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A quantum mechanical study of dehydration vs. decarbonylation of formamide catalysed by amorphous silica surfaces

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(Article begins on next page)

18 April 2024

Formamide decomposition catalyzed by amorphous silica. A quantum mechanical study of dehydration *vs* decarbonylation processes

Electronic Supplementary Information

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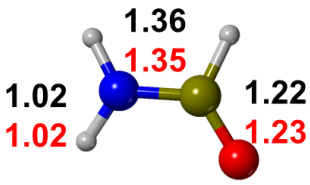
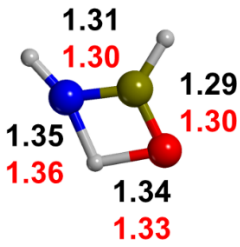
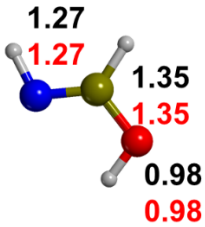
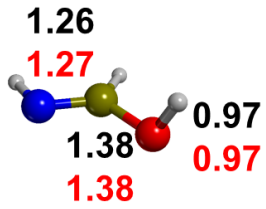
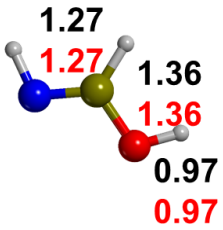
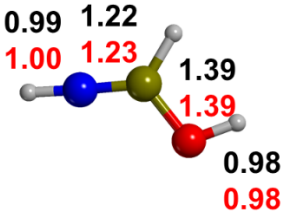
In this document we provide the following supplementary information:

1) Structures and cartesian coordinates of all the optimized steps of the reactions considered in the present work (Figures S1-S10),
2) Energetic values of all the reactions considered in the present work, also including different starting points as reference state (Table S1-S4),
3) Basis sets

Formamide dehydration reaction

Structures (**Gas phase**, **PCM (F)**)	**Gas phase** coordinates	**PCM (F)** coordinates
	6 F_M1_G C -0.161405 0.388237 0.000001 H -0.123992 1.504500 -0.000002 O -1.204573 -0.245520 0.000003 N 1.088652 -0.160090 -0.000022 H 1.918652 0.422350 0.000077 H 1.189792 -1.171476 0.000044	6 F_M1_F C -0.150179 0.387795 0.000000 H -0.116027 1.499664 -0.000002 O -1.210206 -0.242679 -0.000008 N 1.083922 -0.162187 -0.000004 H 1.913120 0.423472 0.000059 H 1.198176 -1.173168 0.000039
	6 F_TS1_G C -0.033977 0.510798 0.000100 H -0.074321 1.607427 -0.000060 O -1.096575 -0.222848 -0.000043 N 1.018032 -0.266205 -0.000195 H 1.988728 0.048633 0.000538 H -0.064171 -1.074631 0.000629	6 F_TS1_F C -0.024627 0.513989 -0.000094 H -0.055961 1.609306 -0.000266 O -1.099825 -0.219221 -0.000031 N 1.014150 -0.272809 0.000086 H 1.985309 0.043233 0.000256 H -0.082035 -1.073045 0.000214
	6 F_M2_G C -0.092409 0.409577 -0.000091 H -0.057027 1.509587 0.000126 O 1.166226 -0.087766 0.000031 N -1.116374 -0.344129 -0.000019 H -1.978950 0.208499 0.000264 H 1.075237 -1.064518 0.000041	6 F_M2_F C -0.093679 0.405776 0.000327 H -0.072090 1.504501 -0.000471 O 1.168054 -0.083148 -0.000112 N -1.120479 -0.347703 0.000010 H -1.972785 0.222390 -0.000654 H 1.105874 -1.062444 -0.000008
	6 F_TS2_G C -0.110769 0.385386 0.007629 H -0.103780 1.491712 0.040243 O 1.148504 -0.160331 -0.115000 N -1.139376 -0.352181 0.003797 H -1.981032 0.238354 0.041171 H 1.537024 -0.294467 0.766232	6 F_TS2_F C -0.111660 0.388352 0.012317 H -0.116190 1.490211 0.063725 O 1.152342 -0.149170 -0.115600 N -1.137644 -0.355523 -0.003923 H -1.979523 0.233190 0.051681 H 1.510447 -0.371490 0.762958
	6 F_M3_G C 0.094555 0.367859 0.000010 H 0.015378 1.472128 -0.000185 O -1.109283 -0.273288 -0.000101 N 1.162005 -0.313982 0.000071 H 1.974042 0.310731 -0.000182 H -1.816525 0.394170 0.000618	6 F_M3_F C 0.091610 0.370546 0.000162 H 0.020611 1.470153 -0.000189 O -1.106606 -0.273340 0.000047 N 1.162349 -0.315971 -0.000106 H 1.968576 0.317081 -0.000508 H -1.822443 0.388013 0.000094
	6 F_TS3_G C 0.080322 0.390908 0.000011 H -0.113568 1.490013 0.000035 O -1.110919 -0.325436 0.000013 N 1.181783 -0.144002 -0.000027 H 2.092519 -0.541730 0.000076 H -1.846013 0.317766 -0.000094	6 F_TS3_F C 0.079496 0.395567 0.000005 H -0.118380 1.489017 0.000003 O -1.110285 -0.327211 -0.000042 N 1.184048 -0.141769 0.000048 H 2.088340 -0.561064 0.000029 H -1.852988 0.308724 -0.000063

