798380767	-1.597896155

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TS involving *P*-OMe-aziridine

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Fe	1.124283888	-2.545015830	0.497701064
Cl	-0.800990862	-2.861078668	1.706773561
Cl	1.028305781	-4.452442837	-0.889852535
Cl	1.994230327	-0.692175686	1.628151393
N	1.310997052	1.359426808	-1.378362022
Se	0.284383560	-1.230509393	-1.545895909
C	1.585048366	2.643635160	-0.888726014
C	1.748993408	2.878355088	0.482407949
C	1.779769477	3.689084414	-1.795342737
C	2.074328691	4.152612105	0.929986457
H	1.649086391	2.044238210	1.176851011
C	2.084194749	4.963195037	-1.334268248
H	1.680127948	3.480653247	-2.858727696
C	2.230980763	5.202712364	0.029306943
H	2.210315076	4.324825763	1.995947366
H	2.219460413	5.773930065	-2.047330358
C	0.345805885	0.643834209	-0.967264470
C	-1.238115437	0.471304317	0.984056409
C	-2.228121613	-0.426197155	0.357360863
C	-3.574733877	-0.161118935	0.080700002
C	-4.272638032	-1.073534908	-0.758319966
C	-4.285709873	0.945984937	0.604086400
C	-5.592008388	-0.882344151	-1.065809820
H	-3.728424181	-1.926328281	-1.159531062
C	-5.614006356	1.146648978	0.301331012
H	-3.782412067	1.639927442	1.273315369
C	-6.273932359	0.233930377	-0.543396273
H	-6.141643369	-1.563261200	-1.708989339
H	-6.141955516	1.997905354	0.718549330
C	-1.333115045	2.429640454	-0.538331048
H	-2.431505344	2.350843970	-0.569110877
H	-1.049240197	3.195540046	0.199190146
H	-0.993907695	2.754606141	-1.524133284
H	-0.432524600	-0.075089363	1.486514573
H	-1.644784421	1.219835599	1.674188480
H	-1.807830284	-1.350045793	-0.038506126
N	-0.760296238	1.137308705	-0.228377015
O	2.348049788	-3.826258379	1.813323993
O	3.254974990	-2.452651407	-0.449285835
H	3.230382120	-3.530013339	1.546736391
H	2.218689710	-4.683226510	1.379554096
H	3.050107831	-2.859033545	-1.303856918
H	3.333126223	-1.500037153	-0.601753070
H	2.481374926	6.198679890	0.387032178
O	-7.549571892	0.340939924	-0.904415404
C	-8.316546089	1.438976294	-0.437560547
H	-7.887611488	2.390950268	-0.773391078
H	-9.309939685	1.317190307	-0.870067456
H	-8.392696348	1.431142165	0.656411927

