

Why simple vanadate is inefficient as a catalyst in oxidation of alkanes with H₂O₂ – the long-standing puzzle is resolved

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Electronic Supplementary Information

Analysis of the HO• capture

Analysis of the HO• radical capture by the V atom during its liberation from **10•H₂O** was performed in accord with the following procedure. First, the singlet biradical PES scan for the VO–OH cleavage in **10•H₂O** was carried out. The VO–OH bond was increased with the step of 0.03 Å, all other internal coordinates being fully relaxed. Second, the point on the scan curve corresponding to the VO–OH distance of 1.789 Å – which is soon after the formation of **TS21** – was selected as the first point for the second singlet biradical PES scan. The V•••OH_{leaving} distance was reduced with the step 0.06 Å with all other internal coordinates being fully relaxed. Results are presented on Figure 6.

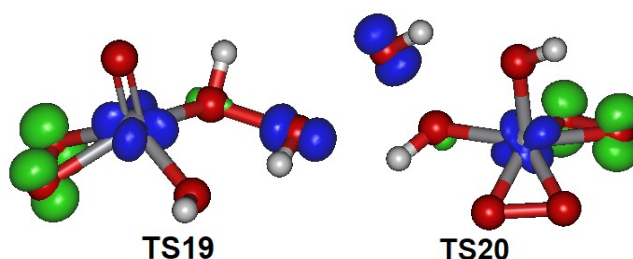
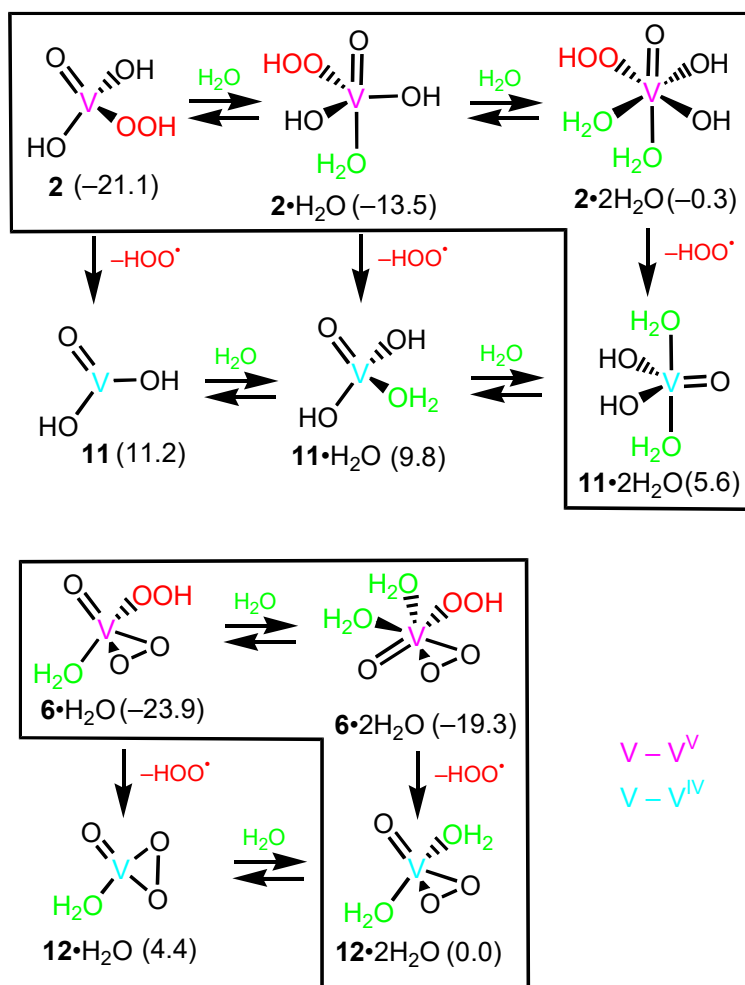


Figure S1. Equilibrium structures and plots of spin densities for **TS19** and **TS20**.



Scheme S1. Elimination of the HOO[•] radical from complexes **2** and **6•H₂O** (Gibbs free energies are indicated in parentheses in kcal/mol relative to HVO₃, the most favourable pathways are boxed).

Table S1. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures (nuclear charges of the atoms are given in the first column).