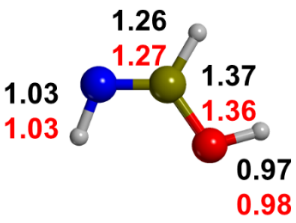
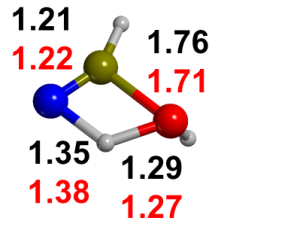
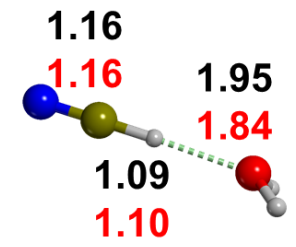
	6 F_M4_G C 0.092930 0.409586 0.000037 H -0.028965 1.502966 -0.000234 O -1.080550 -0.304510 0.000018 N 1.249873 -0.101121 0.000039 H 1.199968 -1.130607 -0.000318 H -1.833288 0.314048 -0.000092	6 F_M4_F C -0.086124 0.413308 0.000211 H 0.043249 1.503859 -0.000142 O 1.071991 -0.306788 -0.000033 N -1.249227 -0.100314 -0.000084 H -1.192087 -1.129950 -0.000074 H 1.834250 0.302749 -0.000197
	6 F_TS4_G C 0.458145 0.561574 0.007153 H 0.377148 1.647228 -0.031064 O -1.161276 -0.123848 -0.109099 N 1.138795 -0.440024 0.023133 H -0.133635 -0.903005 -0.023343 H -1.673734 -0.042712 0.722353	6 F_TS4_F C 0.423852 0.556889 0.001392 H 0.335978 1.643909 -0.021305 O -1.138623 -0.134972 -0.109824 N 1.145201 -0.422131 0.024448 H -0.146350 -0.919184 -0.007466 H -1.640165 -0.031368 0.727880
	6 F_M5_G C 1.016091 0.000385 -0.019147 H -0.074741 0.000589 -0.051094 O -2.024233 0.000034 -0.060114 N 2.176135 -0.000254 0.023564 H -2.531358 0.771161 0.241273 H -2.529532 -0.772551 0.240668	6 F_M5_F C -0.965377 -0.000489 -0.006241 H 0.139781 -0.001009 -0.022964 O 1.974944 -0.000128 -0.093864 N -2.126285 0.000286 0.014986 H 2.370712 -0.767898 0.353998 H 2.366216 0.770872 0.352415

Figure S1: PBE-D2/TZVP optimized geometries for the non-catalysed (intramolecular) formamide dehydration reaction. In the first column the optimized structures with the most representative bond lengths (in Å) in gas phase (black), and in PCM (F) (red) are shown. In the second and third columns the cartesian coordinates of the optimized structures in gas phase, and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue.