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TS involving Ph-isocyanate

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Fe	0.796158085	-2.391538560	0.154592425
Cl	-1.297364874	-3.247681653	0.480829804
Cl	1.356806847	-3.803077664	-1.685202498
Cl	0.958821842	-1.047427312	2.077703040
N	1.784162862	0.807852766	-0.891828573
O	0.218468433	-0.843513157	-0.927844106
C	2.163590619	2.093367769	-0.476196103
C	3.407134286	-4.777113803	-0.888785044
H	2.940640551	-1.897195965	0.861983166
H	0.343324886	-3.782685318	-1.980404245
H	4.607285594	-3.715561887	0.550141079
H	2.001915205	-5.609424961	-2.291674848
H	4.136811158	-5.571630754	-1.027334828
H	0.256026525	-2.407666819	1.721571790
C	1.859784952	2.570242803	0.805316217
C	2.924809159	2.890216637	-1.336447833
C	2.281637387	3.835059798	1.195560270
H	1.319259326	1.919552543	1.492575219
C	3.335953834	4.157294300	-0.939889224
H	3.177314646	2.497619326	-2.319808859
C	3.012270177	4.639773376	0.325074744
H	2.045324770	4.191024758	2.196467446
H	3.918635128	4.770668910	-1.624240925
H	3.340188985	5.628571317	0.636455753
C	0.565940382	0.388381396	-0.812134075
C	-1.620273222	0.849757095	0.277311232
C	-2.229027912	-0.156995383	-0.610116598
C	-3.064754894	0.063233463	-1.726167403
C	-3.225773237	-1.028506414	-2.612742365
C	-3.748544471	1.274356882	-1.981457665
C	-4.027871922	-0.903332828	-3.730990291
H	-2.687529014	-1.952459512	-2.400511890
C	-4.558732285	1.384048302	-3.095888820
H	-3.669894444	2.100832906	-1.278635253
C	-4.689904243	0.301310767	-3.969214112
H	-4.142680979	-1.736200361	-4.418896666
H	-5.098720555	2.306468005	-3.290783939
H	-5.327232544	0.397914522	-4.845466318
C	-0.683372494	2.509140877	-1.342050407
H	-1.542258467	2.464157738	-2.034407816
H	-0.820589836	3.357301182	-0.656690981
H	0.213695601	2.684597233	-1.938321949
H	-1.211613211	0.403656330	1.192373032
H	-2.245116432	1.715886856	0.522651135
H	-1.927437230	-1.192317643	-0.432140874
N	-0.543616829	1.271123980	-0.619433887
O	1.889326432	-3.857672905	1.301413941
O	2.882896107	-1.692833947	-0.256501481
H	2.620979207	-3.346211135	1.674687158
H	2.256829738	-4.422730120	0.604234965
H	2.995113216	-2.108846620	-1.125352734
H	2.742609139	-0.733982311	-0.447831646

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TS involving Ph-isothiocyanate

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Fe	1.087212990	-2.170299430	0.155115735
Cl	0.560687470	-1.199173756	2.135360702
Cl	-1.014763331	-3.548358702	-0.050924630
Cl	3.255566805	-1.643067482	-0.155320651
N	1.503929906	1.201076999	-0.430801941
S	-0.072312064	-0.691889725	-1.451571442
C	1.855055018	2.445766204	0.093846514
C	2.411856415	2.435667769	1.380042357
C	1.732099248	3.658684750	-0.596760979
C	2.786793480	3.626586610	1.984740610
H	2.527805945	1.474053855	1.877226057
C	2.140925267	4.840483979	0.007581934
H	1.335081440	3.658041847	-1.608472127
C	2.655904088	4.833075674	1.300943512
H	3.201726419	3.610972070	2.990094279
H	2.056387801	5.778083079	-0.538225606
H	2.967926288	5.763671044	1.769494575
C	0.401842278	0.955621296	-1.008187831
C	-1.351788628	2.127564914	0.152237467

C	-1.788477918	0.781529477	0.599491184
C	-3.041306793	0.179645866	0.424028147
C	-3.176655934	-1.164015782	0.862824740
C	-4.146916804	0.828669695	-0.184023738
C	-4.369551424	-1.835684966	0.683122427
H	-2.312582941	-1.665860639	1.298275617
C	-5.333548855	0.148488848	-0.350455190
H	-4.056989412	1.860468037	-0.516566683
C	-5.441413783	-1.180906857	0.078614234
H	-4.456044040	-2.873461275	0.993389717
H	-6.184587674	0.637146263	-0.816660392
H	-6.380055071	-1.710948745	-0.067824550
C	-1.529580460	1.806800800	-2.284032634
H	-2.237259774	0.961422228	-2.234709349
H	-2.091355430	2.742829425	-2.396057118
H	-0.913993159	1.663302318	-3.177422737
H	-0.648155324	2.569250056	0.870877245
H	-2.174764413	2.832779341	-0.010212819
H	-1.034687824	0.182650987	1.122127419
N	-0.654486864	1.927289685	-1.133750688
O	1.713359411	-4.051998994	1.075672201
O	1.438614104	-3.503189980	-1.678319114
H	2.339029085	-4.411866009	0.432543756
H	0.888612224	-4.557745272	0.974503758
H	0.515348081	-3.691742119	-1.913119729
H	1.797904080	-2.899320324	-2.341247258

