SUPPLEMENTARY INFORMATION – THEORETICAL INVESTIGATION OF THE SIDE-CHAIN MECHANISM OF THE MTO PROCESS OVER H-SSZ-13 USING DFT AND AB-INITIO CALCULATIONS

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S 1 FURTHER COMPUTATIONAL DETAILS

The Brillouin zone was sampled at the Γ-point and Gaussian smearing with a width of 0.1 eV was used. All atoms in the unit cell were structurally optimized with a the convergence criterion of 0.001 eV/Å for the norm of the force on each atom and 10^{-8} eV for the total energy. Hessian matrices were calculated for all studied structures, obtaining ZPE corrections to the calculated energy. The vibrational frequencies were obtained in the harmonic oscillator approximation using a central finite difference scheme with displacements of ±0.01 Å. Adsorbate species in the gas phase were calculated in a cubic cell with a separation of 20 Å of vacuum to the next periodic image.

As described in the main text, 46T cluster models were constructed from the periodic structures. All energy corrections in this work were then computed as single point energies on these structures. DLPNO-calculations were performed using cc-pVXZ basis set for X = D, T, Q (i.e. double, triple, quadruple). Restricted Hartree-Fock energies for X = T, Q were computed within the RIJCOSX approximation with grid X6. For subsequent correlation treatment (X = D, T), an SCF-convergence criterion of 10^{-9} Hartree was employed and 10^{-7} Hartree to obtain only the Hartree Fock energy (X = Q). DLPNO-calculations were run using the 'TightPNO' setting.

S 1A SYMMETRY NUMBER OF GAS PHASE MOLECULES

Table S1 contains symmetries and corresponding symmetry numbers for the studied gas-phase species used for calculation of thermal corrections via the ideal gas approach. (Abbreviations: MeOH = methanol.)

Table S1. Symmetries and corresponding symmetry numbers σ of the studied gas-phase species

| Molecule	Symmetry	σ
H_2O	C_{2v}	2
MeOH	C_s	1

S 2 ZEOLITE STRUCTURE

S 2A ADDITIONAL INFORMATION

The CHA zeolite crystalizes in R$\bar{3}$m (#166) space group. The framework contains 4, 6 and 8-membered silicon rings and its unit cell consists of 108 atoms. Present tetrahedral atoms (T-atoms) are crystallographically indistinguishable and equal, i.e. there is only T1. Optimization of the framework was carried out for the kinetic cutoff of 800 eV with the convergence criterion set for the net force on each atom being 0.01 eV/Å. Optimized lattice constants obtained this way are a = 13.625 Å, b = 13.625 Å and c = 15.067 Å. For comparison, experimental data[1] are a = 13.675 Å, b = 13.675 Å and c = 14.767 Å. These optimized lattice parameters were used for calculations of the Al-substituted framework, H-SSZ-13.

S 2B FIGURES OF THE FRAMEWORK

Figures S1 and S2 were produced by VESTA.[2]
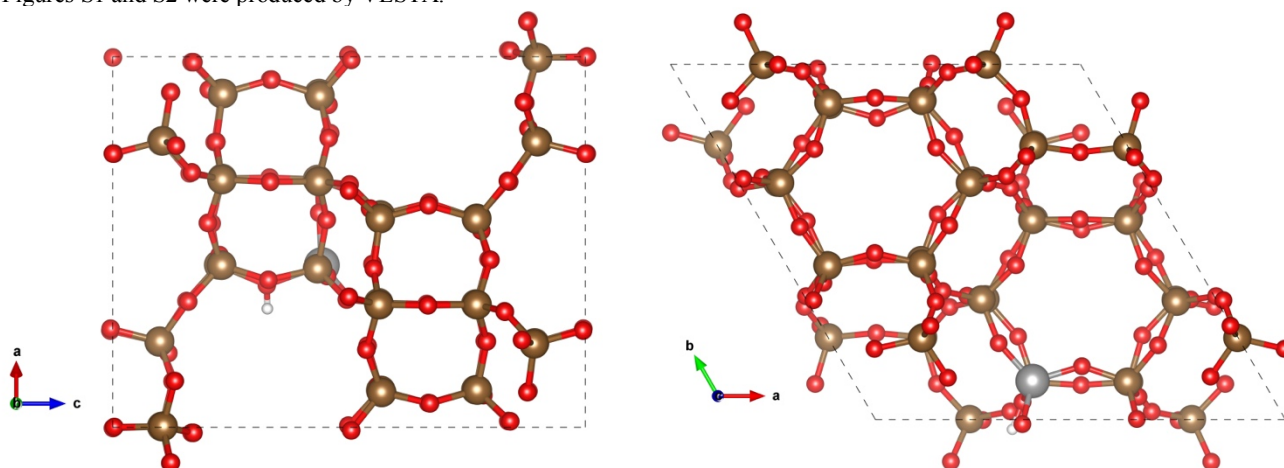
Figure S1. Unit cell of H-SSZ-13 used in the present study viewed along *b* and *c* directions respectively. Colour code: H = white, O = red, Si = brown, Al = gray.
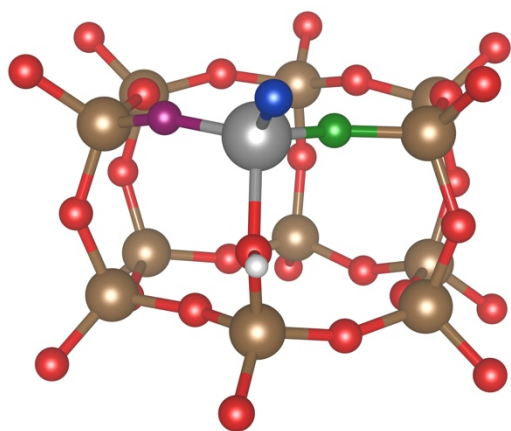
Figure S2. A double 6-ring of the CHA framework with color distinguished available active O-sites, shown in the perspective regime of the VESTA program. Active O-sites (numbering according to IZA): purple = O1, blue = O2, green = O3, red (with attached H) = O4.

S 2C COMPARISON OF O-SITE ENERGIES

Table S2 shows PBE-D3 energy differences of different O-sites neighboring with the substituted Al atom of empty H-SSZ-13, zeolite with adsorbed PMB and adsorbed HMB, all relative to the most stable O-site – O2. Except for O3, which is basically inaccessible, the stability is in the range of 0.1 eV.

Table S2. PBE-D3 energy differences of different active O-sites of empty H-SSZ-13 (ΔE_{empty}), H-SSZ-13 with adsorbed PMB (ΔE_{PMB}) and with adsorbed HMB (ΔE_{HMB}). All energies are relative to O4-site and are in eV.

O-site	E_{empty} [eV]	E_{PMB} [eV]	ΔE_{HMB} [eV]
O1	+0.038	+0.133	-0.005
O2	+0.111	-0.087	-0.001
O3	+0.407	X	X
O4	+0.000	+0.000	+0.000

S 3 CLUSTER MODELS AND CORRECTIONS

Non-periodic calculations carried out with the ORCA and TURBOMOLE program packages were performed on 46T (46 tetrahedra atoms) cluster systems. TURBOMOLE rather than ORCA was used for the PBE-D3 calculations on cluster models for backward compatibility with existing calculations from previous publications.[3-4] The clusters were cut out of the studied H-SSZ-13 framework so they capture the whole CHA pore in which the active Brønsted O-site is located. All used cluster models were terminated by hydrogen atoms for proper valences. Figure S3 shows an example of 46T containing one HMB molecule. Figure S4 shows the Gibbs free energy profiles of HMB mediated side-chain mechanism of the MTO process (a) with cluster corrections, and (b) at the PBE-D3 level of theory.
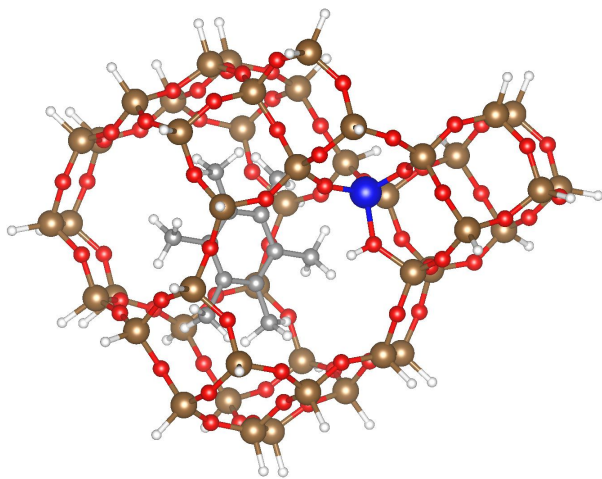
Figure S3. Example of a 46T cluster used during calculations. Here, the pore contains one hexamethylbenzene molecule. Color code: H = white, O = red, Si = brown, Al = blue, C = gray.
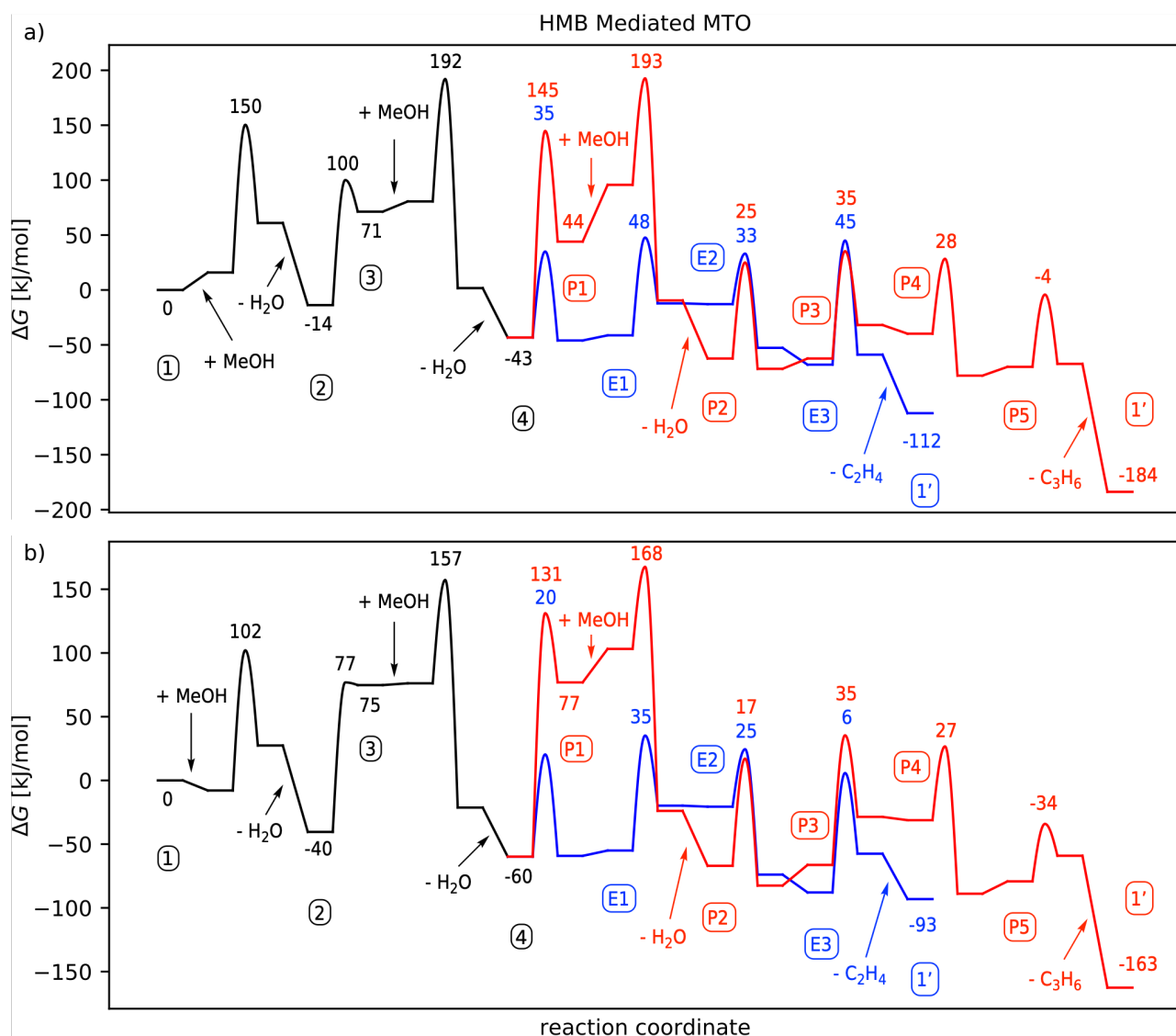
Figure S4. The Gibbs free energy profiles of HMB mediated side-chain mechanism of the MTO process with cluster corrected free energies (a), and at the PBE-D3 level of theory (b). All free energies are in kJ/mol and were obtained for 400 °C and a reference pressure of 1 bar. Indices (numbers in boxes) and colours are taken from Figure 1(a) from the main text.

S 4 PENTAMETHYLBENZENE ISOMERS

In the case of PMB, the arrangement of 5 methyl groups gives rise to 4 different PMB isomers. These are shown in Figure S5 for TS(3-4). Table S3 shows PBE-D3 energy differences of these isomers for the rate-determining step (i.e. step 3-4). Structures of the investigated tetramethylbenzenes (TMBs) were taken from the most stable PMB isomer – iso 1.
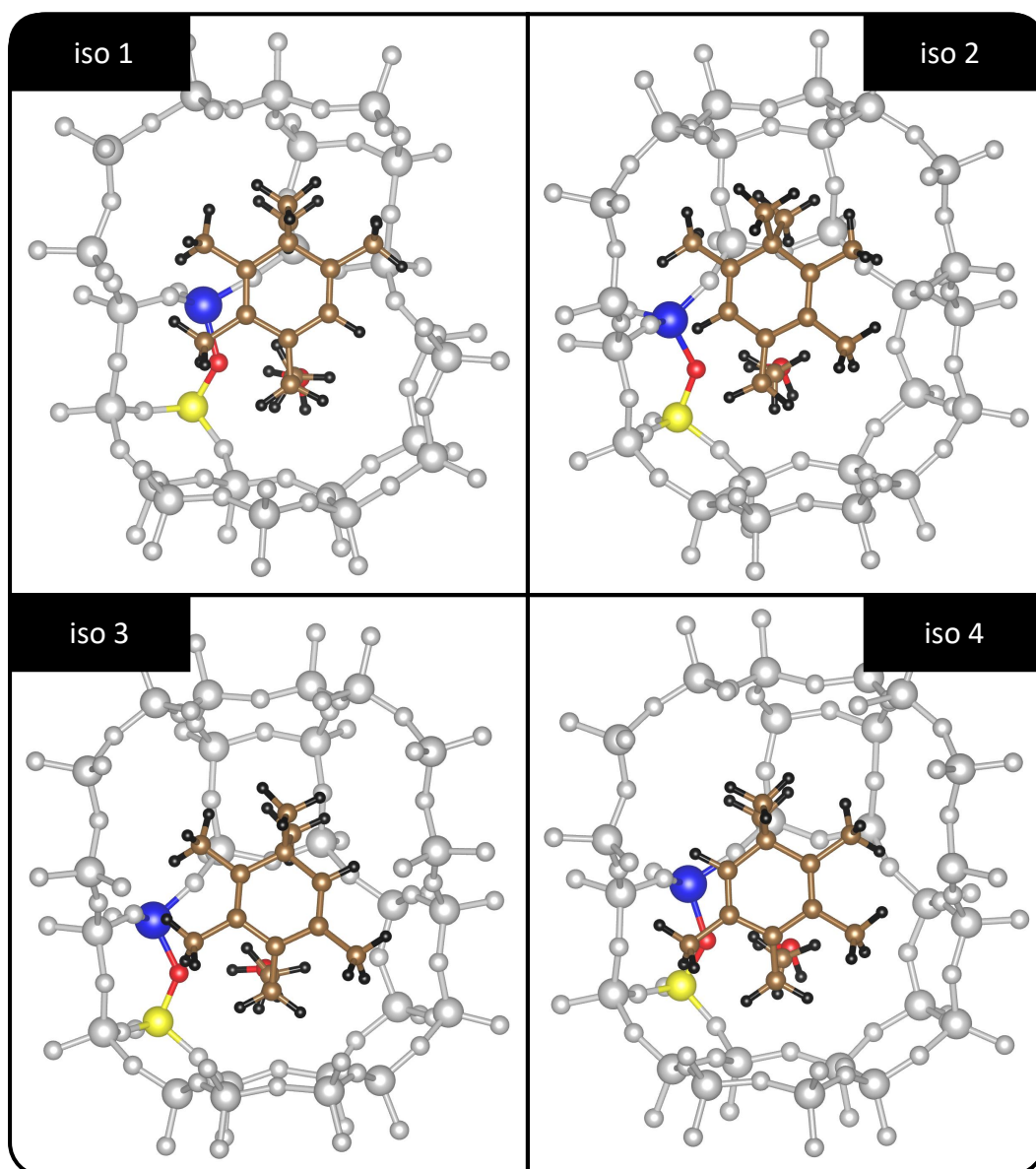
Figure S5. Transition state of step 3-4 from the main text shown for all four considered PMB isomers. Only the active site with the corresponding PMB isomer is color distinguished – Al = blue, Si = yellow, O = red, C = brown, H = black – other atoms are greyed for better readability. For all these isomers, the gem-methylated site is in para position to the site that is being methylated.

Table S3. PBE-D3 energy differences (ΔE_{PBE-D3}) of the rate-determining step (step 3-4 from the main text) for all the four considered PMB isomers relative to the most stable of them. Energies are in kJ/mol.