Formamide decarbonylation reaction

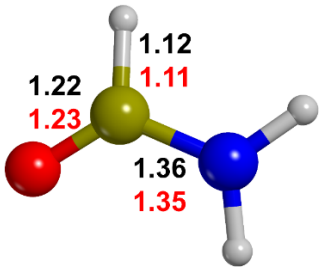
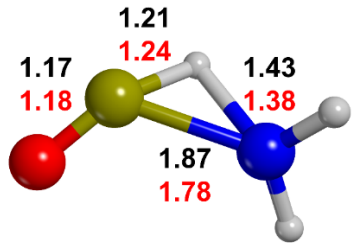
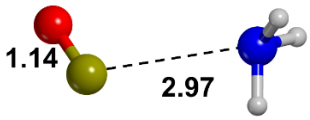
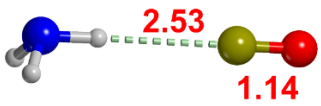
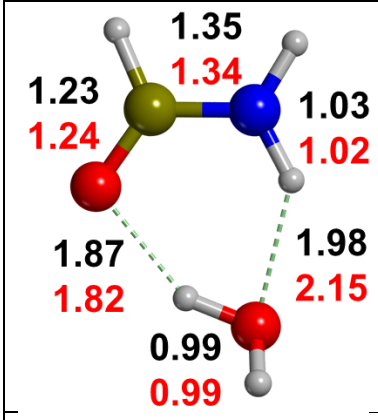
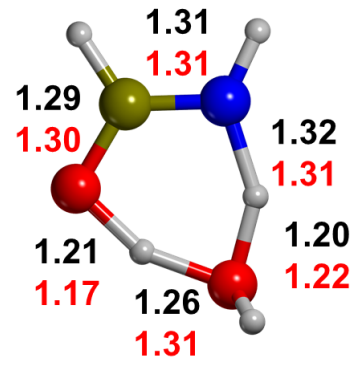
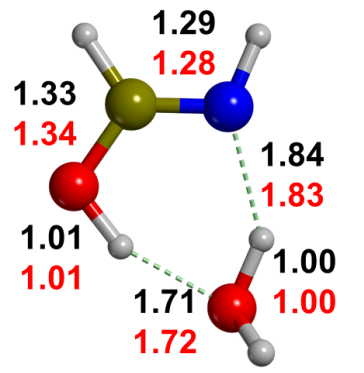
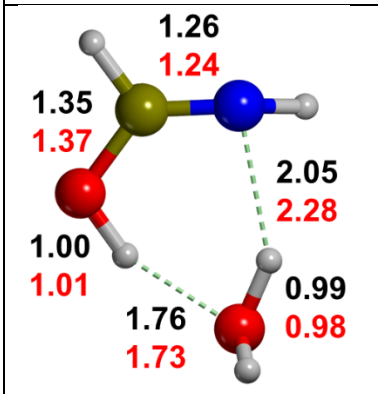
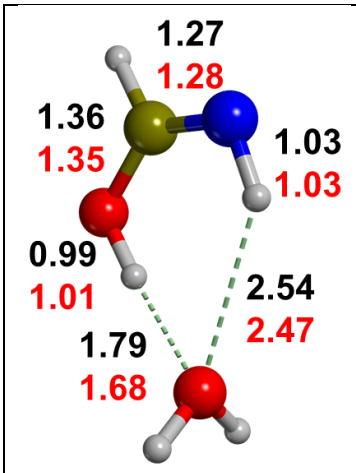
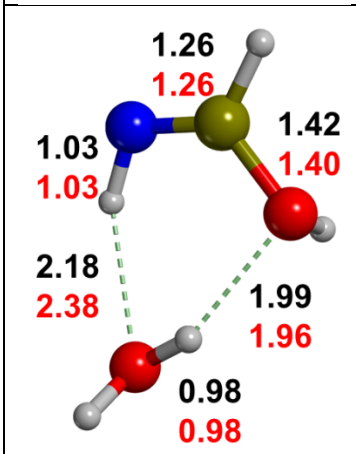
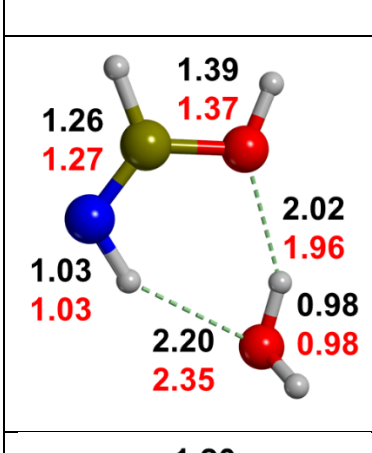
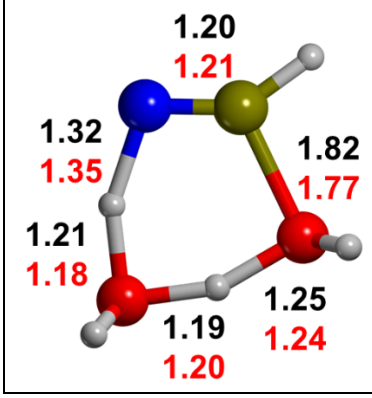
Structures (**Gas phase**, **PCM (F)**)	**Gas phase** coordinates	**PCM (F)** coordinates
	6 F_R_G C -0.095794 0.404515 0.000119 H -0.058229 1.520816 0.000066 O -1.139189 -0.228834 0.000100 N 1.154382 -0.143443 -0.000409 H 1.984304 0.439134 0.001516 H 1.256311 -1.154644 0.001092	6 F_R_F C -0.084324 0.404209 0.000043 H -0.050690 1.516095 0.000014 O -1.144542 -0.226284 0.000044 N 1.149891 -0.145613 -0.000165 H 1.979793 0.439102 0.000638 H 1.263982 -1.156563 0.000421
	6 F_TS_G C -0.359603 0.483937 -0.002796 H 0.617264 0.957542 -0.531184 O -1.246850 -0.277664 0.028911 N 1.414296 -0.114568 -0.014320 H 2.060108 0.296433 0.667882 H 1.745657 -1.021204 -0.363273	6 F_TS_F C -0.319781 0.496189 0.007432 H 0.678376 0.932875 -0.582440 O -1.217770 -0.272378 0.021996 N 1.351980 -0.128117 -0.010333 H 2.020031 0.310805 0.632844 H 1.654483 -1.052538 -0.344525
	6 F_P_G C -0.912735 -0.599852 0.004821 H 2.001837 -0.859322 -0.387160 O -1.485890 0.385230 -0.003176 N 1.979139 0.087704 -0.005204 H 2.668571 0.644063 -0.514160 H 2.288903 0.029666 0.966622	
		6 F_P_F C 0.930493 0.027109 -0.004518 H -1.599805 0.017944 -0.083278 O 2.066424 -0.016039 0.038103 N -2.623518 -0.003577 -0.097621 H -2.933350 0.798391 0.457143 H -2.898280 -0.835052 0.431664