1

23	1.120915	-0.547897	-0.408714
8	0.667303	-1.322031	0.909085
8	0.589615	1.159575	-0.161173
8	0.285662	-1.153424	-1.622353
1	0.232995	1.604197	-0.941687

1•H₂O

23	0.372303	-0.509690	-0.477759
8	-1.580614	-1.005076	-0.456949
8	0.946682	-0.978483	0.933463
8	0.568404	1.248804	-0.774838
8	1.004901	-1.360152	-1.671267
1	-2.105099	-1.017946	-1.274748
1	-2.166126	-0.723426	0.265595
1	0.682468	1.819588	-0.003107

1•2H₂O

23	-0.562276	-0.267028	-0.111632
8	0.208930	-2.518491	-0.282221
8	-0.581110	1.285020	0.267877
8	-1.547117	-1.106670	1.172104
8	1.496059	-0.293098	-0.141840
1	-0.238493	-2.949683	0.459191
8	-1.199632	-0.442182	-1.569194
1	1.947953	-1.054206	-0.535379
1	1.982038	0.513295	-0.369183
1	-0.221808	-2.868358	-1.073881
1	-1.810944	-0.542600	1.908836

1•H₂O₂

23	-0.377008	-0.864579	0.060889
8	1.547739	-0.294385	-0.297684
8	-1.217425	-0.335665	-1.180426
8	-0.960964	-0.343780	1.666518
8	-0.146843	-2.449817	-0.015292
8	2.465160	-1.212472	0.277690
1	-1.544109	0.426040	1.721852
1	2.012050	-2.071690	0.132377
1	1.839920	-0.195742	-1.226926

1•H₂O₂•H₂O

23	0.230662	0.400606	-0.862944
8	0.173840	-1.464781	0.035046
8	0.971519	1.667220	-0.184230
8	-1.534432	0.544429	-0.535203
8	2.396201	-0.476479	-0.785454
1	0.954198	-1.920703	0.383509
8	0.408449	0.398731	-2.446619
1	2.722439	-0.332912	-1.691563
8	3.224003	0.377847	-0.006860
1	-0.606160	-1.735295	0.541672
1	-1.768102	1.014391	0.276735
1	2.602073	1.141577	0.095480

1•2H₂O₂

23	0.102289	0.626648	0.235636
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8	0.261220	-1.539475	-0.093120
8	0.348113	1.706873	1.403852
8	-1.693321	0.226555	0.252492
8	2.113223	-0.081556	0.740030
1	0.555050	-2.055031	0.681043
8	0.449043	1.269999	-1.170452
1	2.747494	0.232398	0.067725
8	2.599635	0.500383	1.942370
8	-0.979046	-2.142060	-0.443886
1	-2.155951	0.434728	1.074899
1	1.911844	1.198383	2.071161
1	-1.586214	-1.396213	-0.186321

2

23	0.185606	-0.721072	1.086743
8	0.662986	-1.628279	2.267710
8	-1.172290	-1.505732	0.275934
8	1.402938	-0.772928	-0.293187
8	-0.399054	0.859852	1.630762
8	2.145043	0.064755	0.607443
1	-1.386322	-2.429233	0.473741
1	2.832113	-0.536730	0.954882
1	-0.316148	1.124280	2.557321

2•H₂O

23	-0.173186	0.437070	0.456320
8	0.770918	0.006262	-1.021141
8	-1.883644	-0.074025	0.426726
8	-0.180995	1.995744	0.281669
8	-0.016853	-1.944103	0.503379
8	0.662786	0.211463	2.016128
8	1.344854	0.987606	-1.852008
1	0.744956	-0.728729	2.239484
1	-0.896815	-2.305710	0.330932
1	0.555910	-2.319682	-0.178585
1	0.971713	1.821087	-1.510185
1	-2.551463	0.620907	0.349691

3•H₂O

23	0.804071	-0.997008	-0.119593
8	2.605144	-0.625424	0.222630
8	-0.699553	0.387363	-0.122605
8	0.308679	-2.159520	0.850164
8	0.672745	-1.455502	-1.645022
1	-1.066532	0.680192	0.727718
1	-1.455478	0.184277	-0.698084
8	1.944370	0.464731	0.891414
1	2.041011	0.245877	1.839042

3•2H₂O

23	0.440954	-0.883096	0.597068
8	0.157496	-2.446394	0.398539
8	0.810607	1.388503	-0.011013
8	2.242636	-0.793563	1.086999
8	-0.664555	-0.420748	-1.101581
8	-0.399072	-0.361602	1.855408
1	1.755895	1.581312	-0.072364
1	0.492276	1.913805	0.735608

1	-0.414653	0.398429	-1.554945
1	-0.771623	-1.118087	-1.762807
8	2.443097	-0.818904	-0.338932
1	2.707452	-1.741984	-0.507060

4

23	0.206109	-0.391782	-0.042144
8	0.720102	-0.231348	1.429735
8	-1.511474	0.201168	-0.285423
8	-1.390279	-1.184647	0.009034
8	1.153685	-1.626390	-0.917859
1	1.986778	-1.937629	-0.532588

4•H₂O

8	1.592641	-0.940162	0.884101
23	0.427867	0.301378	-0.273466
8	0.697434	1.661770	0.465820
8	-1.118213	-0.449322	0.170563
8	1.581350	-0.244254	-1.593369
1	-1.677731	-0.054276	0.855313
8	0.509578	0.571211	-2.041935
1	1.598071	-0.748179	1.836839
1	2.523063	-1.002836	0.612326