Table S2: Vibrational frequencies of the investigated structures

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1
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-54.46 92.11 100.87 113.07 123.79 133.23
146.39 156.45 162.79 165.21 209.48 239.64
254.55 297.16 325.38 346.69 354.57 363.38
542.07 583.84 599.53 618.36 661.54 691.00
1566.28 1588.27 1606.81 3789.24 3794.03 3795.27
3918.02 3919.95 3926.05 3177.10 3186.05 3193.57

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N-Me-phenyl aziridine
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51.45 105.12 160.40 223.90 267.34 326.18
392.40 412.46 432.75 539.71 590.18 624.49
707.49 757.10 772.54 840.26 856.63 920.60
950.01 966.52 970.84 992.07 1009.83 1043.54
1056.88 1077.57 1093.94 1102.22 1119.93 1159.97
1164.30 1180.33 1207.55 1248.36 1300.43 1328.93
1380.08 1426.58 1436.79 1466.98 1470.35 1480.96
1508.40 1539.71 1660.06 1683.94 2954.67 3074.60
3077.45 3079.19 3124.90 3154.88 3167.65 3176.76

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Ph-isoselenocyanate
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41.11 67.70 246.88 286.03 357.94 400.17
416.02 460.59 507.34 614.35 627.62 694.52
769.10 846.09 858.81 921.65 969.40 996.34
1007.64 1049.56 1096.60 1163.92 1175.49 1261.88
1314.81 1363.60 1481.69 1520.09 1643.21 1661.10
2188.01 3164.53 3172.28 3182.07 3189.05 3193.15

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2
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55.93 75.98 90.84 124.54 141.60 144.94
173.31 237.98 246.56 321.05 329.41 364.38
376.16 382.02 463.92 544.48 565.82 661.58
1535.79 1623.97 3795.52 3814.71 3911.28 3958.03

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3
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16.55 37.59 45.01 51.66 75.87 78.83
84.07 87.33 93.51 101.87 126.52 130.98
152.38 159.05 169.14 181.79 198.94 248.80
276.74 279.37 293.08 329.04 339.19 350.54
360.50 378.87 410.96 477.82 506.44 525.29
573.79 597.21 622.04 625.77 671.73 687.15
764.04 839.09 842.82 927.89 972.87 999.27
1008.01 1051.58 1101.99 1164.86 1177.91 1239.13
1320.62 1377.07 1485.39 1517.43 1559.64 1580.32
1651.65 1664.89 2277.92 3180.27 3189.94 3195.08
3201.60 3207.44 3797.06 3798.59 3926.80 3933.29

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3-TS
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-231.61 13.21 17.32 25.67 29.30 33.82
47.09 52.93 56.13 58.47 78.33 80.33
87.60 95.52 100.44 116.01 128.80 132.34
138.58 148.54 153.83 158.78 163.39 185.28
192.35 199.37 204.81 232.01 260.17 263.76
267.86 293.11 319.75 335.45 343.54 345.02
377.17 397.50 410.37 413.74 437.96 465.78
488.51 527.31 533.42 538.12 590.98 594.04
614.15 623.02 624.19 629.96 675.51 693.05
706.91 752.68 765.88 770.42 810.17 829.63
850.41 855.58 914.20 923.46 928.45 966.74
974.08 977.76 996.34 1001.34 1001.72 1010.03
1023.99 1045.98 1057.67 1084.21 1098.98 1113.61
1123.55 1132.37 1152.55 1162.46 1163.85 1175.24
1189.18 1209.43 1239.94 1249.27 1314.83 1320.76
1345.91 1364.43 1378.35 1416.06 1417.32 1455.63
1462.44 1472.60 1483.29 1493.86 1515.06 1540.60
1560.43 1580.70 1640.64 1656.21 1661.75 1680.68
2111.28 3014.86 3097.31 3105.71 3119.10 3120.00
3157.06 3158.21 3163.62 3164.47 3172.23 3175.15
3175.34 3184.75 3193.61 3194.96 3195.63 3785.66
3792.99 3919.58 3929.67