PMB isomer	ΔE_{PBE-D3} [kJ/mol]
iso 1	0
iso 2	+10
iso 3	+7
iso 4	+5

S 5 DIFFERENT GEM-METHYLATION POSITIONS

Three possible gem-methylation possitions with respect to the site where the side-chain is going to be formed - ortho, meta and para - were considered. Their corresponding structures are shown in Figure S6. ZPE corrected energy differences at the PBE-D3 level of theory referenced to the most stable - para-position - are shown in Table S4.
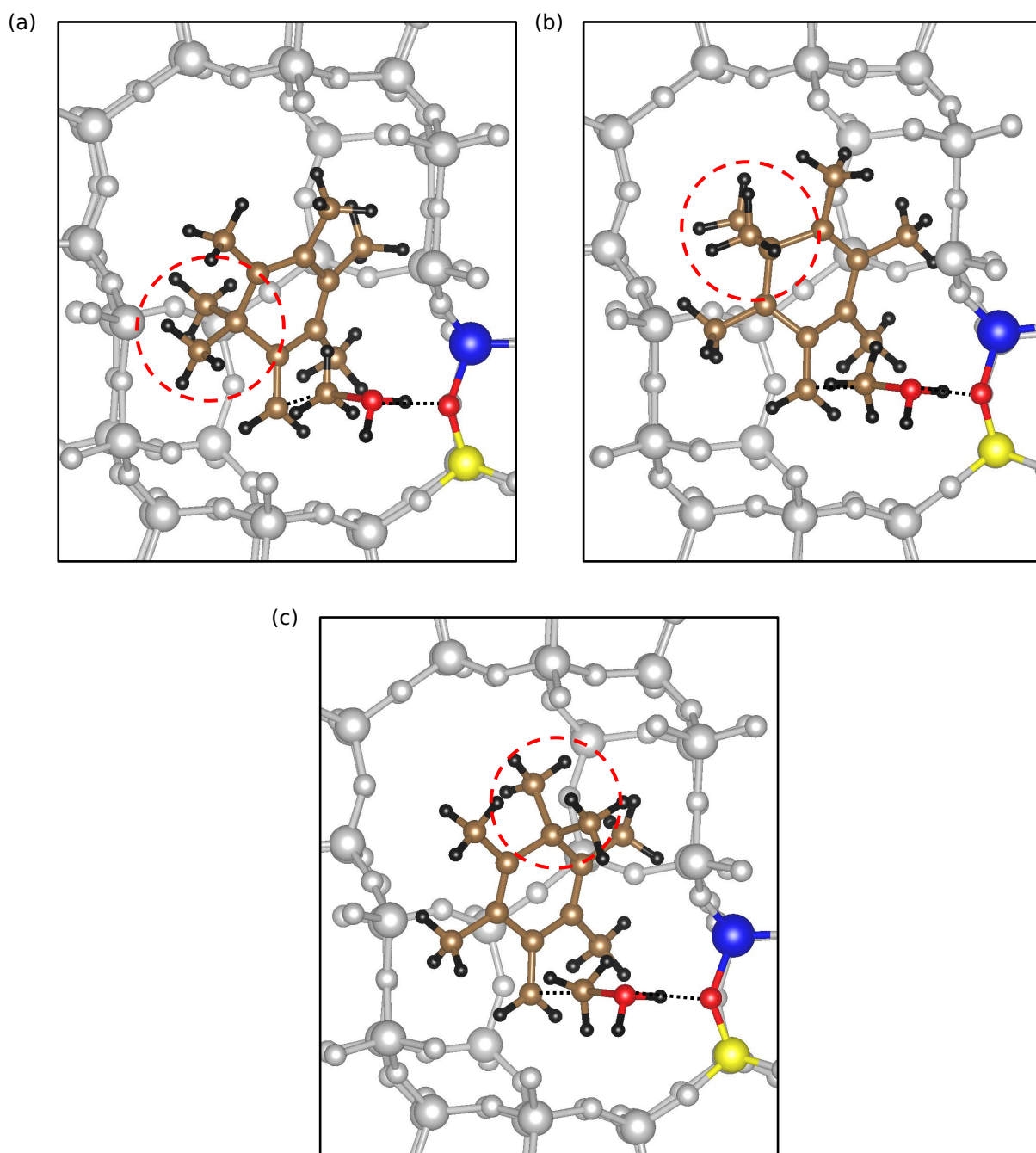
Figure S6. Considered possible gem-methylation positions - (a) ortho, (b) meta, and (c) para - with respect to the side-chain methylated site. The gem-methylated positions are highlighted by red dashed circle. Only the active site with the reactants are color-distinguished - red = O, blue = Al, yellow = Si, black = H, brown = C.

Table S4. PBE-D3 energy differences (ΔE_{PBE-D3}) and the Gibbs free energy differences - at the PBE-D3 level of theory (ΔG_{PBE-D3}) and cluster corrected (ΔG) - of the three considered gem-methylation positions referenced to the most stable of them. All values are in kJ/mol and ZPE corrected.

gem-position	ΔE_{PBE-D3} [kJ/mol]	ΔG_{PBE-D3} [kJ/mol]	ΔG [kJ/mol]
ortho	30	32	26
meta	131	112	140
para	0	0	0

Observed high energy difference of the meta-position is due to the fact that the corresponding structure is not conjugated unlike those corresponding to the ortho- and para-positions.

S 6 STEPWISE METHYLATIONS

The methylation of the first cross-conjugated intermediate (step 3-4) was also investigated proceeding via the stepwise mechanism. The corresponding PBE-D3 energies and the Gibbs free energies (at the PBE-D3 level of theory, and cluster corrected) are shown in Table S5 together with values for the concerted methylation from the main text. All these energies were obtained for 673 K, are in kJ/mol and are referenced to HMB*. Numeric indices were taken from Figure 1(a) from the main text.

Table S5. Energies at the PBE-D3 level of theory (ΔE_{PBE-D3}) and the Gibbs free energies - at the PBE-D3 level of theory (ΔG_{PBE-D3}) and cluster corrected (ΔG) - of the methylation of the first cross-conjugated intermediate. All energies are in kJ/mol, were obtained for 673 K and are referenced to HMB*.

step[a]	ΔE_{PBE-D3} [kJ/mol]	ΔG_{PBE-D3} [kJ/mol]	ΔG [kJ/mol]
3-4 (sw1)	56	204	214
3-4 (sw2)	86	145	148
3-4 (conc)	8	157	192

[a] Used abbreviations: sw = stepwise methylation, sw1 = SMS formation, sw2 = methylation via SMS, conc = concerted methylation.

S 7 COMPARISON WITH DATA FROM LITERATURE

Table S6 shows comparison of the energy span (i.e. the highest barrier versus the lowest energy state) of ethene production cycle of our work with those reported in literature

Table S6. Comparison of energy (ΔE) and free energy (ΔG) spans without applied cluster corrections obtained in this work with results reported in literature. The corresponding sources are in the column "reference".

mol	ΔE [kJ/mol]	ΔG(400 °C) [kJ/mol]	zeolite	reference
HMB	70	198	H-SSZ-13	this work
	147	202	H-SAPO-34	5
Durene[a]	92	177	H-SSZ-13	this work
	143	196	H-SAPO-34	5
	131	182	H-SSZ-13	5
	190	235	H-ZSM-5	6

[a] Durene = 1,2,4,5-tetramethyl-benzene.

S 8 TOTAL ENERGIES AND VIBRATIONS

Tables S7-9 summarize total energies of the used structures. Table S7 shows PBE-D3 total energies of periodic and cluster structures. Table S8 shows HF energies obtained for cc-pVXZ (where X is D, T or Q) basis set and Table S9 contains MP2 energies obtained for cc-pVDZ and cc-pVTZ basis set together with CCSD(T) using cc-pVDZ basis set. All energies given in eV. Table S10 shows lists of frequencies of the studied structures in cm^{-1}. Numerical indices were taken from Figure 1(a) from the main text.

Table S7. Overview of periodic PBE energies, corresponding D3 contributions, 46T cluster PBE-D3 energies and ZPE corrections of the studied structures. Numerical indices taken from Figure 1(a) from the main text. All values are in eV.

		PBE	D3	ZPVE	PBE-D3 46T
empty zeolite					
H-SSZ-13		-856.713	-5.887	0.611	-509092.873
gas phase					
H2O		-14.224	0.000	0.574	-2078.416
MeOH		-30.221	-0.015	1.362	-3146.534
ethene		-31.972	-0.013	1.357	-2136.159
propene		-48.671	-0.040	2.105	-3204.972
prehnitene		-142.382	-0.296	5.567	-10588.646
isodurene		-142.462	-0.285	5.558	-10588.719
durene		-142.526	-0.287	5.568	-10588.782
PMB		-158.947	-0.351	6.299	-11657.360
HMB		-175.328	-0.418	7.021	-12725.896
HMB mediated side-chain					
1		-1030.816	-8.081	7.759	-521819.291
1-2	IS	-1061.901	-8.607	9.153	-524967.204
	TS	-1060.840	-8.637	9.163	-524966.087
	FS	-1061.470	-8.581	9.169	-524966.573
2		-1047.139	-8.376	8.508	-522887.792
2-3	IS	-1047.066	-8.370	8.533	-522887.688
	TS	-1046.096	-8.414	8.411	-522886.937
	FS	-1046.138	-8.412	8.502	-522887.000
3-4	IS	-1076.883	-8.867	9.892	-526034.548
	TS	-1076.169	-8.889	9.906	-526033.826
	FS	-1077.940	-8.913	9.954	-526035.511
3-4 (ortho)	TS	-1075.830	-8.921	9.897	-526033.434
3-4 (meta)	TS	-1074.859	-8.845	9.808	-526032.387
4-E1	IS	-1063.400	-8.610	9.302	-523956.341
	TS	-1062.620	-8.605	9.264	-523955.474
	FS	-1063.320	-8.622	9.289	-523956.207
E1-E2	IS	-1063.318	-8.622	9.293	-523956.210
	TS	-1062.486	-8.602	9.270	-523955.310
	FS	-1063.044	-8.639	9.323	-523955.998
E2-E3	IS	-1063.043	-8.640	9.324	-523955.998
	TS	-1062.553	-8.618	9.274	-523955.407
	FS	-1063.564	-8.628	9.266	-523956.551
E3-1'	IS	-1063.592	-8.647	9.268	-523956.575
	TS	-1062.288	-8.690	9.060	-523955.497
	FS	-1063.008	-8.649	9.173	-523956.189
4-P1	IS	-1063.291	-8.650	9.319	-523956.247
	TS	-1061.441	-8.713	9.181	-523954.745
	FS	-1061.957	-8.675	9.280	-523955.214
P1-P2	IS	-1092.706	-9.173	10.695	-527102.814

	TS	-1092.087	-9.191	10.700	-527102.160
	FS	-1093.782	-9.151	10.686	-527103.670
P2-P3	IS	-1079.389	-8.937	10.057	-525024.800
	TS	-1078.492	-8.889	10.003	-525023.767
	FS	-1079.418	-8.917	10.020	-525024.733
P3-P4	IS	-1079.354	-8.917	10.055	-525024.629
	TS	-1078.456	-8.894	10.050	-525023.678
	FS	-1079.041	-8.926	10.090	-525024.385
P4-P5	IS	-1079.048	-8.951	10.101	-525024.407
	TS	-1078.412	-8.902	10.037	-525023.699
	FS	-1079.492	-8.912	10.041	-525024.878
P5-1'	IS	-1079.524	-8.926	10.044	-525024.880
	TS	-1078.732	-8.987	9.862	-525024.291
	FS	-1079.041	-8.994	9.970	-525024.670
PMB and TMBs mediated methylations					
prehnitene					
1		-998.854	-7.576	6.223	-519682.596
3-4	TS	-1044.089	-8.379	8.356	-523896.960
isodurene					
1		-998.797	-7.561	6.226	-519682.551
3-4	TS	-1043.965	-8.408	8.391	-523896.876
durene					
1		-999.125	-7.560	6.212	-519682.859
1-2	TS	-1029.099	-8.101	7.611	-522829.628
2		-1015.274	-7.838	6.962	-520751.211
3-4	TS	-1044.424	-8.367	8.346	-523897.294
4		-1031.423	-8.104	7.744	-521819.669
PMB					
1		-1015.214	-7.841	6.982	-520751.343
1-2	TS	-1045.123	-8.372	8.372	-523898.018
2		-1031.375	-8.099	7.726	-521819.588
3-4	IS	-1061.207	-8.614	9.115	-524966.468
	TS	-1060.416	-8.663	9.122	-524965.652
	FS	-1062.152	-8.632	9.167	-524967.270
4		-1047.655	-8.381	8.507	-522888.225
stepwise methylation of 3-4					
SMS formation	IS	-1076.410	-8.911	9.945	-526033.795
	TS	-1075.658	-8.903	9.901	-526033.337
	FS	-1076.234	-8.904	9.924	-526034.018
methylation	IS	-1061.883	-8.627	9.297	-523955.085
	TS	-1061.344	-8.682	9.250	-523954.564
	FS	-1063.269	-8.643	9.330	-523956.259

Table S8. Overview of HF energies of the studied structures. Numerical indices taken from Figure 1(a) from the main text. All values are in eV.

	HF/cc-pVDZ	HF/cc-pVTZ	HF/cc-pVQZ
empty zeolite			
H-SSZ-13	-507910.355	-508017.027	-508040.639
gas phase			
H2O	-2068.762	-2069.584	-2069.792

MeOH		-3130.617	-3131.699	-3131.956
ethene		-2123.570	-2124.205	-2124.350
propene		-3185.959	-3186.870	-3187.079
prehnitene		-10527.204	-10529.838	-10530.478
isodurene		-10527.354	-10529.988	-10530.632
durene		-10527.423	-10530.060	-10530.699
PMB		-11589.446	-11592.352	-11593.061
HMB		-12651.416	-12654.593	-12655.370

HMB mediated side-chain

1		-520560.646	-520669.957	-520694.132
1-2	IS	-523691.919	-523801.801	-523826.108
	TS	-523690.434	-523800.177	-523824.481
	FS	-523691.437	-523801.229	-523825.551
2		-521622.528	-521731.590	-521755.748
2-3	IS	-521622.383	-521731.532	-521755.722
	TS	-521620.934	-521730.183	-521754.369
	FS	-521621.343	-521730.777	-521754.986
3-4	IS	-524752.604	-524862.767	-524887.125
	TS	-524751.514	-524861.561	-524885.912
	FS	-524753.798	-524863.707	-524888.055
3-4 (ortho)	TS	-524751.058	-524861.175	-524885.544
3-4 (meta)	TS	-524749.206	-524859.413	-524883.796
4-E1	IS	-522684.456	-522793.797	-522818.016
	TS	-522683.283	-522792.620	-522816.835
	FS	-522684.301	-522793.660	-522817.899
E1-E2	IS	-522684.309	-522793.657	-522817.896
	TS	-522683.049	-522792.387	-522816.591
	FS	-522684.039	-522793.345	-522817.564
E2-E3	IS	-522684.040	-522793.349	-522817.568
	TS	-522683.241	-522792.517	-522816.711
	FS	-522684.604	-522793.982	-522818.187
E3-1'	IS	-522684.642	-522793.972	-522818.183
	TS	-522682.706	-522792.119	-522816.326
	FS	-522684.159	-522793.953	-522818.190
4-P1	IS	-522684.277	-522793.759	-522817.995
	TS	-522681.955	-522791.266	-522815.478
	FS	-522683.193	-522792.979	-522817.254
P1-P2	IS	-525814.135	-525924.420	-525948.832
	TS	-525813.123	-525923.372	-525947.755
	FS	-525815.328	-525925.600	-525950.000
P2-P3	IS	-523746.275	-523855.832	-523880.082
	TS	-523744.923	-523854.465	-523878.695
	FS	-523746.111	-523855.700	-523879.973
P3-P4	IS	-523746.015	-523855.536	-523879.804
	TS	-523744.714	-523854.223	-523878.474
	FS	-523745.727	-523855.177	-523879.440
P4-P5	IS	-523745.824	-523855.243	-523879.498
	TS	-523744.812	-523854.191	-523878.404
	FS	-523746.192	-523855.656	-523879.907
P5-1'	IS	-523746.108	-523855.576	-523879.822

		TS	-523744.999	-523854.677	-523878.924
		FS	-523745.723	-523855.633	-523879.906
PMB and TMBs mediated methylations					
prehnitene					
	1		-518437.400	-518546.416	-518570.512
	3-4	TS	-522628.116	-522737.902	-522762.199
isodurene					
	1		-518437.432	-518546.340	-518570.430
	3-4	TS	-522628.022	-522737.783	-522762.067
durene					
	1		-518437.737	-518546.791	-518570.882
	1-2	TS	-521567.564	-521677.005	-521701.235
	2		-519499.576	-519608.300	-519632.384
	3-4	TS	-522628.547	-522738.354	-522762.652
	4		-520561.450	-520670.418	-520694.545
PMB					
	1		-519499.343	-519608.381	-519632.484
	1-2	TS	-522629.177	-522738.739	-522763.018
	2		-520561.153	-520670.077	-520694.198
	3-4	IS	-523691.350	-523801.316	-523825.642
		TS	-523690.076	-523800.083	-523824.408
		FS	-523692.364	-523802.297	-523826.627
	4		-521623.151	-521732.410	-521756.580
stepwise methylation of 3-4					
SMS formation		IS	-524751.850	-524861.745	-524886.082
		TS	-524751.454	-524861.369	-524885.720
		FS	-524752.339	-524862.508	-524886.854
methylation		IS	-522683.278	-522792.889	-522817.122
		TS	-522682.133	-522791.682	-522815.927
		FS	-522684.300	-522793.716	-522817.931

Table S9. Overview of MP2 and CCSD(T) energies of the studied structures. Numerical indices taken from Figure 1(a) from the main text. All values are in eV.