4•H₂O₂

8	-0.904856	-0.182375	0.693326
23	0.738185	0.995592	0.250340
8	0.018404	2.364764	-0.017349
8	1.178290	0.089953	-1.210417
8	1.140374	0.540177	1.983170
1	0.916265	0.410570	-2.085856
8	2.155000	1.268768	1.310026
8	-1.919867	-0.056814	-0.292181
1	-1.365481	0.039394	1.526443
1	-1.993653	-0.981207	-0.596476

5

23	0.546152	-0.475571	0.489624
8	0.822167	-2.172780	0.885024
8	2.208215	0.086627	0.468073
8	-0.386291	0.850872	1.185965
8	-0.195205	-0.572183	-1.098540
8	-0.461346	-0.309900	1.996690
1	2.381378	1.013459	0.230506
1	0.366616	-2.639280	1.599139
1	-0.010966	-1.337245	-1.667542

5•H₂O

23	0.417661	-0.485162	0.259826
8	0.940364	1.753577	0.117597
8	0.797206	-2.246320	0.072420
8	1.599578	-0.304324	1.568085
8	-1.111083	0.328655	0.681157
8	0.817732	-0.195947	-1.459814
8	-1.231193	-1.058795	0.750605
1	0.234729	2.363277	0.379884
1	1.095032	1.920226	-0.824621
1	1.902803	0.611439	1.670520
1	0.081377	-2.875201	0.224658

1	0.876723	-1.011935	-1.975336
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6•H₂O

8	-0.724546	0.724779	1.078148
23	0.657474	0.310237	-0.121820
8	0.008673	0.107814	-1.531087
8	1.831028	-1.390877	0.058778
8	1.225311	2.041506	0.010445
8	2.265467	1.139174	-0.316242
8	-0.642466	-0.708175	1.083862
1	-0.240323	-0.917266	1.951201
1	1.485722	-2.206130	-0.341412
1	2.748710	-1.300482	-0.244653

7

8	-0.747309	-0.169406	-0.812959
23	0.739986	0.270468	0.162969
8	1.993655	0.375968	-0.764695
8	1.011812	-0.855950	1.519021
1	1.866881	-1.298269	1.608678
8	0.732323	1.779991	1.227490
8	-0.164105	-1.456837	-1.010840
1	-0.615292	-2.009104	-0.344895
8	-0.000885	2.206533	0.074732
1	0.631353	2.775987	-0.409590

8

8	0.748477	0.240027	1.466615
23	0.405216	0.201627	-0.317842
8	-1.309342	-0.134230	-0.431523
8	1.580941	-0.930930	-0.982927
8	0.864961	1.953648	-0.222370
1	1.502534	-1.885306	-0.822247
8	0.553888	1.489414	-1.520560
8	0.317990	-1.113253	1.520910
1	1.151540	-1.607029	1.651425
1	-1.716165	-0.729678	0.219479

9•H₂O

8	-0.810747	0.007488	1.576405
23	0.599996	0.113779	0.450640
8	0.935369	1.787055	0.083515
8	0.673470	-0.382445	-1.582374
8	1.702700	-0.423353	1.780777
8	2.129068	-0.821591	0.496277
8	-1.147611	-0.222403	0.227662
1	-0.028370	0.002768	-2.131603
1	1.510964	-0.183512	-2.031457
1	1.052471	2.394104	0.833839

9•H₂O₂

8	-0.538207	-2.589321	0.107532
23	0.890076	-1.485644	0.097831
8	1.225738	-0.775247	1.671471
8	0.995730	0.525963	-0.598868
8	1.995015	-2.888619	-0.188890
8	2.405893	-1.688114	-0.809283
8	-0.833680	-1.282915	-0.323756
1	0.155236	1.016650	-0.512367

8	1.926376	1.330949	0.107429
1	1.479985	-1.339055	2.421368
1	1.906077	0.915562	0.996073

10•H₂O

8	0.937455	-0.679037	-1.982473
23	0.729595	-0.413925	-0.235797
8	-0.484140	1.156940	-0.930050
8	1.698011	0.923921	0.497307
8	-0.740008	-0.799398	0.655933
8	0.328644	-1.565722	1.167086
8	1.402486	-1.783137	-1.242219
8	2.665501	-0.102660	0.688787
1	-0.116703	1.700361	-1.646066
1	2.566898	-0.334355	1.634781
1	-0.809500	1.775172	-0.255399

11

23	0.901156	-1.102806	-0.530150
8	2.634800	-1.483771	-0.076236
8	1.042833	0.734844	-0.583900
8	0.603630	-1.668824	-1.981752
1	0.436669	1.178793	-1.189809
1	3.289213	-0.809157	-0.291834