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4
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15.46 25.94 26.55 38.69 41.77 50.94
62.32 65.26 73.17 76.06 84.01 96.86
109.74 113.18 124.46 131.46 141.92 148.83
156.53 160.50 163.67 170.46 196.01 200.42
210.17 213.94 242.42 255.86 274.80 295.81
300.70 313.61 327.16 339.07 345.23 405.33
409.56 410.11 433.61 455.79 486.10 520.32
550.05 555.68 581.00 606.86 615.87 622.89
638.32 642.62 649.95 684.82 699.53 705.26
730.29 757.22 776.69 792.65 812.16 836.74
846.60 858.03 879.44 904.98 933.44 961.85
975.06 982.92 990.01 1002.09 1004.46 1007.13
1012.07 1050.51 1057.86 1095.62 1097.88 1124.59
1132.85 1146.89 1160.28 1161.80 1166.37 1174.65
1193.55 1231.43 1241.66 1247.60 1310.54 1313.69
1335.23 1368.52 1382.18 1408.45 1418.54 1445.48
1459.97 1466.80 1480.26 1494.50 1516.29 1541.16
1559.04 1581.75 1645.78 1656.66 1665.77 1679.42

1781.44 3058.40 3124.29 3133.48 3150.37 3161.96
3164.51 3167.59 3177.16 3178.25 3179.47 3182.88
3190.06 3192.22 3199.21 3200.51 3231.46 3763.04
3784.92 3916.29 3924.12

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4-TS

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-164.31 14.20 25.19 30.96 35.54 39.61
50.77 70.13 75.31 83.65 90.84 96.77
97.88 119.17 123.10 129.26 139.16 144.19
151.91 154.20 158.17 172.65 181.78 189.67
204.72 215.10 224.21 256.95 259.11 279.84
282.04 304.33 318.89 332.45 337.52 343.83
388.17 410.67 412.71 428.83 461.59 476.57
514.63 546.13 556.48 605.84 616.47 620.05
622.84 639.12 647.35 671.25 677.92 687.69
704.18 755.92 772.74 802.20 822.41 836.39
848.08 856.89 882.22 916.40 958.22 963.10
985.00 986.54 993.11 1005.95 1007.33 1016.26
1034.67 1050.54 1053.28 1096.53 1100.35 1110.32
1119.78 1157.33 1158.95 1171.42 1175.54 1189.80
1226.69 1253.38 1275.92 1311.85 1315.24 1324.82
1340.99 1368.57 1405.51 1425.54 1446.88 1458.23
1463.59 1465.54 1481.96 1496.36 1518.86 1552.15
1581.81 1615.97 1630.64 1646.17 1663.03 1666.41
1694.18 2991.55 3052.99 3063.65 3125.81 3162.21
3166.55 3172.16 3178.97 3179.68 3182.50 3185.15
3186.70 3192.01 3195.61 3204.20 3208.79 3781.47
3783.98 3901.20 3906.67

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5

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8.23 19.50 28.35 36.12 40.07 49.15
57.26 68.67 78.41 81.31 87.28 97.72
110.28 121.65 129.97 132.60 140.00 153.87
160.17 175.62 182.13 187.82 198.67 205.42
227.73 239.28 242.27 257.30 269.79 309.87
319.21 329.09 349.18 357.29 366.48 381.13
410.54 411.15 420.50 461.71 502.15 506.55
531.77 547.34 592.73 611.90 615.48 616.78
622.88 649.16 678.97 695.67 702.55 709.79
744.47 769.06 784.55 788.33 827.74 846.76
856.52 901.19 917.82 926.42 962.23 969.04
983.85 996.80 1002.97 1005.74 1011.03 1025.33
1052.05 1058.35 1083.68 1096.68 1109.45 1121.58
1158.15 1162.11 1163.60 1177.11 1189.09 1214.83
1235.27 1240.27 1286.45 1311.89 1314.39 1330.25
1363.03 1366.15 1382.56 1403.66 1433.77 1452.08
1464.16 1482.65 1488.73 1491.59 1522.62 1530.18
1553.37 1621.81 1644.05 1654.19 1667.02 1675.42
1798.45 3009.38 3021.48 3076.96 3092.33 3103.14
3151.70 3151.84 3155.20 3162.31 3165.66 3173.33
3173.66 3181.80 3184.94 3193.87 3194.45 3741.25
3786.34 3864.12 3931.18