		MP2/cc-pVDZ	MP2/cc-pVTZ	CCSD(T)/cc-pVDZ
empty zeolite				
	H-SSZ-13	-508366.308	-508599.699	-508388.189
gas phase				
	H2O	-2074.278	-2076.729	-2074.624
	MeOH	-3139.856	-3143.376	-3140.748
	ethene	-2131.059	-2133.344	-2132.147
	propene	-3197.339	-3200.748	-3198.889
	prehnitene	-10564.590	-10575.186	-10568.379
	isodurene	-10564.667	-10575.254	-10568.468
	durene	-10564.730	-10575.319	-10568.523
	PMB	-11630.853	-11642.570	-11635.090
	HMB	-12696.935	-12709.790	-12701.615
HMB mediated side-chain				
	1	-521064.088	-521310.035	-521090.585
	1-2 IS	-524205.677	-524454.763	-524232.958
	TS	-524204.368	-524453.383	-524231.624

	FS	-524204.841	-524453.864	-524232.245
2		-522130.140	-522376.774	-522157.212
2-3	IS	-522129.959	-522376.675	-522157.045
	TS	-522129.162	-522375.946	-522156.229
	FS	-522129.295	-522376.221	-522156.420
3-4	IS	-525270.465	-525520.683	-525298.428
	TS	-525269.480	-525519.659	-525297.402
	FS	-525271.470	-525521.518	-525299.331
3-4 (ortho)	TS	-525269.081	-525519.326	-525296.987
3-4 (meta)	TS	-525267.854	-525518.134	-525295.570
4-E1	IS	-523196.202	-523443.991	-523223.742
	TS	-523195.518	-523443.329	-523222.869
	FS	-523196.036	-523443.848	-523223.585
E1-E2	IS	-523196.048	-523443.846	-523223.597
	TS	-523195.375	-523443.205	-523222.716
	FS	-523195.958	-523443.754	-523223.464
E2-E3	IS	-523195.955	-523443.754	-523223.460
	TS	-523195.544	-523443.331	-523222.902
	FS	-523196.355	-523444.187	-523223.884
E3-1'	IS	-523196.459	-523444.228	-523223.978
	TS	-523195.211	-523443.124	-523222.543
	FS	-523195.940	-523444.129	-523223.407
4-P1	IS	-523196.007	-523443.955	-523223.548
	TS	-523194.642	-523442.428	-523222.176
	FS	-523195.029	-523443.228	-523222.676
P1-P2	IS	-526336.360	-526587.638	-526364.759
	TS	-526335.405	-526586.709	-526363.762
	FS	-526337.062	-526588.341	-526365.403
P2-P3	IS	-524262.266	-524511.159	-524290.287
	TS	-524261.379	-524510.294	-524289.218
	FS	-524262.154	-524511.036	-524290.153
P3-P4	IS	-524262.113	-524510.973	-524290.126
	TS	-524261.369	-524510.276	-524289.170
	FS	-524261.972	-524510.812	-524289.956
P4-P5	IS	-524262.042	-524510.874	-524290.043
	TS	-524261.553	-524510.327	-524289.358
	FS	-524262.394	-524511.227	-524290.341
P5-1'	IS	-524262.488	-524511.299	-524290.400
	TS	-524261.445	-524510.537	-524289.302
	FS	-524262.099	-524511.327	-524289.955

PMB and TMBs mediated methylations

prehnitene				
1		-518932.084	-519175.904	-518957.724
3-4	TS	-523137.243	-523385.311	-523164.310
isodurene				
1		-518932.123	-519175.838	-518957.770
3-4	TS	-523137.184	-523385.260	-523164.254
durene				
1		-518932.295	-519176.091	-518957.937
1-2	TS	-522072.563	-522319.391	-522098.979

2		-519998.276	-520242.659	-520024.517
3-4	TS	-523137.492	-523385.557	-523164.580
4		-521064.258	-521309.814	-521090.959
PMB				
1		-519998.553	-520243.284	-520024.610
1-2	TS	-523138.644	-523386.538	-523165.502
2		-521064.239	-521309.785	-521090.902
3-4	IS	-524204.760	-524453.826	-524232.306
	TS	-524203.531	-524452.720	-524231.034
	FS	-524205.385	-524454.509	-524232.840
4		-522130.342	-522377.128	-522157.471

stepwise methylation of 3-4

SMS formation	IS	-525269.872	-525519.869	-525297.804
	TS	-525269.244	-525519.307	-525297.273
	FS	-525270.028	-525520.262	-525298.027
methylation	IS	-523195.032	-523443.020	-523222.731
	TS	-523194.228	-523442.224	-523221.868
	FS	-523196.107	-523443.968	-523223.629

Table S10. Frequencies of the studied structures.

	list of frequencies [cm^{-1}]
empty zeolite	
H-SSZ-13	245.5, 286.5, 294.1, 354.6, 510.7, 601.9, 628.6, 701.2, 722.7, 779.2, 1029.4, 3701.6
gas phase (first 6 frequencies discarded)	
H2O	1577.2, 3698.9, 3814.2
MeOH	298.0, 1010.5, 1056.2, 1128.0, 1325.3, 1419.6, 1439.8, 1452.0, 2918.7, 2970.1, 3043.7, 3728.1
ethene	808.9, 936.2, 939.2, 1034.5, 1199.3, 1342.0, 1420.9, 1638.2, 3051.2, 3065.2, 3124.3, 3153.8
propene	199.8, 417.5, 570.8, 898.6, 912.9, 914.4, 989.9, 1024.9, 1154.2, 1285.3, 1349.2, 1395.5, 1421.1, 1437.6, 1660.1, 2946.8, 2997.5, 3031.4, 3051.1, 3057.1, 3141.8
prehnitene	44.9, 57.8, 121.0, 134.3, 186.4, 195.8, 259.7, 309.8, 314.5, 319.9, 393.9, 458.4, 474.3, 494.7, 501.0, 550.3, 636.8, 715.1, 720.5, 787.5, 844.2, 907.1, 919.0, 965.9, 981.6, 982.6, 1001.7, 1023.1, 1023.8, 1051.2, 1056.6, 1159.3, 1195.4, 1240.7, 1248.1, 1320.2, 1346.6, 1353.1, 1359.0, 1367.8, 1392.7, 1416.8, 1417.9, 1422.6, 1433.5, 1437.8, 1443.0, 1450.6, 1460.7, 1462.0, 1577.4, 1597.4, 2946.8, 2947.9, 2953.5, 2955.5, 2993.3, 2994.7, 2999.0, 3001.7, 3041.2, 3042.5, 3068.7, 3075.2, 3080.6, 3093.7
isodurene	36.2, 46.2, 109.6, 161.2, 172.4, 189.1, 224.6, 271.2, 301.5, 315.8, 352.8, 448.4, 492.6, 509.7, 540.5, 543.6, 570.5, 704.1, 732.4, 834.1, 864.0, 890.4, 954.3, 971.9, 984.7, 998.4, 1001.1, 1014.2, 1015.6, 1025.5, 1061.5, 1135.2, 1199.5, 1236.3, 1291.3, 1328.3, 1351.1, 1354.9, 1356.2, 1362.1, 1396.3, 1410.5, 1419.3, 1430.4, 1431.7, 1436.8, 1443.0, 1450.3, 1456.1, 1475.9, 1574.2, 1606.7, 2945.0, 2949.4, 2950.8, 2952.8, 3001.1, 3002.0, 3011.3, 3016.3, 3039.5, 3040.9, 3042.4, 3050.9, 3068.0, 3070.0
durene	116.0, 136.0, 136.8, 150.6, 168.1, 188.8, 255.6, 281.9, 288.4, 301.5, 332.9, 425.1, 438.0, 500.4, 515.8, 577.2, 658.3, 703.4, 735.9, 805.0, 847.8, 856.4, 964.7, 973.6, 986.1, 994.7, 1003.3, 1015.3, 1023.5, 1028.6, 1068.4, 1184.4, 1188.6, 1259.7, 1271.7, 1329.6, 1348.3, 1350.4, 1361.5, 1362.6, 1378.6, 1419.3, 1421.1, 1427.9, 1434.4, 1436.2, 1438.1, 1445.0, 1453.7, 1493.7, 1559.0, 1617.5, 2945.7, 2947.2, 2948.2, 2949.3, 2992.6, 2993.7, 2998.2, 2999.2, 3040.0, 3041.6, 3042.2, 3044.4, 3064.7, 3067.3
PMB	63.9, 92.6, 109.0, 117.6, 138.5, 170.1, 172.0, 195.3, 286.2, 295.3, 326.3, 339.3, 344.0, 378.2, 439.2, 481.0, 520.7, 546.4, 565.9, 570.6, 678.8, 713.4, 798.4, 843.5, 887.4, 966.3, 974.7, 975.6, 992.4, 998.2, 1011.7, 1020.6, 1024.4, 1056.3, 1063.0, 1065.8, 1208.7, 1228.6, 1291.7, 1321.9, 1349.7, 1350.9, 1353.3, 1356.8, 1362.1, 1390.5, 1410.2, 1415.3, 1422.3, 1424.0, 1435.2, 1443.6, 1445.2, 1449.9, 1454.8, 1464.4, 1474.7, 1568.2, 1598.3, 2946.5, 2948.7, 2949.9, 2951.3, 2951.7, 3000.0, 3001.6, 3003.9, 3004.5, 3013.3, 3038.9, 3039.3, 3061.3, 3062.4, 3065.8, 3069.0
HMB	57.2, 61.8, 65.9, 71.4, 75.5, 77.6, 124.2, 131.8, 168.6, 191.4, 333.9, 335.6, 341.7, 342.9, 393.4, 395.9, 434.3, 445.6, 446.8, 549.3, 568.4, 568.8, 573.3, 584.9, 720.3, 795.1, 795.6, 954.8, 955.5, 965.1, 965.3, 989.2, 990.2, 1018.2, 1019.4, 1025.7, 1043.8, 1044.6, 1063.7, 1064.3, 1070.8, 1235.0, 1303.2, 1315.9, 1347.7, 1348.5, 1352.2, 1354.9, 1355.6, 1363.0, 1397.7, 1397.9, 1413.2, 1414.1, 1420.5, 1427.8, 1438.7, 1439.3, 1440.1, 1455.5, 1455.9, 1464.6, 1466.5, 1479.3, 1571.4, 1571.6, 2942.8, 2943.3, 2944.0, 2944.3, 2945.2, 2945.8, 3016.8, 3018.5, 3019.3, 3023.6, 3023.9, 3027.5, 3045.2, 3049.8, 3050.8, 3056.2, 3057.1, 3059.1
HMB mediated side-chain	
1	40.7, 52.0, 56.0, 85.0, 86.4, 103.0, 110.2, 127.3, 131.8, 156.8, 168.8, 177.7, 186.3, 193.5, 209.3, 226.9, 241.1, 284.8, 291.6, 329.5, 337.3, 344.9, 352.9, 355.5, 374.2, 413.3, 436.2, 453.5, 463.9, 511.4, 563.6, 570.5, 571.5, 573.0, 588.9, 601.3, 619.8, 703.5, 720.2, 721.6, 782.8, 806.6, 813.0, 951.1, 968.8, 978.6, 983.0, 992.8, 1003.4, 1018.1, 1031.3, 1033.5, 1033.6, 1050.2, 1072.3, 1073.5, 1080.0, 1101.7, 1252.7, 1329.7, 1335.9, 1349.1, 1349.9, 1355.3, 1356.4, 1359.2, 1366.3, 1407.1, 1408.4, 1415.3, 1418.7, 1429.4, 1431.5, 1435.3, 1445.6, 1454.5, 1457.3, 1463.0, 1469.3, 1470.0, 1470.6, 1582.0, 1599.5, 2943.5, 2945.2, 2973.6, 2973.9, 2976.6, 2979.7, 3016.6, 3017.4, 3022.6, 3025.8, 3034.2, 3037.6, 3060.1, 3061.6, 3146.9, 3154.0, 3183.2, 3188.1, 3695.9
1-2 IS	39.4, 60.3, 73.9, 91.0, 92.8, 95.2, 103.0, 109.1, 118.3, 120.3, 132.8, 141.8, 149.6, 161.4, 169.2, 173.1, 178.9, 192.4, 195.0, 215.6, 229.8, 247.1, 281.2, 329.2, 331.9, 346.0, 351.6, 353.1, 372.4, 416.6, 437.8, 454.5, 462.1, 466.6, 565.8, 570.8, 571.4, 572.3, 574.2, 596.0, 601.1, 626.0, 684.5, 701.7, 722.5, 758.6, 807.0, 814.1, 858.9, 951.4, 955.4, 969.4, 977.7, 983.1, 994.6, 1004.7, 1019.9, 1032.0, 1034.8, 1050.3, 1070.5, 1073.0, 1074.2, 1080.9, 1090.9, 1101.5, 1149.0, 1253.7, 1325.3, 1328.7, 1336.6, 1350.1, 1351.9, 1356.3, 1358.1, 1361.2, 1365.5, 1368.2, 1405.7, 1407.2, 1415.0, 1417.4, 1426.8, 1428.3, 1431.1, 1435.5, 1440.3, 1443.4, 1445.7, 1453.4, 1457.6, 1463.4, 1468.4, 1469.4, 1471.3, 1579.8, 1580.4, 1597.6, 2942.5, 2947.5,