11•H₂O

23	1.139955	-0.952948	-0.915265
8	0.259981	-1.069818	0.917717
8	2.860965	-1.375012	-0.446874
8	0.746431	0.806527	-1.266444
8	0.375130	-2.017625	-1.815066
1	-0.298031	-0.351058	1.253683
1	0.746870	-1.435923	1.672521
1	0.518704	1.438882	-0.575487
1	3.267116	-1.050744	0.365455

11•2H₂O

23	0.356750	-0.017993	0.292446
8	-0.293116	-1.715656	-0.140165
8	-0.731818	1.467751	0.606520
8	0.120768	0.202786	-1.795729
8	-0.094468	-0.322492	2.333152
8	1.936122	0.174821	0.398221
1	0.657040	-0.499150	2.918491
1	-0.482241	0.517515	2.627963
1	0.882165	0.554945	-2.277546
1	-0.018715	-0.700862	-2.122718
1	-1.008342	1.981350	-0.159603
1	-0.540165	-2.292744	0.589988

11•H₂O₂•H₂O

23	-0.130667	0.120149	-0.081562
8	1.062007	0.206356	1.329456
8	0.444560	0.117996	-1.836304
8	0.103251	2.255677	0.106298
8	0.034210	-1.942847	-0.280021
8	-1.700553	0.312047	0.221314
1	-0.576957	-2.517760	0.204770
1	-0.018163	-2.200472	-1.214434

8	-1.152493	2.925459	0.108656
1	0.430695	2.366715	1.019409
1	0.530597	0.965793	-2.286508
1	1.552987	-0.584089	1.580311
1	-1.749815	2.146515	0.204525

12•H₂O

23	0.128073	0.538729	-0.077015
8	-0.644284	0.976922	-1.399899
8	1.586382	-0.870443	-0.686498
8	0.129506	1.695686	1.356198
8	1.351584	1.706222	0.591962
1	1.473152	-1.338445	-1.528142
1	2.499567	-0.543951	-0.674836

12•2H₂O

23	0.402795	0.161480	-0.712832
8	0.350383	-0.997650	-1.807586
8	1.724372	-0.411579	0.810768
8	-0.131509	1.852063	-1.194236
8	1.307549	1.710500	-1.108622
1	1.755893	-1.329404	1.122567
1	2.646106	-0.127257	0.711693
8	-1.152612	-0.119120	0.661249
1	-1.351505	-0.990203	1.037335
1	-2.005893	0.290431	0.452016

13•H₂O

8	-1.091040	-0.711240	-1.670114
23	0.149118	-0.411711	-0.312477
8	-0.884753	1.402393	0.016853
8	-0.765372	-1.419055	0.940582
8	0.588798	-1.823792	0.697005
8	0.228317	-0.362307	-2.093610
1	-1.498935	1.532666	-0.724044
1	-0.415863	2.242246	0.146976

13•H₂O₂

8	1.893378	-0.777116	-0.528674
23	0.583261	-0.742865	0.853594
8	0.679854	1.410242	0.546963
8	-0.836748	-0.804478	-0.332605
8	-0.891093	-1.735917	0.745494
8	2.274524	-1.296430	0.738360
1	0.065116	1.665513	-0.167127
8	1.963552	1.751624	0.033852
1	2.216596	0.867098	-0.361878

13•H₂O₂•H₂O

8	-0.451439	-1.474417	0.774679
23	0.230424	-0.302488	-0.490444
8	2.230177	-0.416862	0.174886
8	0.558967	1.807264	-0.434382
8	0.498969	-1.504251	-1.881774
8	-0.341753	-0.370728	-2.169846
8	-0.661972	-0.077460	1.045430
1	0.428632	2.303014	0.396100
8	1.816182	2.247325	-0.922187
1	2.757005	-1.075051	-0.309292

1	2.444725	1.665901	-0.451797
1	2.307733	-0.659267	1.114326

14•H₂O

23	-0.269209	0.768828	-0.043296
8	-0.567328	-1.116577	-0.128335
8	1.346362	1.672933	-0.302592
8	0.189964	0.433292	1.943105
8	-0.066224	0.511793	-2.111811
8	-1.583249	1.649794	0.067303
8	-0.698814	-1.799533	1.132131
1	-0.013993	-0.535241	2.010655
1	-0.093199	-2.548345	1.011608
1	-0.095833	-0.405220	-2.425724
1	0.807061	0.863614	-2.348665
1	1.111234	0.562060	2.207463
1	1.739377	2.182623	0.413447