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11.57 19.37 27.50 36.12 43.70 50.25
67.90 74.90 80.76 81.87 95.80 100.60
106.09 115.83 121.25 126.45 135.38 154.03
157.09 161.54 176.14 192.68 212.61 216.88
225.87 231.08 244.02 256.95 271.02 273.47
294.46 315.08 342.75 347.42 351.18 373.54
412.53 414.53 440.74 483.72 520.21 521.56
537.59 550.23 599.63 602.92 611.31 623.07
629.18 632.14 665.12 667.62 699.98 709.58
718.49 766.03 773.23 814.39 843.40 848.86
861.19 887.94 903.99 928.28 938.92 959.87
972.10 983.18 996.81 1005.32 1009.72 1033.88
1051.23 1056.54 1086.59 1094.37 1103.29 1119.76
1153.12 1158.85 1163.15 1173.24 1182.33 1204.76
1224.57 1246.70 1265.76 1309.98 1311.50 1321.16

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4-TS'

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-276.44 14.63 30.17 32.00 47.67 58.24
63.60 68.61 73.86 82.92 91.37 97.37
107.76 113.37 115.68 131.27 147.54 151.10
153.89 163.17 165.34 167.26 182.53 198.55
215.20 225.04 234.78 247.41 252.37 259.16
274.36 297.35 323.59 326.60 344.70 347.60
365.28 405.64 410.13 418.46 428.36 507.07
527.98 546.93 594.99 600.60 610.58 614.65
620.40 638.13 662.90 675.89 697.53 710.07
711.78 729.71 765.04 777.22 825.03 841.58
864.93 877.14 903.19 925.85 958.20 968.92
982.48 983.54 986.59 997.89 1002.66 1007.24
1017.69 1043.57 1046.80 1051.66 1080.35 1092.66
1110.39 1122.71 1151.37 1157.95 1169.94 1171.05
1186.12 1231.50 1244.51 1257.51 1307.68 1316.95
1338.42 1367.54 1385.61 1414.29 1434.06 1445.85
1470.29 1476.10 1480.68 1491.92 1509.13 1518.43
1559.39 1568.84 1631.15 1643.19 1652.02 1665.50
1715.84 3021.48 3087.47 3111.67 3145.43 3150.86
3156.28 3159.92 3164.99 3170.19 3175.55 3183.78
3188.87 3196.70 3199.17 3205.51 3272.64 3739.56
3776.29 3900.73 3920.97

1361.11 1364.38 1368.39 1390.45 1418.69 1440.93
1451.50 1469.75 1483.03 1489.19 1521.54 1531.12
1557.94 1591.28 1643.11 1661.03 1665.55 1680.01
1799.52 2994.26 3035.40 3083.31 3121.37 3155.89
3156.28 3158.13 3159.55 3165.73 3170.55 3173.30
3174.94 3182.87 3184.58 3191.62 3195.67 3794.98
3798.21 3919.64 3933.82

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TS involving *P*-OMe-aziridine