		2973.0, 2975.6, 2984.0, 2985.9, 2994.2, 3020.6, 3023.1, 3023.6, 3027.2, 3040.6, 3042.1, 3063.6, 3065.2, 3092.4, 3115.0, 3135.0, 3162.2, 3177.6, 3192.5, 3333.1
	TS	365.5i, 45.6, 61.2, 72.8, 92.0, 97.1, 108.0, 111.7, 126.8, 138.1, 143.2, 155.6, 170.3, 172.5, 184.5, 188.6, 193.8, 206.9, 214.5, 227.3, 240.2, 256.5, 274.4, 302.2, 334.4, 336.4, 350.2, 357.5, 379.6, 388.5, 393.9, 414.1, 440.9, 451.0, 461.3, 513.6, 552.7, 553.2, 567.5, 567.8, 574.4, 579.8, 602.2, 637.7, 661.9, 682.0, 704.0, 719.9, 802.8, 814.5, 873.2, 937.2, 952.3, 958.0, 969.3, 975.6, 986.1, 993.2, 1005.9, 1016.7, 1019.7, 1025.4, 1033.0, 1054.1, 1074.8, 1077.7, 1081.8, 1101.8, 1106.9, 1259.5, 1316.0, 1335.4, 1342.6, 1348.7, 1352.5, 1353.4, 1360.9, 1362.8, 1366.2, 1370.3, 1388.8, 1401.7, 1408.2, 1416.7, 1424.0, 1430.1, 1435.6, 1441.1, 1450.8, 1456.1, 1458.6, 1464.5, 1470.9, 1472.7, 1544.3, 1590.3, 1614.4, 2956.3, 2958.4, 2980.0, 2987.2, 2989.3, 2998.7, 3013.4, 3029.6, 3032.2, 3042.9, 3048.0, 3051.5, 3069.4, 3077.7, 3105.0, 3146.1, 3170.5, 3173.4, 3196.4, 3204.0, 3237.2, 3267.6, 3568.6
	FS	30.5, 48.2, 62.1, 66.7, 80.3, 86.3, 89.2, 95.9, 108.6, 112.8, 133.9, 137.7, 147.2, 166.4, 173.3, 198.6, 238.4, 248.6, 256.0, 262.6, 267.4, 289.5, 301.4, 312.8, 321.5, 333.3, 345.5, 364.3, 365.1, 378.6, 392.1, 396.3, 414.8, 437.2, 445.4, 454.3, 535.3, 548.4, 552.9, 562.2, 568.7, 569.7, 598.0, 602.9, 646.4, 661.3, 679.2, 680.7, 772.7, 795.9, 836.6, 918.9, 944.3, 953.0, 961.8, 963.4, 976.5, 989.9, 993.5, 1012.4, 1017.0, 1034.2, 1046.7, 1054.0, 1075.1, 1083.1, 1087.6, 1111.0, 1213.3, 1257.8, 1321.6, 1326.9, 1334.7, 1336.3, 1343.3, 1355.2, 1359.4, 1371.3, 1377.0, 1399.0, 1400.2, 1406.2, 1417.6, 1422.8, 1424.2, 1430.4, 1434.1, 1443.8, 1447.4, 1448.8, 1451.7, 1462.9, 1469.0, 1487.7, 1523.0, 1599.2, 1615.8, 2967.1, 2968.2, 2968.6, 2976.3, 2988.0, 3004.6, 3018.3, 3021.3, 3031.4, 3035.0, 3037.5, 3043.9, 3086.7, 3091.9, 3096.3, 3101.1, 3146.2, 3148.0, 3187.5, 3210.1, 3232.7, 3537.1, 3732.1
2		20.8, 49.4, 61.9, 74.1, 82.8, 93.5, 106.0, 131.8, 154.6, 168.9, 175.4, 191.2, 197.5, 206.0, 208.2, 225.8, 254.2, 261.9, 285.8, 290.1, 300.6, 320.0, 331.0, 355.1, 363.2, 380.1, 382.9, 411.1, 429.0, 440.4, 466.8, 535.8, 540.7, 555.3, 567.4, 571.4, 591.6, 599.5, 634.4, 658.8, 677.7, 684.5, 785.4, 800.6, 849.3, 929.8, 936.1, 949.0, 954.4, 972.6, 984.0, 994.0, 998.3, 1020.4, 1029.2, 1039.2, 1069.6, 1075.8, 1080.9, 1093.1, 1094.9, 1107.0, 1213.2, 1263.5, 1323.2, 1330.0, 1333.7, 1344.6, 1348.2, 1358.1, 1359.7, 1365.7, 1374.1, 1384.9, 1397.5, 1400.1, 1414.6, 1417.7, 1422.4, 1424.7, 1427.2, 1435.3, 1448.3, 1454.2, 1459.6, 1459.9, 1467.5, 1486.1, 1525.2, 1591.5, 2948.7, 2970.3, 2976.1, 2988.7, 2990.5, 2995.6, 2996.3, 3018.7, 3034.2, 3047.0, 3054.6, 3057.7, 3077.0, 3084.4, 3084.5, 3085.7, 3103.1, 3159.1, 3169.1, 3173.7, 3194.6
2-3	IS	45.1, 58.4, 77.2, 84.9, 87.0, 98.1, 108.8, 123.8, 135.5, 163.9, 200.1, 212.9, 225.8, 247.2, 255.5, 260.0, 277.8, 287.1, 297.9, 303.7, 309.3, 333.9, 343.1, 363.8, 366.8, 381.6, 390.9, 422.3, 432.3, 448.4, 469.5, 537.3, 540.7, 560.8, 565.0, 574.9, 589.9, 595.8, 636.8, 660.7, 676.3, 687.2, 784.1, 799.4, 851.4, 931.4, 938.7, 946.5, 954.0, 965.7, 978.5, 991.5, 997.5, 1019.7, 1027.6, 1035.4, 1067.4, 1071.7, 1077.0, 1087.7, 1092.0, 1111.8, 1213.8, 1265.4, 1318.6, 1328.5, 1334.7, 1347.4, 1350.7, 1357.4, 1363.3, 1368.6, 1374.7, 1380.4, 1398.2, 1404.2, 1416.5, 1421.3, 1424.3, 1425.2, 1428.9, 1436.8, 1439.0, 1443.3, 1458.0, 1459.9, 1468.1, 1489.1, 1520.9, 1594.7, 2947.2, 2971.1, 2978.8, 2981.9, 2982.7, 2988.7, 2990.6, 3011.9, 3032.4, 3039.2, 3044.6, 3046.6, 3067.9, 3078.7, 3083.4, 3095.4, 3096.4, 3179.4, 3194.7, 3214.4, 3218.4
	TS	716.6i, 55.3, 71.0, 78.5, 89.8, 99.5, 106.9, 148.4, 157.8, 180.7, 207.9, 226.2, 230.4, 262.4, 273.8, 275.6, 283.7, 295.9, 325.3, 329.5, 338.6, 346.6, 352.2, 362.8, 367.8, 394.4, 402.2, 432.7, 457.5, 465.6, 509.2, 550.7, 553.3, 570.0, 584.0, 598.1, 604.0, 624.7, 632.7, 654.8, 672.2, 710.5, 737.1, 781.7, 795.4, 868.9, 899.0, 921.5, 933.7, 958.3, 969.6, 982.5, 995.9, 1004.8, 1011.4, 1026.6, 1032.2, 1069.2, 1074.0, 1078.3, 1095.6, 1110.9, 1131.8, 1144.8, 1211.4, 1269.8, 1284.0, 1339.9, 1346.2, 1346.8, 1356.2, 1358.8, 1364.4, 1369.1, 1380.8, 1396.3, 1416.1, 1417.5, 1425.7, 1431.3, 1433.3, 1437.7, 1440.7, 1444.7, 1451.0, 1454.3, 1465.9, 1472.5, 1522.5, 1572.3, 1641.3, 2968.7, 2970.2, 2974.9, 2975.0, 2976.0, 2979.8, 3019.8, 3023.5, 3030.0, 3042.2, 3048.7, 3054.1, 3062.7, 3076.9, 3079.6, 3133.3, 3137.5, 3144.0, 3211.1, 3215.6
	FS	58.9, 62.2, 80.9, 86.1, 96.3, 110.2, 132.7, 144.1, 163.2, 192.2, 201.3, 225.1, 256.2, 264.7, 265.5, 273.3, 290.1, 301.4, 324.9, 333.2, 340.8, 344.2, 352.9, 358.4, 367.9, 390.5, 403.5, 434.2, 455.0, 470.2, 545.8, 548.6, 549.0, 572.5, 588.7, 593.4, 612.3, 622.9, 661.2, 687.4, 709.9, 721.4, 765.1, 773.3, 792.0, 808.6, 831.7, 900.6, 918.2, 929.0, 956.8, 974.3, 981.3, 996.6, 1005.5, 1026.4, 1032.3, 1073.8, 1076.4, 1084.1, 1101.7, 1113.8, 1136.6, 1210.4, 1235.4, 1263.9, 1278.4, 1338.2, 1344.7, 1355.7, 1359.0, 1364.5, 1368.4, 1382.2, 1388.3, 1416.6, 1418.2, 1426.1, 1431.4, 1432.5, 1435.7, 1440.9, 1445.5, 1448.5, 1452.7, 1464.7, 1473.1, 1532.0, 1600.1, 1651.4, 2619.1, 2963.8, 2964.9, 2971.7, 2971.9, 2974.8, 2977.6, 3019.2, 3020.4, 3023.3, 3033.0, 3041.5, 3059.0, 3070.3, 3073.3, 3073.8, 3138.4, 3149.6, 3159.7, 3202.9, 3216.5
3-4	IS	35.7, 47.8, 56.7, 72.1, 73.8, 87.6, 93.9, 96.2, 109.2, 113.5, 115.4, 125.1, 135.6, 139.8, 152.4, 165.5, 174.4, 213.1, 230.8, 244.6, 246.0, 271.2, 272.9, 276.5, 324.9, 338.3, 344.1, 351.4, 364.7, 374.5, 394.9, 411.2, 436.1, 440.2, 455.0, 460.9, 560.8, 563.1, 570.3, 576.9, 578.8, 592.7, 609.8, 644.3, 689.9, 698.1, 704.7, 710.4, 739.0, 777.3, 785.7, 815.3, 854.5, 901.5, 902.6, 916.0, 948.8, 965.4, 966.3, 975.1, 991.8, 1004.2, 1020.8, 1029.7, 1066.7, 1068.3, 1075.7, 1082.8, 1089.2, 1101.1, 1118.0, 1130.8, 1174.6, 1199.0, 1207.3, 1262.7, 1294.8, 1334.0, 1343.7, 1347.7, 1354.2, 1357.2, 1364.8, 1370.1, 1389.7, 1405.2, 1418.1, 1423.5, 1428.1, 1429.4, 1430.5, 1437.8, 1438.1, 1440.2, 1442.0, 1448.0, 1453.7, 1460.3, 1462.2, 1468.1, 1475.2, 1568.2,

		1613.9, 1628.5, 1657.0, 2961.1, 2967.4, 2973.2, 2990.8, 2993.7, 3002.4, 3007.9, 3014.5, 3016.0, 3051.5, 3052.0, 3059.1, 3064.2, 3068.7, 3072.2, 3094.0, 3113.5, 3122.3, 3123.8, 3166.6, 3193.2, 3218.2, 3225.6, 3409.4
	TS	434.1i, 34.0, 56.4, 61.7, 74.7, 81.7, 94.5, 100.8, 113.2, 120.8, 126.2, 153.6, 161.0, 169.6, 171.5, 187.5, 218.6, 238.4, 242.8, 246.4, 254.3, 265.6, 279.0, 285.4, 290.4, 323.4, 336.2, 343.0, 357.3, 362.8, 388.8, 393.1, 405.0, 414.1, 436.9, 451.4, 464.4, 507.1, 561.0, 562.9, 566.8, 579.7, 581.0, 590.4, 617.7, 621.9, 665.1, 679.0, 719.6, 753.4, 776.2, 781.9, 790.8, 877.8, 907.2, 915.7, 920.2, 952.2, 964.8, 972.9, 978.3, 991.7, 995.5, 1004.1, 1008.8, 1026.3, 1031.9, 1062.7, 1069.8, 1077.8, 1080.7, 1089.9, 1100.4, 1114.6, 1133.1, 1200.8, 1266.4, 1305.2, 1334.9, 1338.5, 1345.7, 1349.6, 1353.6, 1359.4, 1362.4, 1372.8, 1381.9, 1414.7, 1417.2, 1426.6, 1429.3, 1430.6, 1435.8, 1439.9, 1445.0, 1451.9, 1453.8, 1461.5, 1464.0, 1476.5, 1526.7, 1596.9, 1602.8, 1645.2, 2809.4, 2966.9, 2972.8, 2981.5, 2987.0, 2998.3, 2999.5, 3014.4, 3019.2, 3047.1, 3055.5, 3060.7, 3063.9, 3067.3, 3070.7, 3078.8, 3112.2, 3134.5, 3166.1, 3194.6, 3208.1, 3215.5, 3240.3, 3265.9, 3639.7
	FS	54.0, 63.4, 68.9, 72.8, 77.9, 86.8, 87.6, 104.6, 106.2, 113.2, 127.8, 151.9, 154.0, 166.0, 178.5, 188.1, 196.5, 215.4, 227.0, 239.7, 247.1, 260.7, 267.3, 271.8, 298.3, 317.9, 333.6, 342.8, 359.3, 366.2, 373.4, 378.8, 385.5, 396.8, 402.1, 437.2, 456.4, 463.5, 521.7, 564.5, 564.6, 573.0, 586.3, 588.3, 593.9, 624.4, 644.1, 651.4, 680.6, 739.5, 776.8, 779.7, 829.7, 884.8, 927.8, 935.1, 942.2, 958.1, 963.5, 974.3, 995.4, 1002.8, 1006.1, 1016.0, 1033.6, 1041.1, 1045.1, 1068.9, 1081.0, 1091.9, 1099.8, 1107.4, 1200.3, 1220.3, 1248.2, 1272.8, 1330.0, 1338.2, 1343.9, 1344.8, 1348.7, 1360.9, 1362.4, 1366.8, 1378.3, 1404.9, 1413.6, 1416.6, 1418.6, 1428.2, 1430.9, 1433.3, 1439.3, 1444.5, 1447.4, 1451.4, 1455.1, 1457.8, 1465.9, 1482.7, 1488.6, 1527.3, 1588.9, 1610.0, 2977.4, 2989.8, 2991.2, 3001.3, 3001.7, 3005.9, 3006.4, 3010.2, 3043.4, 3044.1, 3057.1, 3074.4, 3076.4, 3078.0, 3078.8, 3079.2, 3089.7, 3092.0, 3100.6, 3110.0, 3151.5, 3178.6, 3218.1, 3532.2, 3731.3
3-4 (ortho)	TS	396.1i, 51.5, 55.5, 66.4, 77.1, 92.6, 99.6, 103.8, 114.2, 127.2, 138.4, 156.2, 162.6, 169.7, 182.2, 204.3, 209.6, 220.4, 224.8, 232.8, 236.4, 261.8, 286.6, 291.8, 302.4, 309.9, 337.6, 340.3, 347.2, 355.7, 376.9, 393.2, 401.0, 405.5, 416.4, 444.9, 458.9, 470.6, 514.0, 557.8, 561.3, 581.4, 583.0, 609.2, 622.3, 628.0, 671.6, 677.7, 718.3, 736.0, 770.6, 771.2, 797.7, 892.1, 906.4, 920.3, 939.4, 953.4, 962.7, 973.3, 987.7, 998.0, 1003.4, 1007.1, 1012.2, 1021.5, 1023.4, 1026.6, 1060.7, 1073.3, 1085.7, 1086.9, 1098.9, 1114.6, 1147.2, 1229.4, 1263.5, 1305.7, 1313.4, 1336.5, 1344.9, 1353.8, 1355.2, 1358.4, 1364.9, 1366.3, 1377.1, 1392.9, 1415.2, 1417.4, 1426.4, 1429.0, 1432.9, 1435.8, 1440.1, 1448.1, 1455.3, 1461.4, 1466.4, 1469.2, 1555.8, 1563.8, 1599.6, 1641.6, 2922.0, 2955.5, 2974.9, 2982.1, 2989.0, 2991.2, 2991.9, 3022.0, 3034.9, 3046.5, 3055.8, 3057.7, 3058.7, 3069.7, 3070.2, 3098.0, 3107.2, 3127.3, 3147.9, 3153.6, 3161.1, 3191.7, 3238.9, 3289.3, 3663.4
3-4 (meta)	TS	429.8i, 43.5, 52.2, 57.1, 63.8, 84.1, 87.4, 91.7, 97.2, 103.6, 113.1, 126.8, 136.1, 153.9, 179.3, 187.1, 209.7, 219.5, 235.7, 242.8, 245.7, 254.8, 268.3, 277.5, 294.6, 296.9, 322.2, 325.1, 330.9, 342.5, 346.9, 379.3, 385.8, 391.7, 434.9, 451.5, 457.8, 517.5, 544.1, 545.5, 553.5, 576.7, 591.7, 595.4, 614.1, 633.0, 661.3, 678.7, 680.8, 681.8, 735.9, 770.8, 808.8, 857.3, 907.0, 923.0, 930.9, 946.3, 957.6, 968.7, 969.7, 977.9, 987.8, 994.6, 995.6, 1018.7, 1052.7, 1059.9, 1064.8, 1077.7, 1085.1, 1094.4, 1134.2, 1175.3, 1197.0, 1222.0, 1249.2, 1308.8, 1331.3, 1332.3, 1341.9, 1350.6, 1352.2, 1358.2, 1364.4, 1368.1, 1380.3, 1387.4, 1402.6, 1412.9, 1415.3, 1419.5, 1422.7, 1428.6, 1433.1, 1436.7, 1443.3, 1449.6, 1452.6, 1459.9, 1468.2, 1537.7, 1563.5, 1612.0, 2320.2, 2943.5, 2953.8, 2957.1, 2978.6, 2979.2, 2984.3, 2998.9, 2999.1, 3004.9, 3027.1, 3053.5, 3071.8, 3082.8, 3091.1, 3092.4, 3117.0, 3147.0, 3156.0, 3172.3, 3174.6, 3194.6, 3230.3, 3273.8, 3647.0
4-E1	IS	17.3, 53.8, 64.3, 76.2, 86.8, 90.0, 100.2, 122.4, 140.4, 182.0, 190.3, 200.7, 223.6, 225.1, 237.5, 239.5, 242.9, 255.3, 263.6, 267.2, 289.0, 302.4, 310.5, 347.4, 360.0, 363.1, 376.5, 385.4, 400.3, 427.5, 439.3, 466.5, 467.3, 539.5, 554.2, 560.6, 562.0, 579.3, 582.9, 615.5, 632.7, 655.1, 688.7, 737.1, 770.8, 776.4, 822.6, 835.7, 922.4, 930.9, 939.4, 951.0, 957.3, 964.3, 994.0, 996.6, 1004.8, 1019.9, 1021.3, 1035.8, 1063.0, 1072.5, 1090.9, 1092.0, 1097.0, 1107.5, 1216.7, 1218.6, 1247.3, 1269.2, 1318.2, 1325.9, 1338.5, 1345.8, 1349.2, 1357.4, 1358.5, 1370.2, 1375.2, 1391.3, 1399.8, 1410.3, 1419.1, 1420.7, 1423.2, 1424.8, 1433.1, 1433.6, 1438.0, 1448.3, 1454.5, 1455.5, 1462.9, 1480.4, 1481.4, 1515.8, 1588.6, 2954.7, 2966.8, 2978.9, 2991.1, 2991.9, 2996.7, 3003.9, 3013.9, 3020.3, 3025.0, 3045.5, 3050.5, 3052.0, 3066.6, 3073.7, 3075.1, 3089.3, 3101.0, 3103.1, 3211.8, 3215.3, 3231.3, 3234.0
	TS	455.7i, 46.2, 56.7, 64.6, 77.2, 92.2, 101.5, 103.5, 126.7, 152.9, 172.2, 177.8, 194.5, 211.6, 218.6, 232.2, 242.0, 252.3, 253.2, 258.0, 258.5, 300.7, 315.1, 316.7, 350.5, 363.3, 368.6, 384.4, 394.1, 428.7, 442.1, 455.0, 459.3, 473.3, 510.0, 539.7, 560.4, 563.8, 581.0, 593.3, 598.3, 635.3, 658.0, 688.9, 724.7, 765.8, 794.8, 818.1, 884.7, 914.4, 934.4, 960.5, 971.0, 981.3, 992.4, 1005.2, 1010.0, 1023.2, 1029.8, 1032.0, 1060.5, 1070.1, 1078.5, 1089.7, 1095.0, 1107.6, 1231.0, 1237.9, 1246.2, 1288.8, 1294.7, 1343.8, 1352.1, 1356.5, 1357.8, 1359.3, 1364.7, 1368.0, 1376.3, 1385.5, 1389.9, 1412.0, 1416.1, 1417.1, 1422.0, 1426.3, 1435.0, 1437.1, 1442.4, 1446.2, 1449.9, 1452.6, 1462.8, 1464.6, 1480.6, 1547.0, 1582.2, 2976.0, 2981.4,