15•H₂O

23	0.062693	-0.111041	0.371132
8	0.204934	-0.374630	-1.186911
8	1.666329	0.226111	1.262136
8	-1.616527	0.372649	1.101925
8	-0.965114	1.620108	0.760172
8	2.048453	1.559284	0.889687
8	0.159945	-1.956478	1.277866
1	1.038063	-2.363153	1.353472
1	-0.448320	-2.659674	1.000684
1	2.730021	1.390550	0.219886
1	-0.718887	2.008814	1.620771

16•H₂O

23	-0.224561	-0.791908	0.260504
8	-1.148263	0.705958	0.079953
8	1.560341	-0.608642	-0.043373
8	-0.990230	-2.269427	0.970816
8	-0.239054	-1.496412	1.923126
8	2.146844	0.105428	1.044445
8	-0.239777	-1.603928	-1.650845
1	-0.794765	-2.381431	-1.821387
1	0.617926	-1.779987	-2.069694
1	2.512396	-0.615587	1.584216
1	-0.826188	1.488395	-0.387421

17•H₂O

8	-0.523783	0.410618	1.217260
23	-0.243382	-1.127632	0.267146
8	1.600725	-1.418809	1.178972
8	0.643420	-0.766914	-1.285122
8	-0.597094	-2.843238	0.703241
8	-1.666267	-2.228070	-0.024976
8	-1.419995	0.598573	0.107390
8	2.047007	-1.044405	-1.339733
1	2.225603	-1.428415	0.422258
1	2.408874	-0.176054	-1.586632
1	1.731045	-2.239355	1.677913
1	-0.976312	1.283521	-0.431117

23	0.476368	0.694453	-1.120218
8	0.790287	2.413414	-1.352737
8	-1.040668	0.402923	-0.257359
8	1.852656	-0.082537	-0.354079
8	0.282563	0.257309	-2.618651
1	2.481654	-0.644117	-0.831649
1	-1.034697	0.530442	0.705929

19•H₂O

8	1.835950	0.227273	0.059947
23	0.292985	0.444391	0.391742
8	-0.004891	0.256997	1.943863
8	-0.491894	-1.212554	-0.508592
8	-0.147253	2.285737	-0.048984
8	-0.942923	1.542305	-0.756480
1	-0.003854	-2.041601	-0.369092
1	-1.431460	-1.418019	-0.366114

20•H₂O

8	0.674960	-0.720623	-2.204855
23	0.846243	-0.364988	-0.429537
8	-0.258967	1.313200	-0.930041
8	2.229301	0.289173	-0.120468
8	-0.161262	-0.404330	1.258841
8	0.525863	-1.490364	1.144963
8	1.050482	-1.850989	-1.446065
1	-0.732898	1.836386	-0.264602
1	-0.835275	1.237739	-1.706977

21•H₂O

23	0.369694	0.276505	-1.006171
8	0.057055	-1.658021	-0.154578
8	1.029362	1.907969	-0.781870
8	-1.275581	0.633145	-0.360787
8	2.089944	-0.154710	-0.499809
1	0.816466	-2.021810	0.325574
8	0.171721	0.046203	-2.544678
1	2.756238	-0.062265	-1.197204
1	-0.733071	-1.796848	0.388715
1	-1.333215	0.925039	0.561755

22

8	-0.682105	0.364251	0.478029
23	0.416994	-1.003790	0.212407
8	0.414185	-1.942151	1.448207
8	2.023162	-0.280322	-0.001999
8	-0.712292	-1.882205	-1.143917
1	2.764273	-0.595631	0.536471
8	0.531997	-2.187161	-1.360034
1	-1.229580	0.384798	1.276913

23

8	-0.383157	-2.500032	-0.050398
23	0.781251	-1.177319	0.203365
8	1.110639	-0.947974	1.900363
8	0.919731	0.490696	-0.379120
8	2.221882	-2.545313	0.027503
8	2.130963	-1.829553	-1.043655
8	-0.977059	-1.215311	-0.094006

1	0.377618	0.844494	-1.100668
1	1.593918	-1.625991	2.401654

³24

8	2.387124	-0.530273	-1.547889
23	1.427157	-0.370983	0.179625
8	1.288327	1.160532	0.380518
8	-0.327298	-1.086948	0.613444
8	0.378865	-1.075969	1.692094
8	1.119396	-0.693432	-1.707468
8	2.942955	-1.006456	0.935668
1	2.967514	-1.026737	1.902524

1,124

8	2.385959	-0.525505	-1.548556
23	1.427775	-0.370281	0.180093
8	1.289144	1.161278	0.381177
8	-0.324785	-1.090138	0.610753
8	0.376433	-1.071119	1.692584
8	1.118930	-0.698046	-1.704789
8	2.942384	-1.007992	0.935202
1	2.968201	-1.028463	1.902052