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-52.82 6.02 20.01 24.95 33.97 43.41
47.34 59.77 68.05 77.70 83.90 94.50
95.91 114.47 115.83 123.47 128.05 134.47
139.28 142.68 152.51 155.82 171.85 180.86
191.13 203.67 209.53 219.64 227.55 251.23
256.95 260.57 274.04 276.81 294.55 300.65
315.46 331.74 345.09 371.52 385.12 398.29
414.15 433.82 451.17 506.58 515.04 525.39
525.91 555.49 602.22 620.18 621.77 632.12
639.27 647.83 672.74 689.18 704.63 725.19
745.34 772.89 811.45 822.45 826.93 848.07
850.46 873.60 887.04 916.42 962.59 965.00
983.62 985.49 992.65 1006.82 1009.82 1041.28
1053.13 1086.95 1096.27 1109.11 1113.69 1127.05
1158.30 1160.95 1161.06 1175.51 1184.12 1195.04
1230.53 1259.36 1278.27 1311.91 1313.67 1328.76
1334.96 1354.13 1368.54 1407.88 1425.96 1449.16
1456.52 1465.59 1467.49 1468.22 1471.08 1482.28
1490.74 1518.33 1520.00 1579.14 1594.72 1607.45
1616.74 1645.53 1664.19 1676.55 1696.01 2988.83
3024.72 3053.76 3060.06 3113.60 3126.70 3157.15
3163.55 3169.67 3172.50 3177.11 3177.48 3185.52
3186.22 3192.84 3194.64 3213.81 3222.80 3780.36
3784.11 3899.23 3907.99

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TS involving Ph-isocyanate

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-96.99 8.16 24.34 34.12 44.05 52.53
60.81 70.62 79.93 93.95 102.10 110.38
118.04 122.59 130.71 133.35 151.28 154.13
184.21 185.73 193.05 208.40 215.03 222.59
232.15 258.21 273.29 304.13 309.25 316.79

332.34 333.67 353.23 394.98 413.13 415.27
428.41 436.33 446.10 469.38 502.16 521.98
541.58 612.70 615.79 621.10 626.17 666.57
680.70 681.84 707.79 716.39 733.98 762.20
772.62 780.92 800.49 846.87 853.59 884.15
913.30 940.55 952.54 960.87 968.66 982.55
992.83 996.70 1002.99 1008.00 1019.75 1025.05
1047.60 1053.56 1094.79 1099.10 1114.78 1130.96
1157.47 1162.04 1172.12 1175.08 1190.14 1223.98
1248.92 1285.06 1310.56 1329.69 1338.68 1352.90
1365.99 1384.81 1408.97 1426.11 1442.86 1451.73
1465.10 1472.16 1482.05 1501.33 1527.17 1560.79
1583.09 1628.06 1635.54 1645.24 1659.78 1666.74
1685.07 2975.05 3046.24 3060.35 3117.28 3127.50
3162.46 3166.37 3168.72 3170.34 3176.97 3183.12
3183.69 3189.69 3195.51 3203.68 3208.12 3452.16
3769.70 3805.05 3905.38

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TS involving Ph-thioisocyanate

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-86.17 12.67 19.73 25.01 38.73 42.64
62.25 70.51 80.86 82.24 97.54 97.98
109.12 111.95 124.88 139.00 142.16 155.76
159.20 168.91 174.88 184.61 203.07 216.93
228.42 254.39 259.96 263.33 298.83 306.98
314.42 319.22 327.07 351.00 375.24 385.37
412.27 413.02 419.04 449.26 492.20 513.93
521.50 553.96 577.28 588.10 612.99 616.85
640.41 665.66 667.11 675.28 698.04 710.55
714.08 772.98 774.50 801.10 836.40 839.92
840.85 892.35 916.27 951.39 961.07 973.47
985.82 986.34 994.90 1002.25 1006.69 1015.80
1020.75 1046.54 1052.22 1088.06 1096.63 1116.99
1127.24 1159.28 1161.84 1169.62 1173.64 1191.54
1207.94 1254.26 1280.12 1309.00 1312.66 1319.79
1347.44 1371.30 1413.86 1427.07 1450.92 1457.73
1463.66 1467.74 1480.14 1498.29 1515.82 1563.66
1566.10 1595.41 1618.20 1641.09 1656.20 1664.96
1699.69 2982.20 3035.33 3073.90 3097.66 3114.14
3132.85 3168.48 3175.87 3176.42 3182.19 3185.71
3189.42 3194.17 3200.74 3202.82 3207.15 3728.15
3748.25 3901.06 3914.23