		2984.2, 2984.6, 2990.4, 2995.7, 2998.0, 3016.3, 3024.6, 3034.7, 3038.0, 3042.8, 3059.6, 3061.3, 3064.1, 3091.5, 3097.4, 3109.4, 3155.8, 3195.2, 3202.7, 3232.0, 3236.2
	FS	30.3, 54.4, 61.9, 77.8, 84.1, 95.2, 95.9, 106.4, 134.6, 141.4, 152.6, 165.3, 177.0, 186.4, 203.5, 216.7, 236.1, 239.9, 252.4, 260.7, 276.6, 306.0, 309.3, 334.4, 351.6, 361.9, 364.2, 378.8, 410.3, 430.2, 447.3, 453.3, 476.7, 545.2, 549.7, 558.8, 565.0, 575.7, 599.6, 634.4, 636.5, 657.0, 694.8, 707.5, 754.7, 787.7, 807.8, 898.4, 910.1, 937.6, 954.1, 960.9, 962.3, 971.1, 985.5, 996.2, 1012.0, 1020.5, 1036.7, 1041.9, 1062.2, 1078.3, 1088.8, 1091.2, 1096.7, 1117.1, 1190.0, 1236.4, 1256.4, 1297.6, 1321.1, 1326.9, 1336.1, 1337.3, 1340.5, 1350.2, 1364.1, 1371.9, 1374.8, 1398.3, 1399.5, 1409.7, 1416.2, 1422.3, 1430.6, 1432.8, 1435.1, 1442.5, 1444.0, 1448.2, 1450.8, 1454.8, 1466.7, 1473.7, 1487.0, 1524.7, 1601.7, 2964.5, 2976.3, 2978.2, 2981.3, 2992.0, 2999.3, 3010.0, 3018.1, 3024.2, 3029.0, 3030.1, 3032.6, 3044.5, 3050.5, 3074.4, 3088.4, 3088.7, 3106.2, 3146.3, 3148.7, 3161.5, 3243.8, 3249.6
E1-E2	IS	43.9, 59.8, 68.3, 77.2, 89.7, 95.6, 98.4, 108.2, 137.9, 139.1, 151.4, 163.9, 177.7, 192.2, 206.9, 219.1, 235.7, 235.9, 253.2, 259.5, 277.2, 306.7, 308.8, 335.4, 351.7, 361.5, 369.9, 381.4, 410.9, 429.1, 447.0, 453.1, 476.6, 544.0, 544.7, 561.9, 564.3, 575.1, 599.1, 632.9, 634.6, 658.5, 697.6, 706.9, 754.5, 787.9, 807.3, 897.4, 910.4, 939.3, 954.5, 961.2, 962.7, 972.0, 985.6, 997.0, 1012.4, 1020.5, 1036.9, 1042.4, 1063.0, 1078.8, 1088.9, 1093.4, 1096.8, 1117.6, 1190.1, 1237.5, 1256.8, 1298.1, 1320.7, 1326.5, 1335.3, 1337.2, 1340.7, 1350.6, 1364.6, 1373.3, 1374.9, 1398.6, 1399.8, 1409.0, 1416.0, 1423.0, 1431.2, 1432.8, 1434.6, 1442.3, 1443.0, 1447.6, 1451.7, 1455.3, 1467.1, 1473.5, 1487.3, 1524.3, 1601.7, 2961.8, 2976.3, 2977.0, 2981.7, 2991.3, 2998.4, 3010.8, 3019.1, 3022.3, 3028.9, 3029.1, 3031.8, 3043.9, 3051.1, 3073.6, 3088.1, 3089.4, 3107.4, 3146.4, 3149.7, 3161.5, 3244.3, 3253.3
	TS	431.8i, 56.6, 68.3, 76.0, 84.6, 85.6, 96.4, 99.1, 111.3, 136.2, 145.3, 166.0, 171.6, 206.5, 222.9, 235.5, 244.5, 256.2, 264.4, 265.8, 286.6, 305.6, 307.2, 345.8, 356.7, 358.9, 365.5, 375.7, 403.1, 430.7, 438.7, 453.6, 466.8, 472.6, 512.8, 537.2, 559.6, 560.5, 563.0, 598.7, 635.4, 636.4, 657.7, 697.5, 716.1, 760.2, 788.0, 815.3, 897.1, 914.3, 933.7, 958.3, 972.2, 980.3, 999.3, 1006.4, 1010.4, 1020.1, 1025.7, 1037.8, 1057.6, 1075.3, 1082.0, 1090.2, 1091.1, 1107.3, 1232.2, 1246.8, 1249.1, 1288.9, 1304.0, 1336.7, 1348.2, 1352.6, 1356.9, 1361.5, 1365.0, 1367.2, 1371.3, 1391.7, 1394.8, 1409.7, 1416.2, 1422.1, 1423.9, 1427.6, 1431.4, 1437.9, 1439.5, 1447.6, 1450.7, 1452.6, 1456.8, 1466.7, 1480.3, 1532.1, 1586.9, 2956.7, 2984.0, 2987.5, 2995.6, 3000.4, 3003.2, 3004.8, 3008.7, 3034.1, 3035.8, 3045.2, 3045.8, 3056.5, 3057.5, 3063.8, 3095.3, 3099.9, 3102.4, 3164.1, 3181.8, 3207.9, 3235.0, 3255.0
	FS	55.4, 62.1, 68.5, 76.9, 90.7, 103.7, 117.0, 124.8, 139.7, 153.0, 166.8, 173.7, 184.6, 212.2, 225.6, 236.4, 247.0, 254.3, 260.7, 271.5, 290.4, 298.9, 310.8, 348.4, 357.2, 361.2, 366.6, 389.1, 406.3, 425.3, 438.2, 460.5, 472.7, 544.3, 547.7, 561.0, 567.8, 573.1, 603.7, 638.9, 643.0, 661.2, 700.0, 736.6, 766.1, 790.1, 814.4, 844.2, 925.2, 949.5, 956.0, 961.3, 972.6, 983.5, 991.8, 1002.8, 1011.5, 1020.5, 1026.5, 1050.2, 1062.2, 1084.8, 1085.4, 1090.2, 1091.7, 1119.9, 1216.4, 1242.6, 1251.6, 1275.6, 1324.4, 1332.5, 1335.8, 1338.5, 1351.0, 1361.0, 1366.0, 1368.7, 1377.0, 1390.2, 1403.6, 1407.5, 1412.6, 1420.9, 1425.9, 1435.4, 1438.4, 1438.7, 1441.3, 1455.0, 1458.2, 1461.1, 1465.5, 1482.3, 1491.9, 1522.5, 1602.0, 2968.2, 2970.8, 2973.6, 2997.0, 2998.0, 3006.7, 3009.8, 3016.0, 3018.9, 3024.7, 3042.8, 3051.7, 3061.6, 3073.2, 3096.5, 3098.5, 3102.1, 3103.1, 3125.3, 3162.3, 3183.9, 3223.9, 3257.8
E2-E3	IS	47.5, 55.6, 68.3, 75.0, 91.1, 103.4, 121.4, 124.2, 141.9, 157.1, 169.5, 177.2, 184.1, 214.7, 225.4, 236.2, 248.0, 255.4, 263.7, 271.6, 289.0, 298.1, 311.4, 346.9, 357.7, 360.5, 368.0, 390.6, 406.2, 422.6, 439.4, 458.4, 472.1, 543.8, 547.1, 565.2, 567.3, 572.5, 602.0, 638.7, 642.0, 658.7, 700.5, 734.0, 765.8, 790.4, 813.6, 842.5, 925.6, 950.7, 956.3, 962.8, 972.9, 984.6, 992.0, 1003.0, 1011.9, 1020.0, 1026.1, 1049.9, 1062.4, 1085.4, 1086.0, 1089.9, 1092.2, 1119.8, 1215.8, 1242.4, 1251.0, 1275.2, 1323.9, 1332.4, 1337.3, 1339.1, 1351.6, 1361.3, 1366.3, 1368.4, 1376.7, 1389.9, 1403.6, 1407.2, 1412.9, 1421.7, 1426.1, 1436.0, 1438.4, 1439.6, 1441.6, 1455.4, 1457.5, 1460.7, 1465.7, 1482.0, 1491.2, 1523.3, 1602.4, 2969.8, 2971.3, 2974.5, 2995.7, 2998.6, 3006.6, 3010.7, 3017.3, 3020.4, 3025.6, 3042.5, 3050.9, 3060.6, 3074.4, 3096.9, 3097.0, 3102.6, 3104.0, 3126.9, 3161.8, 3179.2, 3228.8, 3258.9
	TS	405.2i, 49.3, 58.0, 68.9, 76.0, 80.9, 99.3, 107.2, 119.1, 141.4, 161.1, 167.4, 176.0, 180.3, 198.4, 220.4, 236.6, 247.8, 259.1, 262.9, 271.7, 304.9, 307.5, 340.6, 346.8, 362.8, 365.3, 385.1, 406.3, 423.0, 439.4, 456.4, 476.3, 488.9, 512.9, 537.0, 560.7, 566.9, 575.5, 593.3, 628.5, 638.0, 656.0, 679.8, 694.8, 768.9, 793.3, 826.1, 923.7, 928.2, 949.8, 970.6, 975.8, 978.9, 992.7, 1000.8, 1017.5, 1026.5, 1038.8, 1044.8, 1064.4, 1078.9, 1084.9, 1088.3, 1094.0, 1110.4, 1233.0, 1246.7, 1257.0, 1294.4, 1302.2, 1343.3, 1353.2, 1357.0, 1358.5, 1363.7, 1368.8, 1373.6, 1379.1, 1389.4, 1399.6, 1410.1, 1413.2, 1414.4, 1421.8, 1428.4, 1432.6, 1440.3, 1444.8, 1447.3, 1449.2, 1454.4, 1457.4, 1464.8, 1489.2, 1553.6, 1596.3, 2968.0, 2979.6, 2981.2, 2981.8, 2984.1, 3010.4, 3020.4, 3029.4, 3030.8, 3031.8, 3032.3, 3039.4, 3041.0, 3061.6, 3102.5, 3103.2, 3107.2, 3108.6, 3149.9, 3163.8, 3183.9, 3212.4, 3251.0
	FS	30.7i, 59.1, 62.4, 70.1, 77.7, 84.7, 96.5, 105.1, 116.4, 123.3, 140.5, 146.8, 168.9, 190.9, 206.5, 212.5, 227.8, 238.0, 258.4, 263.6, 294.5, 311.0, 319.8, 350.0, 360.1, 360.7, 371.0, 382.3, 405.8, 410.5, 426.4, 448.6, 458.7, 541.1, 552.2, 554.7, 561.3, 568.2, 596.0, 602.2, 639.6, 659.0, 680.0, 682.0, 747.9, 768.7, 817.4, 845.0, 940.6, 946.0, 960.4, 971.6, 973.6, 977.3, 989.7, 1003.1,

1017.0, 1019.2, 1028.7, 1038.1, 1065.3, 1073.8, 1084.4, 1092.3, 1103.0, 1106.4, 1169.7, 1232.3, 1257.9, 1293.0, 1327.7, 1334.4, 1343.0, 1347.3, 1349.7, 1361.3, 1363.1, 1371.5, 1374.6, 1395.9, 1398.5, 1408.0, 1413.9, 1415.5, 1422.2, 1437.8, 1440.2, 1440.8, 1443.4, 1447.4, 1453.2, 1456.9, 1460.5, 1466.7, 1479.3, 1529.0, 1587.1, 2958.7, 2984.2, 2985.5, 2989.2, 2994.1, 2999.0, 3007.4, 3010.1, 3015.5, 3034.8, 3035.6, 3037.0, 3061.6, 3070.4, 3076.4, 3088.4, 3092.7, 3093.2, 3104.4, 3118.1, 3120.3, 3199.1, 3215.2

E3-1' **IS** 47.7, 50.0, 53.6, 68.2, 85.7, 91.0, 105.7, 121.3, 134.1, 153.1, 164.3, 176.5, 189.3, 201.8, 203.0, 214.2, 229.7, 230.9, 250.0, 255.1, 294.3, 298.8, 321.2, 332.9, 354.4, 360.7, 367.9, 375.0, 391.7, 408.2, 423.9, 438.5, 460.8, 538.3, 547.1, 554.6, 560.4, 573.1, 591.6, 595.0, 642.5, 661.5, 674.1, 678.5, 746.5, 766.7, 815.8, 830.0, 944.9, 949.7, 952.8, 975.2, 978.6, 984.8, 992.6, 1006.8, 1013.4, 1022.2, 1040.0, 1041.0, 1070.4, 1078.1, 1082.2, 1088.3, 1103.1, 1104.8, 1179.4, 1232.9, 1258.8, 1297.2, 1335.0, 1336.1, 1346.8, 1351.6, 1358.1, 1358.7, 1361.5, 1369.9, 1373.3, 1385.9, 1397.2, 1402.7, 1416.6, 1421.4, 1425.7, 1431.6, 1437.9, 1442.8, 1446.5, 1448.2, 1452.2, 1459.7, 1462.3, 1465.7, 1481.8, 1527.9, 1589.7, 2945.4, 2979.6, 2987.0, 2987.3, 2991.4, 2993.9, 2997.3, 3004.8, 3029.8, 3031.7, 3034.0, 3041.8, 3061.8, 3062.7, 3068.0, 3075.9, 3081.5, 3087.9, 3096.3, 3123.1, 3149.1, 3176.9, 3182.0

TS 1055.1i, 23.6, 56.7, 68.7, 69.5, 79.9, 93.1, 98.1, 107.0, 118.5, 127.4, 146.6, 168.1, 170.8, 187.0, 201.5, 205.6, 210.1, 216.7, 232.9, 244.4, 288.0, 299.6, 328.5, 330.2, 347.1, 358.4, 367.6, 378.3, 419.1, 438.3, 449.6, 465.8, 483.7, 495.3, 556.9, 569.2, 571.5, 573.6, 579.6, 580.7, 603.1, 651.4, 674.6, 699.9, 714.0, 779.9, 808.2, 814.7, 865.1, 925.8, 949.0, 956.3, 968.6, 973.1, 982.9, 990.3, 1005.6, 1019.9, 1025.7, 1034.8, 1037.5, 1052.0, 1073.7, 1075.6, 1080.9, 1100.8, 1179.1, 1184.5, 1255.4, 1278.3, 1297.0, 1318.5, 1344.6, 1352.6, 1354.9, 1359.4, 1364.0, 1369.1, 1378.6, 1397.9, 1402.9, 1411.8, 1417.7, 1418.9, 1422.0, 1430.4, 1432.9, 1445.0, 1448.7, 1455.9, 1459.4, 1462.5, 1465.6, 1477.4, 1538.3, 1571.5, 1579.6, 2947.0, 2954.5, 2976.0, 2979.4, 2990.2, 2990.5, 3002.0, 3024.5, 3028.3, 3037.5, 3041.8, 3045.1, 3050.0, 3069.9, 3080.1, 3097.9, 3120.4, 3134.9, 3164.4, 3180.1, 3188.9, 3196.9

FS 35.4, 62.8, 63.8, 68.6, 77.0, 89.3, 99.1, 106.7, 113.3, 129.7, 140.9, 155.3, 159.6, 170.6, 174.6, 181.1, 189.4, 194.0, 196.3, 215.5, 230.9, 256.6, 273.5, 305.3, 330.3, 345.8, 352.8, 354.7, 374.1, 376.4, 413.5, 435.4, 456.5, 465.8, 554.0, 565.5, 572.5, 574.4, 575.3, 590.6, 604.3, 605.7, 668.4, 699.6, 719.0, 722.5, 808.0, 811.6, 816.3, 827.1, 952.5, 970.1, 978.6, 983.2, 989.4, 994.3, 1001.7, 1005.0, 1019.5, 1032.5, 1035.1, 1051.2, 1054.4, 1073.8, 1074.0, 1081.2, 1102.2, 1202.4, 1224.8, 1253.2, 1328.1, 1337.1, 1338.2, 1351.2, 1352.0, 1357.5, 1358.4, 1361.8, 1368.7, 1405.8, 1407.2, 1414.8, 1416.7, 1417.6, 1428.4, 1431.4, 1436.2, 1445.4, 1454.6, 1456.8, 1463.5, 1468.3, 1468.5, 1471.3, 1580.3, 1598.3, 1611.4, 2832.9, 2938.6, 2945.6, 2970.8, 2975.5, 2983.0, 2983.2, 3019.7, 3022.3, 3025.0, 3026.3, 3038.7, 3039.2, 3052.5, 3061.4, 3061.8, 3086.2, 3136.9, 3138.6, 3162.5, 3178.7, 3179.5, 3192.8

4-P1 **IS** 41.8, 52.2, 56.5, 79.3, 91.0, 94.4, 107.3, 132.9, 152.6, 171.6, 198.2, 199.7, 217.3, 234.3, 241.9, 252.2, 262.0, 264.7, 280.8, 285.2, 291.9, 297.6, 319.2, 338.7, 355.5, 361.3, 376.6, 382.7, 397.7, 426.3, 437.6, 455.5, 474.9, 541.2, 561.0, 563.1, 566.1, 571.6, 589.5, 630.7, 637.5, 658.1, 683.6, 738.2, 769.3, 781.4, 826.2, 843.5, 925.8, 934.5, 945.4, 962.0, 966.5, 971.0, 995.6, 1002.9, 1008.4, 1020.0, 1034.2, 1037.4, 1068.7, 1077.7, 1089.4, 1093.4, 1098.2, 1105.7, 1216.0, 1219.5, 1251.1, 1274.5, 1318.0, 1330.9, 1341.8, 1349.2, 1351.8, 1359.0, 1368.6, 1369.3, 1375.9, 1397.6, 1403.6, 1411.2, 1419.7, 1422.7, 1425.0, 1430.5, 1431.8, 1436.1, 1445.8, 1447.4, 1456.7, 1460.4, 1468.6, 1477.8, 1485.9, 1518.5, 1592.6, 2965.2, 2969.9, 2981.6, 2989.5, 2995.9, 3000.2, 3004.6, 3006.9, 3010.1, 3033.2, 3044.4, 3055.0, 3064.6, 3069.5, 3074.5, 3081.8, 3084.3, 3103.2, 3103.8, 3184.0, 3197.2, 3202.1, 3212.1

TS 872.2i, 68.1, 82.1, 84.4, 87.8, 102.5, 109.0, 114.6, 148.2, 154.2, 172.3, 195.4, 216.8, 234.1, 257.6, 269.7, 284.0, 287.7, 289.6, 294.8, 323.2, 325.1, 327.8, 332.8, 348.6, 358.4, 364.9, 377.1, 403.8, 422.0, 437.8, 452.6, 481.5, 519.2, 555.9, 564.5, 574.2, 588.1, 604.2, 611.9, 623.9, 666.2, 673.0, 706.2, 739.8, 777.8, 803.4, 837.6, 899.5, 909.2, 930.6, 934.9, 949.6, 973.9, 978.5, 989.0, 1004.5, 1015.7, 1020.6, 1026.8, 1046.6, 1066.4, 1074.2, 1077.7, 1094.9, 1107.3, 1122.9, 1148.4, 1212.5, 1245.6, 1266.3, 1304.2, 1339.4, 1340.3, 1346.1, 1353.8, 1358.2, 1360.7, 1368.3, 1372.3, 1404.4, 1411.8, 1416.6, 1421.8, 1425.6, 1431.0, 1432.8, 1439.2, 1442.4, 1443.5, 1450.5, 1454.7, 1467.2, 1472.5, 1476.5, 1505.3, 1566.4, 1637.9, 2971.1, 2973.2, 2973.5, 2973.8, 2982.1, 2984.8, 3009.4, 3016.4, 3024.1, 3037.4, 3049.4, 3054.0, 3077.0, 3079.0, 3080.3, 3082.2, 3099.2, 3130.1, 3159.4, 3171.0, 3181.8, 3191.2