25•H₂O₂•H₂O

8	2.026390	0.552842	0.125397
23	0.326048	-0.397970	0.992236
8	0.556770	-1.009224	2.438057
8	0.597827	-1.855147	-0.453008
8	-0.551819	1.240381	0.834659
1	1.426323	-2.353681	-0.530472
8	-1.351986	0.104988	0.436739
1	2.588282	1.062046	0.739193
8	1.492563	1.553214	-0.746015
1	-0.121636	-2.471552	-0.659911
1	0.592218	1.686043	-0.318406

TS1

23	-0.121921	-0.967974	0.861734
8	0.735981	-2.571028	-0.266657
8	0.559685	-1.050792	2.287152
8	-1.579102	-2.041623	0.881623
8	1.517922	-0.206889	-0.114456
1	1.705176	-2.456300	-0.269334
8	-0.755560	0.555244	0.619512
1	1.533814	1.094720	0.155022
8	2.735683	-0.899510	0.142334
1	0.536529	-3.471426	0.022629
1	-1.597284	-2.748179	1.538996
1	2.815451	-0.851470	1.112560
1	0.113724	1.567714	0.588803
8	1.072289	2.079851	0.382799
1	1.434493	2.418943	1.216732

TS2

23	1.003404	-0.736582	-0.056828
8	2.056090	0.680645	-0.962922
8	-0.493708	-1.580884	1.212251
8	2.080026	-0.831736	1.138540
8	-0.470423	0.546006	-0.331795

1	1.475310	1.860024	-0.846143
8	1.140734	-1.988287	-1.026132
1	-0.343939	-2.511338	1.440332
1	-1.397815	-1.530431	0.866397
1	-1.147892	0.302625	-0.975962
8	3.414051	0.793451	-0.548348
1	3.383012	0.324178	0.309038
8	0.656188	2.605484	-0.752757
1	-0.046982	1.761593	-0.519436
1	0.797164	3.146721	0.039196

TS3

23	0.233213	-1.151667	-0.374497
8	0.300611	-2.289213	1.056266
8	1.780040	-0.136046	-0.734453
8	-0.882950	0.042698	-0.148602
8	-0.146432	-2.056598	-1.619137
1	1.357682	1.167386	-0.504527
1	2.253535	-0.284617	-1.563384
8	0.827630	-1.255854	1.903885
1	0.046068	-0.989455	2.421215
8	0.692136	1.961048	-0.178913
1	-0.146193	1.336584	-0.107533
1	0.551000	2.591693	-0.906259

TS4

23	0.284142	-1.476641	-0.269661
8	-0.785130	-0.225466	-0.370289
8	-0.386898	-2.619108	0.928302
8	1.685260	-1.169341	0.837067
8	0.406664	-2.445030	-1.746916
8	1.854969	-0.451052	-0.390600
1	0.094137	-2.847756	1.733625
1	1.335589	1.050481	-0.137970
1	-0.039733	-2.134779	-2.549752
8	0.566408	1.703089	0.004232
1	-0.240920	0.899697	-0.186443
1	0.583503	2.356034	-0.716435

TS5

23	0.484105	-1.488612	-0.172468
8	-0.632411	-0.206618	-1.032320
8	-0.263094	-1.639685	1.200447
8	2.221004	-1.235609	0.297469
8	0.298017	-3.017154	-1.048460
8	1.872212	-0.195753	-0.604023
1	1.372381	0.948232	-0.172160
1	0.702684	-3.054729	-1.930739
8	0.570174	1.726213	-0.122124
1	-0.143306	1.095549	-0.572492
1	-1.568522	-0.366692	-0.851042
1	0.775437	2.471418	-0.710658

TS6

8	1.236126	-0.774494	-0.632508
23	-0.576082	-0.832253	0.035576
8	-1.396357	-1.230167	-1.244894
8	-0.578905	1.042788	0.309105

8	-0.014949	-2.170447	1.153686
1	-1.305720	1.543374	-0.091188
8	-1.321637	-1.682457	1.413850
8	2.259503	-1.526708	-0.012849
1	1.722012	0.620411	-0.543665
1	2.459402	-2.181723	-0.702029
8	1.685119	1.627123	-0.270289
1	0.631440	1.585838	0.015872
1	1.799988	2.179947	-1.062835

TS7

8	1.373942	0.685927	-0.020334
23	0.011652	-0.655568	0.200102
8	-0.095642	-0.711564	1.764171
8	0.701843	-2.129548	-0.503107
8	-0.957393	0.661557	-0.813077
1	1.003074	-2.848951	0.068582
8	-1.705393	-0.455325	-0.364957
8	2.482092	0.343792	0.802398
1	0.728833	1.947743	0.335802
1	3.130943	0.053342	0.139168
8	-0.132069	2.549017	0.442040
1	-0.783650	1.857518	-0.046535
1	-0.045982	3.363629	-0.084412