FS 48.4, 65.7, 76.7, 82.2, 87.6, 93.6, 103.0, 137.5, 153.1, 162.1, 185.2, 199.5, 225.1, 232.2, 248.6, 254.6, 263.1, 265.4, 277.3, 288.1, 290.9, 311.8, 321.3, 323.4, 332.4, 338.5, 357.4, 361.1, 367.6, 372.4, 415.7, 432.2, 448.3, 471.9, 512.7, 538.0, 550.8, 576.4, 598.0, 608.7, 622.6, 631.5, 695.6, 703.5, 720.0, 773.7, 783.2, 787.3, 797.7, 906.2, 922.7, 928.7, 949.4, 978.5, 980.4, 996.5, 1002.9, 1013.4, 1019.3, 1025.7, 1039.1, 1043.1, 1068.8, 1084.9, 1099.2, 1106.9, 1119.0, 1160.2, 1212.0, 1240.5, 1267.4, 1304.9, 1336.4, 1344.0, 1348.1, 1354.1, 1357.7, 1361.9, 1368.8, 1397.3, 1414.4, 1420.3, 1425.3, 1428.3, 1430.9, 1433.8, 1439.9, 1443.6, 1448.2, 1450.8, 1456.5, 1460.4, 1466.7, 1472.1, 1620.4, 1627.7, 1674.3, 2957.5, 2959.5, 2966.3, 2969.1, 2975.2, 2975.9, 2978.9, 3005.2, 3019.2, 3021.1, 3025.2, 3046.5, 3056.5, 3064.4, 3066.9, 3077.0, 3095.3, 3102.2, 3153.3, 3176.2, 3177.9, 3194.2, 3681.1

P1-P2	IS	56.0, 67.0, 69.9, 77.2, 85.4, 95.8, 98.6, 103.8, 112.9, 126.8, 134.4, 154.9, 165.5, 172.9, 174.3, 178.1, 189.3, 209.1, 230.0, 245.2, 247.9, 250.8, 271.6, 276.7, 285.0, 291.9, 322.5, 338.5, 340.3, 352.0, 369.7, 377.0, 386.2, 405.4, 413.9, 420.7, 445.4, 445.9, 482.5, 556.0, 564.9, 571.0, 580.5, 596.7, 599.0, 637.0, 640.9, 698.2, 698.6, 711.2, 732.7, 772.5, 780.1, 807.7, 846.4, 907.1, 914.0, 932.8, 952.7, 963.7, 973.9, 991.3, 1000.3, 1005.7, 1014.0, 1018.3, 1031.6, 1034.6, 1067.7, 1078.9, 1083.4, 1093.5, 1104.6, 1107.5, 1124.9, 1143.4, 1167.6, 1206.8, 1232.9, 1260.6, 1283.9, 1323.5, 1335.2, 1347.7, 1350.8, 1356.3, 1359.9, 1363.6, 1366.1, 1370.0, 1413.6, 1416.7, 1420.1, 1427.0, 1427.8, 1429.4, 1432.1, 1438.1, 1440.4, 1446.4, 1449.9, 1453.8, 1455.9, 1459.2, 1461.9, 1466.2, 1470.4, 1476.8, 1593.4, 1617.7, 1642.0, 1661.7, 2935.4, 2966.7, 2974.7, 2977.5, 2985.7, 2990.3, 2998.5, 3013.6, 3014.1, 3020.7, 3034.1, 3049.3, 3050.5, 3058.5, 3060.1, 3073.9, 3074.7, 3085.0, 3105.7, 3121.4, 3125.1, 3138.9, 3161.4, 3225.9, 3265.3, 3384.9
	TS	421.6i, 60.9, 67.2, 82.3, 84.6, 88.2, 90.6, 100.2, 113.4, 115.9, 131.7, 149.4, 163.7, 171.0, 184.1, 188.5, 196.2, 223.4, 228.0, 238.1, 245.4, 259.4, 269.4, 280.6, 285.6, 295.6, 325.5, 332.2, 337.5, 360.0, 367.7, 373.9, 385.5, 386.1, 401.1, 408.5, 417.1, 421.6, 445.4, 488.2, 494.4, 556.4, 563.8, 572.8, 580.5, 587.9, 603.2, 617.1, 643.0, 669.5, 680.0, 712.7, 780.6, 783.1, 812.0, 827.8, 911.1, 922.9, 938.4, 958.0, 970.0, 976.3, 986.5, 999.0, 1002.3, 1003.3, 1014.6, 1018.5, 1029.2, 1036.3, 1044.1, 1051.6, 1073.2, 1085.4, 1093.8, 1099.2, 1110.4, 1122.2, 1171.8, 1209.2, 1269.6, 1293.8, 1327.0, 1339.6, 1339.8, 1347.9, 1351.9, 1354.3, 1357.7, 1363.4, 1368.7, 1373.4, 1415.3, 1419.9, 1422.9, 1425.9, 1428.7, 1431.1, 1439.8, 1444.0, 1451.8, 1455.2, 1458.1, 1466.4, 1468.3, 1471.2, 1478.7, 1543.9, 1598.3, 1599.9, 1649.2, 2806.0, 2972.9, 2980.2, 2983.2, 2985.0, 2989.5, 2992.5, 3009.3, 3021.4, 3039.3, 3040.8, 3053.3, 3064.2, 3065.0, 3069.4, 3071.0, 3077.8, 3078.4, 3089.4, 3103.4, 3123.3, 3128.2, 3221.6, 3238.2, 3257.0, 3261.7, 3650.9
	FS	45.1, 52.9, 56.0, 70.6, 75.9, 79.1, 83.8, 87.5, 100.5, 103.6, 107.0, 123.5, 142.3, 165.1, 178.1, 186.8, 195.6, 203.4, 214.6, 222.9, 237.8, 240.6, 249.4, 258.7, 273.9, 278.4, 281.4, 287.1, 300.6, 322.2, 327.3, 347.5, 348.5, 357.0, 363.4, 365.6, 377.6, 402.1, 428.4, 458.3, 481.7, 495.0, 544.9, 553.8, 564.9, 573.1, 592.6, 616.5, 636.6, 644.8, 660.8, 666.6, 748.3, 768.4, 815.2, 875.5, 903.7, 927.4, 934.4, 939.5, 953.1, 961.3, 965.9, 982.7, 1000.6, 1002.8, 1017.7, 1019.5, 1034.3, 1048.5, 1070.1, 1072.4, 1089.5, 1091.0, 1097.1, 1121.6, 1166.3, 1199.4, 1252.8, 1291.3, 1315.7, 1333.3, 1343.0, 1344.5, 1348.2, 1348.7, 1350.7, 1364.4, 1366.5, 1370.0, 1382.6, 1405.5, 1411.9, 1419.7, 1422.4, 1427.8, 1429.9, 1434.7, 1437.4, 1440.6, 1447.0, 1448.6, 1450.7, 1457.5, 1461.7, 1462.8, 1465.4, 1491.8, 1527.8, 1596.5, 1598.8, 2982.1, 2987.3, 2987.7, 2993.1, 2993.4, 3001.5, 3006.9, 3008.8, 3013.8, 3037.4, 3065.2, 3065.6, 3069.1, 3070.4, 3077.3, 3080.3, 3081.9, 3086.5, 3099.5, 3100.5, 3104.3, 3109.5, 3133.5, 3176.5, 3203.3, 3586.5, 3764.7
P2-P3	IS	56.9, 69.5, 79.4, 79.5, 86.4, 93.4, 108.7, 110.3, 132.2, 139.9, 172.1, 186.5, 195.5, 201.7, 214.0, 225.7, 241.1, 243.0, 251.6, 257.7, 266.8, 277.4, 282.4, 288.1, 301.5, 326.7, 345.9, 348.5, 356.9, 358.1, 362.6, 380.1, 402.2, 427.7, 458.2, 494.3, 540.6, 552.6, 553.0, 573.7, 591.7, 615.6, 630.3, 643.3, 660.5, 667.7, 749.0, 766.7, 815.1, 872.3, 903.5, 924.2, 934.8, 938.7, 952.5, 957.0, 965.6, 981.8, 1000.6, 1002.4, 1017.1, 1019.5, 1034.3, 1048.7, 1072.1, 1086.2, 1090.7, 1096.2, 1114.2, 1120.1, 1164.6, 1199.5, 1251.8, 1290.0, 1314.6, 1332.7, 1342.3, 1342.7, 1346.8, 1348.0, 1349.9, 1364.1, 1365.6, 1369.3, 1381.0, 1405.4, 1411.7, 1419.5, 1422.3, 1428.2, 1433.2, 1435.5, 1437.5, 1440.4, 1446.8, 1449.2, 1451.0, 1458.3, 1461.6, 1462.8, 1465.5, 1490.7, 1527.1, 1595.9, 2981.7, 2988.9, 2990.0, 2991.8, 2995.1, 2996.4, 3005.5, 3008.8, 3015.0, 3034.3, 3064.3, 3068.1, 3069.7, 3070.7, 3071.5, 3080.5, 3081.6, 3089.0, 3098.0, 3102.1, 3103.0, 3104.3, 3131.1, 3177.3, 3198.6
	TS	471.2i, 48.2, 59.3, 70.6, 71.7, 83.8, 95.2, 102.9, 116.8, 129.1, 155.9, 175.2, 182.5, 184.8, 192.9, 206.9, 219.1, 229.2, 233.3, 244.0, 257.2, 262.7, 268.5, 286.0, 294.1, 302.5, 317.7, 349.0, 357.4, 361.4, 381.1, 392.4, 422.2, 433.1, 435.4, 471.1, 481.4, 534.1, 538.0, 557.4, 558.9, 590.9, 610.2, 625.6, 633.4, 659.3, 669.9, 727.3, 778.8, 811.9, 875.6, 895.7, 909.2, 919.8, 949.1, 959.1, 973.4, 988.3, 997.2, 1003.1, 1018.0, 1023.0, 1031.4, 1040.8, 1069.9, 1078.1, 1093.7, 1113.5, 1116.1, 1123.0, 1169.3, 1236.3, 1250.9, 1299.1, 1303.8, 1334.1, 1344.1, 1352.1, 1357.2, 1361.0, 1364.8, 1367.6, 1370.9, 1375.9, 1382.1, 1385.0, 1394.3, 1410.8, 1416.6, 1418.8, 1429.0, 1433.7, 1434.7, 1436.1, 1444.3, 1448.4, 1451.5, 1453.4, 1457.9, 1459.8, 1465.0, 1471.3, 1559.7, 1591.7, 2963.3, 2982.2, 2984.1, 2988.7, 2990.8, 2993.1, 2995.0, 2996.4, 3017.7, 3041.9, 3062.6, 3064.4, 3067.8, 3069.9, 3071.2, 3074.9, 3084.5, 3092.1, 3098.3, 3123.2, 3134.3, 3149.9, 3155.7, 3166.0, 3215.7
	FS	40.7, 53.8, 68.7, 71.8, 86.5, 89.7, 94.7, 104.3, 116.4, 134.8, 136.9, 148.0, 175.6, 185.3, 197.7, 206.3, 216.3, 236.8, 238.8, 246.8, 258.7, 273.9, 294.2, 302.5, 310.0, 312.0, 334.8, 349.4, 361.4, 362.1, 371.8, 391.4, 405.1, 433.3, 453.6, 503.1, 548.4, 551.7, 561.0, 567.7, 594.2, 611.5, 635.0, 645.6, 655.8, 680.2, 715.9, 758.3, 795.4, 863.7, 890.6, 904.8, 916.0, 935.9, 945.4, 957.1, 966.8, 972.4, 988.9, 994.2, 1005.5, 1019.5, 1032.4, 1045.5, 1076.9, 1078.7, 1087.9, 1093.6, 1097.5, 1119.0, 1160.5, 1205.9, 1256.1, 1287.7, 1318.4, 1321.7, 1334.1, 1337.9, 1341.7, 1345.9, 1350.5, 1356.6, 1369.4, 1374.2, 1375.3, 1403.7, 1405.8, 1413.4, 1420.6, 1423.6, 1427.4, 1433.0, 1435.8, 1438.9, 1444.2, 1450.0, 1451.8, 1455.3, 1456.6, 1461.2, 1466.1, 1488.4,

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	TS	436.9i, 62.0, 70.8, 71.8, 87.6, 97.6, 102.9, 112.8, 121.2, 149.2, 158.9, 173.0, 189.4, 193.0, 207.3, 212.3, 222.7, 255.7, 259.7, 260.4, 269.2, 279.2, 288.3, 301.4, 303.3, 317.3, 359.4, 362.6, 365.2, 373.4, 395.4, 406.3, 433.6, 442.8, 451.8, 461.0, 499.6, 509.6, 555.9, 558.4, 561.9, 598.3, 624.6, 630.8, 633.7, 659.4, 690.7, 710.9, 777.4, 821.6, 882.1, 899.7, 917.6, 920.9, 950.8, 964.1, 981.5, 987.3, 1000.8, 1015.5, 1027.4, 1030.3, 1040.8, 1057.9, 1077.3, 1081.5, 1088.9, 1107.4, 1111.9, 1121.2, 1169.7, 1245.4, 1256.5, 1286.1, 1307.2, 1333.2, 1348.8, 1351.0, 1353.8, 1358.9, 1363.6, 1370.1, 1371.8, 1373.4, 1380.2, 1398.3, 1405.1, 1412.6, 1419.2, 1423.4, 1426.9, 1429.4, 1434.1, 1439.3, 1442.1, 1446.5, 1449.0, 1456.4, 1461.9, 1462.7, 1471.7, 1477.9, 1550.2, 1608.5, 2964.2, 2980.6, 2987.6, 2997.5, 2998.3, 3003.1, 3012.7, 3017.1, 3026.2, 3039.8, 3045.4, 3049.0, 3058.4, 3070.8, 3078.8, 3082.1, 3084.0, 3095.2, 3108.3, 3112.4, 3144.5, 3157.4, 3171.1, 3172.4, 3257.0
	FS	44.7, 60.5, 70.4, 76.6, 91.9, 100.4, 111.2, 116.5, 133.4, 170.1, 172.1, 174.7, 177.5, 196.6, 204.6, 224.4, 228.7, 256.9, 259.3, 262.1, 274.5, 288.3, 293.5, 305.5, 307.4, 323.8, 344.6, 360.5, 372.3, 381.6, 388.2, 409.8, 432.4, 436.6, 457.5, 491.7, 544.8, 557.1, 564.4, 566.0, 607.8, 622.0, 630.9, 645.3, 657.0, 694.5, 735.7, 779.2, 809.5, 849.8, 875.8, 920.0, 936.7, 948.7, 957.7, 961.6, 976.4, 986.8, 997.1, 1016.7, 1036.9, 1043.3, 1054.6, 1063.5, 1079.9, 1089.3, 1092.2, 1098.6, 1103.5, 1118.3, 1164.5, 1237.3, 1255.4, 1273.8, 1309.5, 1323.4, 1334.1, 1338.3, 1344.3, 1348.6, 1365.5, 1371.5, 1374.1, 1378.4, 1380.7, 1389.9, 1401.5, 1418.7, 1420.1, 1425.8, 1430.3, 1436.4, 1438.5, 1442.3, 1444.1, 1447.8, 1460.1, 1464.2, 1467.8, 1475.1, 1481.3, 1493.5, 1539.2, 1620.7, 2961.1, 2963.0, 2992.4, 2995.8, 2997.0, 3004.0, 3014.8, 3017.7, 3025.5, 3028.3, 3050.3, 3063.4, 3071.7, 3077.6, 3083.2, 3085.2, 3085.8, 3099.5, 3105.7, 3110.6, 3121.7, 3126.5, 3149.2, 3180.9, 3225.2
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	TS	420.3i, 49.2, 53.0, 66.4, 78.4, 82.7, 90.1, 96.1, 103.8, 119.1, 133.6, 150.1, 162.3, 185.1, 197.9, 210.3, 221.9, 229.8, 244.3, 259.1, 259.7, 281.4, 291.4, 303.3, 321.9, 333.2, 341.1, 360.8, 363.5, 386.6, 400.6, 408.1, 434.3, 440.2, 452.4, 483.9, 492.2, 514.4, 540.1, 559.5, 561.4, 605.4, 620.1, 629.6, 637.2, 662.0, 675.2, 680.6, 785.8, 828.4, 882.6, 902.3, 915.0, 924.6, 959.1, 972.8, 979.9, 987.2, 994.8, 1016.1, 1019.1, 1034.2, 1042.6, 1061.1, 1074.3, 1089.5, 1094.0, 1105.4, 1114.5, 1136.0, 1178.1, 1243.9, 1257.9, 1271.0, 1305.5, 1334.5, 1347.5, 1353.6, 1358.5, 1360.7, 1361.7, 1372.5, 1376.1, 1381.3, 1384.8, 1390.3, 1398.0, 1411.1, 1413.5, 1417.2, 1423.4, 1429.5, 1431.0, 1437.2, 1440.7, 1448.5, 1449.1, 1456.0, 1459.5, 1468.4, 1476.6, 1484.3, 1562.9, 1605.8, 2982.6, 2985.6, 2990.5, 2991.0, 2991.4, 2997.9, 3009.5, 3011.4, 3040.2, 3040.3, 3042.4, 3055.1, 3059.4, 3063.3, 3073.3, 3081.7, 3086.9, 3098.3, 3108.1, 3134.0, 3138.9, 3152.3, 3182.0, 3193.5, 3211.3
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P5-1'	IS	49.9, 58.8, 70.2, 78.4, 94.4, 98.6, 105.6, 109.3, 126.6, 140.9, 165.7, 178.8, 186.6, 207.1, 214.8, 228.9, 240.2, 254.4, 258.5, 266.0, 286.5, 300.1, 321.7, 324.3, 343.7, 359.1, 363.9, 369.4, 373.8, 384.1, 420.4, 429.6, 436.6, 441.8, 451.9, 470.4, 538.1, 545.6, 549.5, 562.8, 563.9, 587.1, 594.5, 618.0, 638.7, 657.0, 676.4, 707.1, 794.6, 805.1, 903.4, 911.1, 939.0, 951.0, 954.2, 958.2, 970.8, 981.5, 992.2, 1018.6, 1019.8, 1023.2, 1040.3, 1054.8, 1068.8, 1074.1, 1081.3, 1096.2, 1101.7, 1129.0, 1151.7, 1206.9, 1251.8, 1286.7, 1299.6, 1322.9, 1339.2, 1340.5, 1347.0, 1358.2, 1358.5, 1363.1, 1365.4, 1369.9, 1377.0, 1388.1, 1397.6, 1405.9, 1412.3, 1419.4, 1425.2, 1427.5, 1431.0, 1435.6, 1443.6, 1449.1, 1454.5, 1454.9, 1462.9, 1467.9, 1471.6, 1481.8, 1521.2, 1588.6, 2950.0, 2962.1, 2967.7, 2973.1, 2982.5, 2988.6, 2988.9, 3004.8, 3006.3, 3015.1, 3030.3, 3035.9, 3049.7, 3054.9, 3067.3, 3081.2, 3083.6, 3085.4, 3097.0, 3097.8, 3105.0, 3134.6, 3204.0, 3219.0, 3239.1
	TS	266.1i, 43.6, 62.7, 64.2, 74.8, 96.3, 103.7, 109.2, 113.8, 123.4, 129.9, 141.7, 146.7, 150.5, 180.5, 190.2, 199.1, 205.0, 215.9, 225.4, 231.6, 249.2, 271.9, 299.5, 314.3, 328.1, 343.6, 354.5, 358.5, 365.5, 376.7, 414.8, 436.7, 445.5, 452.7, 466.1, 544.4, 566.4, 568.8, 572.1, 573.1, 577.6, 582.8, 603.2, 628.8, 661.4, 697.0, 718.6, 808.0, 814.9, 819.2, 839.0, 897.8, 932.8, 951.8, 960.9, 969.0, 977.1, 983.1, 991.7, 1003.8, 1018.4, 1029.2, 1033.4, 1043.2, 1052.4, 1073.7, 1074.4, 1082.0, 1106.2, 1111.5, 1192.6, 1233.9, 1255.8, 1290.2, 1324.2, 1327.7, 1344.5, 1352.3, 1354.8, 1358.3, 1360.2, 1363.4, 1365.8, 1373.8, 1391.4, 1402.5, 1407.3, 1414.0, 1418.5, 1426.5, 1433.8, 1435.6, 1440.4, 1446.3, 1451.1, 1454.1, 1460.0, 1462.7, 1467.7, 1473.4, 1474.8, 1571.6, 1592.1, 1608.7, 2948.2, 2956.1, 2958.3, 2979.7, 2980.6, 2982.2, 2991.5, 3013.5, 3022.8, 3028.5, 3032.5, 3035.6, 3039.5, 3048.2, 3064.2, 3065.2, 3069.6, 3077.7, 3109.9, 3117.8, 3140.1, 3146.8, 3191.8, 3199.7
	FS	50.6, 59.4, 62.3, 81.7, 90.7, 96.6, 106.7, 115.0, 117.3, 123.5, 138.9, 143.0, 160.2, 172.3, 185.5, 193.5, 196.1, 209.4, 219.9, 232.7, 238.1, 271.7, 277.0, 295.2, 314.3, 329.1, 352.1, 356.7, 363.7, 381.5, 385.9, 417.7, 441.3, 444.2, 453.2, 465.6, 539.2, 563.7, 570.7, 572.9, 576.0, 597.4, 602.3, 604.0, 658.5, 686.9, 714.4, 720.3, 761.5, 805.8, 816.6, 832.6, 928.6, 938.5, 952.2, 967.4, 977.4, 978.8, 983.7, 992.4, 1003.6, 1017.9, 1031.2, 1031.6, 1034.4, 1049.7, 1050.6, 1074.1, 1074.4, 1079.6, 1103.9, 1175.9, 1252.9, 1260.1, 1291.1, 1329.7, 1338.2, 1349.2, 1352.0, 1356.2, 1358.4, 1359.7, 1360.7, 1367.3, 1399.5, 1406.0, 1409.5, 1415.7, 1417.9, 1421.5, 1428.0, 1434.0, 1440.1, 1443.3, 1448.1, 1453.9, 1462.1, 1464.3, 1468.8, 1473.5, 1476.8, 1580.2, 1599.4, 1655.7, 2647.7, 2936.3, 2947.4, 2969.9, 2977.6, 2981.3, 2986.1, 2996.0, 3017.1, 3022.8, 3030.7, 3032.6, 3037.6, 3039.6, 3064.3, 3069.9, 3073.4, 3077.4, 3083.5, 3101.5, 3132.8, 3150.2, 3180.0, 3184.6, 3196.7