TS8

8	1.361680	-0.050889	0.243260
23	-0.065506	-1.213370	-0.278321
8	-0.988385	0.059970	-0.744282
8	-0.536281	-1.938298	1.263869
8	1.128035	-2.001383	-1.410482
1	-1.064495	-1.433855	1.901085
8	-0.182988	-2.535162	-1.468897
8	2.682500	-0.536948	0.274443
1	1.065145	1.389715	-0.274255
1	2.938188	-0.537698	-0.664088
8	0.362964	2.040965	-0.641106
1	-0.394350	1.262917	-0.809874
1	0.678913	2.392596	-1.492834

TS9

8	2.305937	0.110675	0.505161
23	0.691752	-0.400992	-0.172429
8	0.829430	-1.518848	-1.261307
8	-0.562762	0.917782	-0.805637
1	-1.493611	0.712326	-0.656417
8	-0.658614	-0.873409	1.023132
8	2.005755	0.965711	-0.581864
1	1.455129	2.102922	-0.238234
8	0.480969	-1.618850	1.453245
1	0.299856	-2.531857	1.148561
8	0.650067	2.877695	-0.112213
1	-0.098415	2.183648	-0.443811
1	0.759156	3.585617	-0.767466

TS10

8	1.019934	-0.374628	-1.832948
23	-0.295974	0.104372	-0.656394

8	-0.173353	1.737418	-0.512295
8	-0.355434	-0.419281	1.365188
8	-1.554683	-0.304657	-1.913151
8	-2.026737	-0.422924	-0.581788
8	1.511213	-0.414898	-0.494360
1	0.383603	-0.122215	1.918858
1	-1.169870	-0.183659	1.836459
1	2.245034	1.010484	-0.492649
8	2.209934	2.029930	-0.531911
1	1.074662	2.075703	-0.571503
1	2.592251	2.311475	-1.380865

TS11

8	-0.261964	-1.798781	-2.018072
23	0.729519	-1.191568	-0.554981
8	-0.296443	0.350171	-0.276623
8	2.316495	-0.097088	-0.474243
8	0.194614	-2.577064	0.412447
8	1.336629	-1.963384	0.957753
8	1.123421	-1.535588	-2.228089
1	1.944513	1.434966	-0.471430
8	3.314127	-0.281976	0.504259
1	2.821247	-0.304656	1.342840
8	1.250012	2.168443	-0.337190
1	0.378408	1.459010	-0.320001
1	-1.153453	0.360722	-0.732510
1	1.226566	2.724774	-1.135641

TS12

23	0.440605	-0.790643	0.202787
8	-0.463227	0.891055	0.615723
8	0.841807	-2.165659	1.375954
8	2.079860	0.260389	0.675807
8	-1.456439	-1.742276	0.306471
8	0.800450	-1.010703	-1.333765
1	-1.924733	-1.909598	-0.524993
1	-1.306867	-2.609199	0.716441
8	3.235550	-0.177728	-0.033912
1	1.852900	1.501480	0.475580
1	1.705048	-2.106139	1.800465
1	2.852586	-0.443767	-0.890098
8	1.276120	2.488055	0.423953
1	0.295020	1.894468	0.477380
1	1.373054	2.871644	-0.458283
1	-1.417714	0.994090	0.544620

TS13

8	2.026390	0.552842	0.125397
23	0.326048	-0.397970	0.992236
8	0.556770	-1.009224	2.438057
8	0.597827	-1.855147	-0.453008
8	-0.551819	1.240381	0.834659
1	1.426323	-2.353681	-0.530472
8	-1.351986	0.104988	0.436739
1	2.588282	1.062046	0.739193
8	1.492563	1.553214	-0.746015
1	-0.121636	-2.471552	-0.659911

1	0.592218	1.686043	-0.318406
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TS14

23	-1.035190	-0.611925	0.041061
8	-1.537912	-1.750027	-0.944092
8	0.914638	-0.103069	-0.069033
8	-2.218012	0.619585	0.743245
8	-1.553907	1.175040	-0.413972
1	0.932771	1.124147	0.105933
8	1.783980	-0.702073	0.897796
8	-0.530104	-1.549335	1.815995
1	0.440061	-1.663536	1.835557
1	-0.942730	-2.385855	2.076090
1	2.414770	-1.172402	0.327128
8	0.557219	2.227803	0.232283
1	-0.452500	1.968513	-0.025839
1	0.919536	2.806184	-0.456280

TS15

8	-1.229396	0.098008	0.575849
23	0.015554	-0.810281	-0.329456
8	0.730627	-1.502843	1.540934
8	1.552537	0.393843	-0.490554
8	0.045858	-2.494725	-0.917467
8	-0.112642	-1.574385	-2.009661
8	-1.184845	0.690595	-0.729340
1	1.194540	1.545502	-0.477337
8	2.702195	0.205576	0.323988
1	1.161189	-2.372663	1.553511
1	2.340577	0.204559	1.227714
1	0.094699	-1.506402	2.273691
8	0.475818	2.504318	-0.462857
1	-0.380077	1.904962	-0.594741
1	0.595898	3.047085	-1.257426