PMB and TMBs mediated methylations

prehnitene		
1		19.5, 42.4, 45.3, 54.8, 58.6, 64.8, 76.9, 107.9, 136.3, 150.7, 182.6, 215.3, 242.2, 259.3, 288.4, 309.7, 312.5, 316.9, 331.7, 357.1, 362.8, 466.8, 484.2, 500.5, 512.3, 517.6, 546.0, 598.4, 626.7, 648.7, 704.5, 715.9, 725.5, 727.8, 781.6, 789.4, 850.9, 914.4, 921.0, 971.2, 982.8, 995.3, 1008.4, 1026.0, 1028.4, 1037.3, 1060.3, 1063.5, 1165.8, 1203.9, 1247.7, 1259.4, 1329.0, 1353.7, 1354.1, 1360.7, 1364.9, 1394.1, 1417.8, 1423.9, 1425.0, 1438.0, 1441.0, 1441.9, 1455.1, 1458.7, 1480.2, 1581.8, 1599.1, 2946.7, 2951.0, 2953.8, 2969.4, 2993.4, 3004.4, 3005.5, 3030.1, 3046.1, 3054.2, 3069.9, 3095.3, 3110.3, 3123.9, 3697.8
3-4	TS	432.0i, 17.6, 29.7, 43.5, 52.6, 60.3, 68.9, 83.6, 107.7, 120.6, 132.1, 142.5, 158.3, 197.4, 211.1, 235.2, 253.7, 258.0, 259.1, 275.2, 279.6, 284.3, 298.6, 324.3, 336.9, 347.0, 357.8, 376.9, 410.6, 473.9, 478.2, 491.2, 497.7, 502.2, 566.1, 572.6, 580.3, 615.6, 621.3, 663.9, 679.8, 692.3, 724.5, 748.9, 762.6, 812.1, 822.7, 876.2, 891.4, 921.9, 926.0, 955.2, 961.9, 972.4, 974.9, 986.0, 997.7, 1002.1, 1004.2, 1019.7, 1046.8, 1078.0, 1085.7, 1090.5, 1102.3, 1164.3, 1174.5, 1183.8, 1302.2, 1317.0, 1334.5, 1338.8, 1349.5, 1350.1, 1361.3, 1370.6, 1390.3, 1414.7, 1418.6, 1427.5, 1429.5, 1434.1, 1446.7, 1449.9, 1450.4, 1467.1, 1530.1, 1582.1, 1603.8, 1657.6, 2852.6, 2959.1, 2974.6, 2975.7, 2982.1, 3012.6, 3046.0, 3054.5, 3054.8, 3057.0, 3060.2, 3060.9, 3072.0, 3087.5, 3093.0, 3111.4, 3134.8, 3178.2, 3242.4, 3266.0, 3649.7
isodurene		
1		38.1, 46.8, 49.3, 72.4, 84.8, 94.2, 108.9, 125.1, 143.9, 160.6, 180.3, 193.3, 226.1, 237.8, 267.4, 287.6, 292.6, 303.6, 315.7, 335.1, 358.2, 449.0, 494.9, 509.5, 512.6, 541.5, 544.7, 577.5, 594.9, 626.0, 698.7, 705.1, 719.5, 735.9, 779.2, 825.4, 860.1, 893.4, 960.0, 972.1, 987.5, 998.4, 1008.5, 1015.8, 1020.8, 1031.7, 1038.1, 1063.6, 1138.7, 1204.7, 1238.1, 1297.9, 1334.4, 1353.0, 1357.4, 1360.2, 1364.2, 1396.7, 1412.9, 1418.1, 1427.3, 1435.7, 1441.4, 1442.4, 1445.1, 1460.9, 1480.1, 1578.8, 1614.2, 2942.9, 2947.3, 2970.3, 2991.5, 2999.9, 3001.7, 3036.4, 3038.3, 3053.2, 3060.1, 3061.4, 3093.5, 3104.4, 3147.1, 3697.8
3-4	TS	437.2i, 38.0, 48.0, 60.1, 70.2, 79.0, 85.9, 100.4, 113.7, 128.1, 159.1, 163.2, 199.4, 201.7, 216.9, 232.3, 253.1, 257.4, 263.8, 270.7, 281.8, 295.5, 300.7, 316.9, 327.6, 345.6, 355.5, 379.4, 417.5, 460.3, 500.0, 509.5, 513.2, 553.2, 567.7, 576.1, 584.3, 589.6, 622.3, 666.4, 673.8, 684.5, 701.7,

		754.1, 771.5, 826.4, 853.0, 865.6, 882.6, 914.3, 933.0, 952.0, 963.0, 978.1, 987.9, 996.1, 1000.8, 1010.5, 1015.4, 1028.3, 1036.0, 1055.1, 1094.0, 1099.1, 1106.4, 1161.9, 1178.7, 1223.5, 1300.2, 1333.9, 1338.7, 1341.2, 1350.3, 1358.2, 1364.2, 1368.7, 1394.7, 1401.2, 1419.1, 1425.8, 1427.9, 1432.3, 1440.6, 1448.4, 1461.4, 1462.6, 1536.9, 1594.8, 1609.3, 1660.9, 2806.9, 2976.8, 2983.8, 2985.7, 3000.6, 3033.2, 3054.6, 3055.1, 3064.5, 3065.0, 3072.6, 3073.1, 3077.2, 3099.1, 3110.2, 3115.2, 3150.5, 3156.8, 3241.7, 3265.7, 3641.3
durene		
1		21.7, 42.8, 44.9, 52.0, 60.9, 70.6, 121.1, 140.0, 144.1, 148.5, 165.7, 186.7, 240.6, 262.3, 272.9, 288.4, 290.4, 293.6, 308.7, 337.4, 356.8, 429.5, 443.5, 507.7, 516.2, 517.6, 581.4, 601.7, 630.8, 666.1, 704.8, 709.0, 728.2, 740.3, 780.8, 805.9, 859.2, 868.1, 967.0, 975.5, 988.8, 1001.9, 1010.6, 1017.4, 1030.2, 1034.5, 1035.2, 1070.6, 1186.5, 1193.1, 1265.3, 1276.2, 1332.2, 1351.4, 1353.6, 1364.3, 1365.9, 1380.3, 1421.2, 1421.9, 1428.2, 1435.4, 1437.4, 1438.7, 1445.0, 1456.0, 1496.7, 1561.0, 1619.4, 2947.6, 2950.4, 2951.6, 2952.1, 2995.9, 2999.7, 3002.9, 3005.2, 3043.7, 3045.4, 3047.2, 3049.5, 3108.7, 3113.3, 3697.9
1-2	TS	361.2i, 42.1, 65.9, 69.7, 72.9, 80.6, 87.5, 116.7, 131.5, 133.7, 136.5, 158.5, 171.2, 183.4, 189.2, 206.5, 220.2, 248.0, 266.5, 274.3, 284.8, 301.0, 307.7, 324.0, 335.5, 363.6, 394.0, 430.5, 435.4, 504.1, 511.0, 520.4, 559.2, 571.6, 576.6, 636.1, 659.7, 665.9, 687.6, 690.2, 705.4, 729.6, 805.6, 864.0, 869.0, 882.4, 928.3, 959.3, 972.0, 979.9, 995.4, 1002.7, 1011.5, 1013.4, 1015.6, 1028.5, 1033.9, 1075.7, 1100.1, 1192.5, 1195.3, 1261.4, 1275.5, 1333.8, 1343.2, 1353.6, 1356.2, 1363.6, 1364.6, 1369.6, 1374.8, 1417.2, 1418.1, 1422.8, 1429.2, 1436.7, 1441.4, 1447.8, 1452.6, 1487.6, 1523.6, 1611.0, 1611.9, 2958.3, 2959.0, 2964.8, 2966.4, 3008.3, 3013.0, 3020.8, 3032.4, 3042.0, 3060.8, 3061.0, 3064.8, 3070.1, 3108.2, 3126.2, 3177.8, 3232.5, 3250.4, 3583.6
2		29.4, 50.6, 55.1, 57.2, 65.1, 70.1, 84.8, 117.7, 143.7, 153.7, 173.3, 191.6, 219.4, 266.9, 267.1, 277.1, 282.4, 296.8, 313.5, 316.4, 332.9, 337.0, 365.1, 429.9, 444.9, 502.7, 524.1, 551.1, 557.2, 571.2, 639.0, 655.1, 657.6, 658.0, 685.7, 694.7, 782.9, 843.9, 873.7, 905.9, 939.1, 940.1, 973.4, 984.1, 988.0, 1001.1, 1012.6, 1017.3, 1025.1, 1035.2, 1074.3, 1092.2, 1151.8, 1184.1, 1224.0, 1279.4, 1320.1, 1333.1, 1336.1, 1344.3, 1357.7, 1368.0, 1374.7, 1399.3, 1406.2, 1420.3, 1424.6, 1426.4, 1429.4, 1431.9, 1436.6, 1452.3, 1462.8, 1479.3, 1513.0, 1616.4, 2944.3, 2948.2, 2974.4, 2974.6, 2982.0, 3001.4, 3021.1, 3034.3, 3064.6, 3066.4, 3071.0, 3072.4, 3074.1, 3075.3, 3075.3, 3087.8, 3130.8
3-4	TS	432.4i, 28.7, 42.9, 47.0, 54.5, 65.5, 72.1, 80.4, 84.5, 100.6, 119.2, 140.3, 168.1, 193.2, 205.2, 218.0, 242.7, 260.4, 265.6, 278.2, 281.6, 292.3, 303.1, 316.1, 333.6, 341.9, 351.0, 362.9, 413.8, 426.9, 454.2, 498.6, 502.4, 529.1, 566.8, 579.2, 583.2, 624.2, 659.2, 667.1, 679.5, 683.6, 697.1, 749.1, 775.8, 784.0, 869.4, 872.6, 899.3, 911.3, 921.2, 924.6, 958.3, 970.6, 994.7, 997.8, 999.5, 1010.5, 1023.1, 1023.9, 1027.2, 1041.4, 1082.1, 1092.6, 1099.9, 1156.8, 1176.4, 1251.5, 1281.3, 1323.4, 1329.7, 1339.7, 1353.6, 1357.7, 1362.5, 1367.0, 1393.4, 1404.2, 1412.0, 1423.0, 1426.9, 1429.3, 1436.4, 1439.8, 1452.3, 1458.8, 1534.0, 1603.1, 1610.2, 1660.3, 2859.5, 2957.8, 2967.1, 2974.2, 2975.8, 3010.8, 3021.4, 3051.8, 3053.6, 3062.7, 3063.8, 3064.6, 3064.8, 3066.7, 3072.0, 3094.6, 3104.6, 3165.8, 3253.8, 3277.2, 3642.8
4	4	32.7, 39.4, 47.6, 60.3, 62.6, 68.0, 74.6, 95.8, 118.7, 138.5, 175.3, 182.2, 201.6, 213.4, 260.2, 263.2, 276.1, 283.1, 295.4, 306.7, 313.1, 327.8, 348.1, 362.4, 370.2, 428.9, 452.1, 498.2, 527.6, 547.0, 559.4, 596.6, 628.8, 656.0, 656.8, 686.4, 690.4, 728.3, 770.1, 812.7, 884.9, 887.9, 902.4, 934.2, 940.0, 941.7, 977.2, 991.0, 993.7, 1002.5, 1012.5, 1025.4, 1031.4, 1053.0, 1085.2, 1093.5, 1147.9, 1174.6, 1203.1, 1220.1, 1255.6, 1276.4, 1323.2, 1336.0, 1343.2, 1356.5, 1362.6, 1371.5, 1378.2, 1407.1, 1423.3, 1426.9, 1428.8, 1429.3, 1433.6, 1437.3, 1442.6, 1448.1, 1460.1, 1465.5, 1472.3, 1519.4, 1618.0, 2950.7, 2984.1, 2984.2, 2985.3, 2985.9, 2997.2, 3016.9, 3039.9, 3042.7, 3059.3, 3070.7, 3073.0, 3077.9, 3079.2, 3081.0, 3095.1, 3103.9, 3111.6, 3112.9
PMB		
1		36.3, 39.9, 57.6, 66.8, 78.6, 86.0, 89.0, 110.9, 123.2, 143.7, 164.5, 182.6, 211.4, 241.5, 289.5, 296.3, 305.8, 317.9, 342.0, 358.5, 372.0, 375.3, 409.0, 443.6, 486.3, 512.0, 520.3, 536.2, 547.3, 575.1, 582.0, 590.1, 625.2, 685.5, 700.6, 716.7, 720.5, 798.3, 809.7, 847.1, 900.7, 970.0, 976.7, 985.4, 993.8, 1003.7, 1014.3, 1026.2, 1029.1, 1062.6, 1070.0, 1081.6, 1125.7, 1217.0, 1225.8, 1300.7, 1328.7, 1337.5, 1353.6, 1356.1, 1360.7, 1368.6, 1393.4, 1414.4, 1419.1, 1422.8, 1433.7, 1437.8, 1441.1, 1448.8, 1463.3, 1467.7, 1476.4, 1483.2, 1577.0, 1606.0, 2904.6, 2947.1, 2952.6, 2957.5, 2969.5, 2995.1, 3001.4, 3016.4, 3019.5, 3028.5, 3047.1, 3047.9, 3064.6, 3081.4, 3128.0, 3155.3, 3343.0
1-2	TS	380.2i, 35.9, 47.9, 65.3, 67.3, 85.6, 91.8, 103.3, 113.5, 122.7, 128.5, 158.3, 160.9, 178.0, 180.3, 188.5, 199.6, 201.8, 231.4, 258.2, 274.1, 288.4, 311.9, 321.1, 336.2, 337.4, 362.9, 382.0, 388.6, 405.4, 441.0, 482.8, 511.1, 528.5, 542.7, 557.2, 564.3, 571.6, 587.6, 640.5, 655.4, 677.0, 686.4, 700.4, 721.7, 807.2, 857.5, 881.3, 896.6, 935.9, 966.0, 978.5, 981.6, 984.5, 999.7, 1006.1, 1010.3, 1014.3, 1021.0, 1028.0, 1071.7, 1075.2, 1088.6, 1107.3, 1218.2, 1220.8, 1302.0, 1330.8, 1336.3, 1352.9, 1353.8, 1358.4, 1361.7, 1366.1, 1368.0, 1376.0, 1406.1, 1417.0, 1419.9, 1421.9, 1435.2, 1437.0, 1444.3, 1450.1, 1459.1, 1468.0, 1477.4, 1537.4, 1599.4,

		1613.4, 2955.8, 2966.0, 2969.8, 2981.2, 2981.9, 3009.7, 3028.7, 3032.2, 3035.7, 3037.3, 3038.4, 3061.5, 3067.2, 3078.8, 3133.0, 3138.2, 3171.0, 3185.1, 3231.0, 3247.5, 3565.9
2		35.4, 47.3, 55.3, 59.7, 68.6, 73.5, 85.0, 107.3, 124.7, 160.5, 168.5, 183.1, 199.1, 215.4, 232.8, 261.8, 263.5, 278.6, 285.6, 301.4, 326.6, 343.5, 356.4, 362.3, 368.4, 406.8, 437.5, 484.9, 541.5, 547.9, 548.9, 555.9, 571.7, 587.6, 636.2, 658.7, 664.2, 673.5, 686.3, 784.4, 846.4, 857.7, 872.5, 937.4, 954.1, 971.1, 980.6, 990.4, 995.4, 1001.0, 1016.4, 1019.4, 1044.1, 1082.5, 1091.2, 1092.5, 1097.9, 1169.2, 1211.7, 1264.5, 1311.4, 1331.6, 1333.6, 1336.3, 1348.3, 1361.0, 1370.3, 1377.0, 1396.7, 1402.7, 1404.6, 1416.8, 1422.8, 1432.4, 1435.1, 1440.1, 1441.7, 1454.7, 1456.0, 1466.6, 1481.9, 1512.2, 1609.9, 2945.2, 2949.5, 2969.2, 2973.1, 2981.1, 2999.3, 3005.5, 3014.7, 3020.0, 3033.2, 3070.0, 3077.0, 3079.1, 3079.7, 3087.4, 3102.7, 3123.9, 3141.5, 3189.8
3-4	TS	28.4, 32.9, 60.2, 66.1, 71.2, 77.2, 84.7, 99.6, 105.2, 108.0, 112.5, 133.8, 176.1, 184.1, 195.3, 209.7, 222.1, 243.3, 244.7, 252.3, 266.7, 275.1, 292.2, 307.4, 329.4, 339.9, 359.6, 363.2, 388.4, 423.6, 427.5, 432.3, 481.2, 532.1, 553.1, 561.1, 579.7, 585.4, 590.8, 643.1, 652.6, 667.2, 698.1, 704.6, 711.8, 748.3, 766.2, 821.6, 842.4, 847.7, 853.8, 898.0, 923.1, 958.1, 960.7, 968.3, 985.1, 1001.4, 1013.1, 1017.5, 1027.5, 1065.1, 1078.9, 1093.4, 1104.3, 1107.0, 1116.8, 1157.8, 1180.7, 1190.3, 1220.0, 1257.1, 1310.6, 1335.8, 1350.9, 1359.5, 1364.1, 1366.1, 1371.8, 1384.5, 1397.3, 1418.1, 1420.1, 1424.6, 1426.6, 1427.5, 1435.6, 1436.6, 1440.2, 1443.4, 1452.0, 1456.2, 1464.7, 1473.7, 1585.7, 1616.3, 1627.7, 1676.0, 2953.5, 2965.0, 2969.3, 2977.2, 2978.5, 2999.0, 3006.9, 3017.7, 3031.3, 3038.1, 3052.9, 3054.3, 3070.8, 3074.6, 3087.4, 3087.6, 3102.8, 3131.8, 3133.1, 3173.6, 3181.4, 3403.5
4		431.6i, 40.3, 42.0, 55.8, 65.5, 70.3, 80.1, 98.3, 107.7, 117.7, 133.5, 138.2, 161.5, 173.9, 183.0, 190.3, 217.3, 235.6, 242.5, 249.8, 265.6, 279.4, 283.1, 297.7, 332.5, 340.5, 342.8, 363.1, 368.3, 373.4, 395.8, 413.7, 430.3, 484.8, 508.7, 540.4, 566.6, 567.0, 579.9, 581.5, 586.1, 621.3, 663.1, 664.2, 677.9, 695.1, 760.5, 770.3, 777.4, 850.6, 856.0, 881.4, 915.7, 929.0, 956.2, 964.1, 972.2, 981.9, 997.4, 999.8, 1001.5, 1015.3, 1017.6, 1026.1, 1055.0, 1078.8, 1083.8, 1097.2, 1103.7, 1119.6, 1178.8, 1198.3, 1265.0, 1321.5, 1338.7, 1340.5, 1350.7, 1353.9, 1356.8, 1362.3, 1370.1, 1389.4, 1401.4, 1414.5, 1423.3, 1424.1, 1427.2, 1434.2, 1439.1, 1449.0, 1454.6, 1457.1, 1469.2, 1528.1, 1590.1, 1608.5, 1656.3, 2812.2, 2954.8, 2984.6, 2992.1, 2997.0, 3002.6, 3008.7, 3054.9, 3056.0, 3066.4, 3071.2, 3073.9, 3074.2, 3079.0, 3093.7, 3099.0, 3107.4, 3112.4, 3145.0, 3166.8, 3242.6, 3266.9, 3643.4

stepwise methylation of 3-4

SMS formation	IS	37.8, 54.7, 69.5, 82.8, 85.6, 104.4, 107.4, 110.9, 117.4, 122.4, 128.3, 144.5, 151.3, 158.0, 168.8, 180.4, 188.3, 219.1, 232.5, 255.4, 266.3, 267.1, 271.1, 278.5, 311.1, 321.8, 343.5, 359.3, 363.4, 365.7, 385.6, 397.8, 406.5, 437.8, 455.6, 457.7, 547.4, 553.4, 560.1, 564.3, 572.2, 577.2, 610.6, 642.7, 655.5, 677.8, 682.8, 696.4, 727.1, 776.7, 784.1, 842.7, 881.8, 899.4, 909.8, 912.9, 949.2, 953.8, 965.8, 973.4, 993.1, 1005.6, 1016.1, 1030.1, 1052.3, 1063.9, 1073.8, 1076.9, 1083.9, 1090.6, 1099.4, 1130.6, 1136.5, 1195.6, 1259.6, 1292.7, 1308.4, 1337.6, 1348.8, 1350.3, 1357.4, 1362.0, 1373.2, 1389.0, 1394.3, 1397.9, 1416.7, 1423.9, 1429.2, 1431.6, 1432.4, 1437.7, 1438.2, 1439.2, 1443.1, 1447.9, 1454.8, 1461.2, 1465.9, 1477.3, 1572.7, 1590.5, 1606.0, 1647.1, 2663.7, 2828.6, 2973.2, 2976.7, 2979.8, 2991.9, 3008.0, 3019.4, 3021.9, 3024.4, 3025.5, 3056.0, 3061.0, 3066.7, 3067.6, 3073.7, 3083.9, 3110.8, 3121.6, 3136.4, 3150.1, 3194.0, 3204.4, 3207.9, 3208.4
	TS	391.0i, 40.9, 58.2, 65.3, 84.3, 85.0, 95.5, 98.9, 109.1, 136.0, 144.2, 149.9, 151.0, 156.2, 162.8, 189.7, 198.2, 217.5, 235.7, 241.1, 255.2, 267.8, 279.4, 288.6, 317.7, 321.6, 340.8, 353.8, 354.8, 358.3, 381.9, 388.8, 402.0, 405.5, 417.4, 436.7, 453.6, 456.8, 557.2, 565.0, 568.9, 570.3, 576.9, 579.7, 603.0, 612.7, 644.3, 669.8, 691.8, 700.1, 703.2, 756.4, 777.2, 784.4, 836.8, 904.6, 906.3, 913.1, 918.9, 948.3, 964.1, 973.0, 993.4, 1004.7, 1024.2, 1031.9, 1059.3, 1064.1, 1074.6, 1075.4, 1083.0, 1094.5, 1098.9, 1129.8, 1198.0, 1216.6, 1259.6, 1294.2, 1336.1, 1348.1, 1350.4, 1350.9, 1357.9, 1358.9, 1360.6, 1372.9, 1390.6, 1396.8, 1419.7, 1425.3, 1429.1, 1431.8, 1436.7, 1438.8, 1442.8, 1448.2, 1455.1, 1462.5, 1465.1, 1474.2, 1551.3, 1573.8, 1607.2, 1654.4, 2972.0, 2972.7, 2976.3, 2986.4, 2999.8, 3003.8, 3016.3, 3016.9, 3049.0, 3049.4, 3055.5, 3058.1, 3064.1, 3067.4, 3068.7, 3119.0, 3148.0, 3185.6, 3200.1, 3203.1, 3215.0, 3242.0, 3263.3, 3385.2, 3525.9
	FS	50.8, 58.8, 67.0, 74.1, 80.4, 91.9, 97.8, 98.7, 108.0, 114.3, 145.3, 150.3, 159.2, 167.8, 172.7, 184.6, 189.7, 222.8, 235.0, 247.4, 261.3, 269.7, 270.2, 278.8, 287.9, 299.1, 324.3, 339.6, 342.9, 347.7, 353.2, 370.3, 386.0, 395.9, 405.8, 439.5, 457.2, 458.5, 529.3, 553.7, 565.6, 566.7, 578.8, 583.3, 600.6, 607.8, 612.5, 687.3, 709.5, 712.6, 729.6, 746.9, 777.2, 783.6, 816.3, 901.0, 901.2, 909.7, 914.9, 946.5, 963.9, 974.6, 994.5, 1004.6, 1025.4, 1028.6, 1064.4, 1075.0, 1082.1, 1093.8, 1099.4, 1116.6, 1129.0, 1169.4, 1198.7, 1259.6, 1298.3, 1335.9, 1347.4, 1350.8, 1357.1, 1360.3, 1371.6, 1386.8, 1400.9, 1406.1, 1419.3, 1425.5, 1428.4, 1429.2, 1432.4, 1437.1, 1437.4, 1442.0, 1444.1, 1450.0, 1454.1, 1462.1, 1464.5, 1475.0, 1559.6, 1585.5, 1613.0, 1655.8, 2966.5, 2976.2, 2976.9, 2982.1, 2995.7, 3001.6, 3007.2, 3012.0, 3021.4, 3049.4, 3050.7, 3057.1, 3060.9, 3063.4, 3071.1, 3107.5, 3114.1, 3140.3, 3166.9, 3177.5, 3196.6, 3205.1, 3225.0, 3463.0, 3740.5

methylation	IS	56.0, 60.0, 65.9, 80.9, 89.7, 94.4, 105.4, 112.3, 141.9, 163.5, 179.1, 200.7, 212.4, 244.6, 246.1, 252.1, 268.1, 268.3, 287.1, 293.7, 309.7, 322.7, 334.6, 341.4, 352.3, 358.4, 372.0, 378.6, 402.1, 427.4, 442.8, 457.1, 468.5, 520.8, 551.4, 554.7, 566.8, 577.5, 594.4, 608.8, 610.6, 697.4, 699.6, 708.4, 727.4, 742.1, 770.3, 786.7, 827.5, 894.5, 911.7, 916.0, 925.1, 954.4, 967.6, 974.8, 991.6, 1004.8, 1025.3, 1026.4, 1070.3, 1076.1, 1080.1, 1094.5, 1101.8, 1121.0, 1136.7, 1163.6, 1205.3, 1262.1, 1288.4, 1332.3, 1341.6, 1354.8, 1356.2, 1365.2, 1368.9, 1389.9, 1400.1, 1419.6, 1424.3, 1426.0, 1429.7, 1431.1, 1434.5, 1435.1, 1437.8, 1440.6, 1445.3, 1448.3, 1451.7, 1458.1, 1465.3, 1471.4, 1567.6, 1615.7, 1659.8, 2963.3, 2969.5, 2971.9, 2972.7, 2980.2, 2982.0, 2987.4, 3010.9, 3014.6, 3019.8, 3028.6, 3038.3, 3058.4, 3064.3, 3072.9, 3090.7, 3116.4, 3116.9, 3179.9, 3192.8, 3197.0, 3221.0, 3225.8
	TS	463.4i, 55.2, 65.3, 85.2, 92.5, 99.9, 104.9, 127.2, 140.6, 153.1, 186.6, 192.5, 209.0, 219.9, 248.5, 261.8, 272.9, 274.1, 286.1, 298.7, 310.5, 315.1, 326.2, 340.6, 350.1, 354.8, 374.8, 379.3, 384.2, 398.3, 428.2, 441.5, 463.5, 465.8, 554.7, 560.9, 577.6, 578.2, 582.2, 584.8, 591.4, 612.9, 660.8, 706.2, 717.4, 750.2, 777.1, 790.5, 880.1, 888.3, 895.7, 916.6, 922.9, 953.9, 956.8, 970.5, 976.4, 989.7, 997.4, 1004.2, 1024.3, 1029.2, 1070.7, 1073.3, 1078.6, 1093.2, 1101.7, 1112.9, 1136.4, 1207.3, 1266.8, 1293.8, 1337.0, 1338.1, 1347.4, 1357.9, 1360.0, 1366.1, 1367.3, 1369.8, 1383.4, 1413.4, 1415.0, 1422.0, 1426.8, 1428.7, 1434.2, 1434.5, 1443.6, 1446.3, 1447.3, 1454.6, 1466.1, 1470.1, 1527.4, 1591.2, 1643.0, 2974.1, 2974.7, 2974.9, 2977.9, 2981.6, 2982.9, 3019.4, 3023.4, 3024.4, 3031.6, 3047.4, 3056.2, 3066.8, 3068.8, 3083.8, 3117.6, 3185.7, 3189.7, 3197.9, 3211.7, 3231.6, 3234.5, 3268.0
	FS	55.8, 61.4, 63.2, 78.8, 93.1, 99.3, 109.5, 126.3, 144.0, 160.1, 189.8, 203.7, 216.1, 218.2, 248.4, 251.8, 261.9, 272.4, 278.8, 300.5, 301.5, 313.3, 328.7, 349.0, 362.9, 364.1, 383.0, 394.3, 399.0, 425.5, 436.2, 464.7, 467.4, 542.3, 553.5, 562.7, 567.9, 587.8, 594.8, 609.4, 636.1, 658.5, 681.5, 741.2, 772.7, 784.5, 825.2, 851.9, 926.1, 934.3, 940.8, 952.0, 957.9, 965.7, 991.8, 998.9, 1008.8, 1018.1, 1029.2, 1039.9, 1070.3, 1077.1, 1089.4, 1096.0, 1097.3, 1112.8, 1206.8, 1213.6, 1242.9, 1268.3, 1323.8, 1329.1, 1338.0, 1352.0, 1355.7, 1359.2, 1364.5, 1369.9, 1375.6, 1399.3, 1406.0, 1414.8, 1422.8, 1426.0, 1427.3, 1431.1, 1431.9, 1437.6, 1440.0, 1447.0, 1453.3, 1458.9, 1466.7, 1485.0, 1490.8, 1525.0, 1595.8, 2974.0, 2978.0, 2982.2, 2989.7, 2991.1, 2991.7, 2998.4, 3020.5, 3035.6, 3036.8, 3041.1, 3047.6, 3060.3, 3070.5, 3077.5, 3082.9, 3083.5, 3103.9, 3139.3, 3173.4, 3206.2, 3217.8, 3240.7

S 9 DATA OF THE STUDIED STRUCTURES

All the studied structures in CIF and XYZ format are available in the attached ZIP file.

S 10 ADDITIONAL REFERENCES

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3.   Fečík, M.; Plessow, P. N.; Studt, F., A Systematic Study of Methylation from Benzene to Hexamethylbenzene in H-SSZ-13 Using Density Functional Theory and Ab Initio Calculations. *ACS Catal.* **2020,** *10* (15), 8916-8925.
4.   Plessow, P. N.; Studt, F., Unraveling the Mechanism of the Initiation Reaction of the Methanol to Olefins Process Using ab Initio and DFT Calculations. *ACS Catal.* **2017,** *7* (11), 7987-7994.
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6.   Wang, C.-M.; Wang, Y.-D.; Du, Y.-J.; Yang, G.; Xie, Z.-K., Computational insights into the reaction mechanism of methanol-to-olefins conversion in H-ZSM-5: nature of hydrocarbon pool. *Catal. Sci. Technol.* **2016,** *6* (9), 3279-3288.