TS17

23	0.122168	-0.264955	-0.211152
8	1.747700	-1.249134	-1.018250
8	0.114283	-0.996851	1.195099
8	-0.957424	-0.878637	-1.570558
8	1.086058	1.171457	-0.229055
1	2.418122	-0.503631	-0.903558
8	-1.555928	1.009960	0.071951
8	2.795706	1.013134	-0.651056
1	2.057934	-2.007308	-0.504977
1	-0.975614	-1.825337	-1.753128
1	3.094299	1.160631	0.261491
1	-1.373871	1.960675	0.024784
1	-2.179964	0.808297	-0.643581

TS18

23	0.222757	-0.739026	0.069873
8	0.394220	-1.457047	1.678169
8	0.583280	0.888686	-0.031149
8	-0.180107	-1.706397	-1.412357
8	1.220443	-1.576520	-1.169055
8	2.295181	1.080096	0.068523
8	-1.800400	-0.301297	0.217086

1	-2.411123	-1.022671	-0.007719
1	-2.104972	0.471342	-0.286213
1	2.430968	1.060848	-0.894961
1	0.378513	-0.930533	2.489481

TS19

8	-0.210310	-1.283926	1.386955
23	-0.021289	-0.399428	-0.210826
8	1.924862	-1.056251	-0.278696
8	0.554405	1.184419	-0.010362
8	-0.153614	-0.966013	-1.923831
8	-1.377725	-0.471075	-1.400726
8	-1.335656	-0.394361	1.394864
8	2.205606	1.469877	-0.152323
1	2.387510	-0.172779	-0.258092
1	2.316392	1.825753	0.746564
1	2.209703	-1.526144	-1.076941
1	-1.086795	0.287918	2.051166

TS20

8	-0.372154	0.170651	0.721988
23	0.817480	0.513479	-0.462768
8	0.257797	0.337951	-1.927049
8	1.780406	-1.172715	0.057798
8	1.304964	2.369270	-0.188863
8	2.399440	1.663541	-0.138114
8	-0.378568	-1.474660	1.312386
1	-0.329747	-1.210195	2.247670
1	1.056930	-1.595718	0.622242
1	2.078501	-1.801022	-0.618072

TS21

8	0.994676	-0.792182	-2.147359
23	0.575318	-0.378608	-0.296379
8	-0.592330	1.185809	-1.047409
8	1.800361	0.593173	0.242458
8	-0.724083	-0.501007	0.939578
8	0.196144	-1.578929	1.028896
8	1.495653	-1.708899	-1.374102
8	3.107430	-0.212981	1.007230
1	-0.135678	1.933983	-1.465491
1	2.683282	-0.234703	1.883229
1	-1.222533	1.572503	-0.418761

TS22

8	-1.038410	-0.028331	0.957491
23	0.454099	0.993559	0.414385
8	0.036500	2.488572	0.251872
8	0.531563	0.084164	-1.164447
8	1.601287	0.761326	1.992864
1	0.919164	0.475748	-1.957249
8	2.348138	0.888500	0.934802
8	-1.886685	-0.888076	-0.251928
1	-1.820082	0.440348	1.301704
1	-1.182910	-0.726987	-0.918468

TS23

8	-0.514061	-2.529415	0.217861
23	0.882566	-1.404146	0.060454

8	1.409880	-0.868027	1.647872
8	1.090025	0.365021	-0.648982
8	2.047407	-2.900473	-0.327675
8	2.456749	-1.833154	-0.948983
8	-0.885235	-1.198946	-0.104787
1	0.258402	0.837157	-0.827162
8	1.725047	1.666609	0.358211
1	1.375328	-1.503145	2.383598
1	1.762132	1.108729	1.158133

1.1¹TS24

8	1.231367	2.500685	0.488633
23	0.242584	-0.303578	-0.851864
8	-0.692160	0.106776	-2.044364
8	2.134891	0.149014	-1.137602
8	1.921693	-1.086068	-1.477556
8	0.234521	2.038334	-0.004941
8	-0.376700	-0.827414	0.738173
1	-1.298577	-0.891130	1.018711

3¹TS24

8	1.144443	1.265676	-2.125502
23	0.222479	-0.459466	-0.002221
8	0.739439	-0.169828	1.439013
8	-1.532511	0.179559	-0.264661
8	-1.496844	-1.143339	-0.024960
8	0.798844	1.286862	-0.941554
8	1.207115	-1.592306	-0.915489
1	2.025244	-1.985249	-0.570927