Figure S2: PBE-D2/TZVP optimized geometries for the non-catalysed (intramolecular) formamide decarbonylation reaction. In the first column the optimized structures with the most representative bond lengths (in Å) in gas phase (black), and in PCM (F) (red) are shown. In the second and third columns the cartesian coordinates of the optimized structures in gas phase, and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue.

Formamide + H_2O dehydration reaction

Structures (**Gas phase**, **PCM (F)**)	**Gas phase** coordinates	**PCM (F)** coordinates
	9 FW_M1_G C -1.191359 -0.185463 0.007696 H -2.302316 -0.245160 0.011911 O -0.490184 -1.201650 0.000307 N -0.717425 1.080695 0.011883 H 0.303384 1.217293 0.006437 H -1.353159 1.870046 0.001795 O 1.949590 0.124436 -0.089449 H 1.284631 -0.609521 -0.074074 H 2.562348 -0.067039 0.637719	9 FW_M1_F C -1.192454 -0.229437 0.016432 H -2.290339 -0.374987 0.054626 O -0.410954 -1.197493 -0.006767 N -0.815580 1.059578 -0.004070 H 0.183876 1.286474 -0.032729 H -1.508059 1.801350 0.022381 O 2.009456 0.151904 -0.098643 H 1.277238 -0.517261 -0.056207 H 2.413050 0.128709 0.785106
	9 FW_TS1_G C -1.101260 -0.104734 0.013471 N -0.549343 1.085252 0.003427 O -0.395052 -1.186902 0.001542 O 1.659629 0.085013 -0.099567 H -2.195718 -0.234311 0.033426 H 0.757261 0.879435 -0.026119 H -1.182297 1.881568 0.002255 H 0.740226 -0.780710 -0.027057 H 2.216881 0.100767 0.696877	9 FW_TS1_F C -1.108737 -0.095081 0.017613 N -0.544345 1.082058 -0.005816 O -0.398638 -1.188365 -0.002693 O 1.672060 0.082044 -0.098912 H -2.200043 -0.220971 0.054802 H 0.747733 0.872034 -0.028288 H -1.166282 1.887756 0.018561 H 0.706094 -0.797100 -0.023739 H 2.187957 0.104932 0.726539
	9 FW_M2_G C -1.179565 -0.051314 0.010278 H -2.264509 -0.237159 0.021319 N -0.625812 1.108861 0.003720 O -0.492339 -1.192248 0.005151 H -1.320072 1.858961 0.001798 H 0.493926 -0.958033 -0.014398 O 1.862981 0.058828 -0.097260 H 2.399962 0.154580 0.705873 H 1.183635 0.794869 -0.065419	9 FW_M2_F C -1.185640 -0.048804 0.013848 H -2.269360 -0.229268 0.040065 N -0.624998 1.106238 -0.002479 O -0.492751 -1.194358 -0.000014 H -1.319203 1.857274 0.011963 H 0.491506 -0.954425 -0.018393 O 1.873872 0.067345 -0.099965 H 2.361008 0.105690 0.741086 H 1.175908 0.785987 -0.040633
	9 FW_TS2_G C -1.205713 -0.048592 0.049994 N -0.787826 1.138708 0.039400 O -0.495340 -1.193373 -0.053310 O 1.910289 0.062666 -0.074923 H -2.259352 -0.319337 0.252623 H 0.472170 -0.958198 -0.177746 H -0.454359 1.923732 -0.485421 H 1.228292 0.751287 0.128030 H 2.442720 -0.031228 0.732614	9 FW_TS2_F C -1.236232 -0.095562 0.017823 N -0.902710 1.103498 0.025484 O -0.425548 -1.194003 -0.016585 O 1.954759 0.097417 -0.094913 H -2.282603 -0.451990 0.080248 H 0.528666 -0.878464 -0.056041 H -0.590351 2.032039 -0.169962 H 1.364136 0.872420 0.030962 H 2.482829 0.047565 0.721457

	9 FW_M3_G C -1.338780 -0.142641 0.000300 N -1.200464 1.124195 -0.000150 H -0.203591 1.389983 -0.000770 H -2.342601 -0.585168 0.000599 O -0.396709 -1.125026 -0.000185 H 0.501370 -0.703097 -0.000655 O 2.049759 0.207187 -0.000076 H 2.626688 0.114135 0.776061 H 2.629656 0.113345 -0.773898	9 FW_M3_F C -1.307953 -0.165551 0.001421 N -1.195686 1.109396 -0.002471 H -0.201980 1.386959 -0.007478 H -2.303998 -0.627129 0.006444 O -0.344778 -1.112833 0.000393 H 0.559797 -0.668561 -0.002357 O 1.978034 0.234229 -0.003031 H 2.529020 0.108340 0.789333 H 2.568628 0.056749 -0.756072
	9 FW_TS3_G C 1.280936 -0.047217 -0.088815 O 0.509604 1.141736 -0.041165 N 0.850635 -1.220153 0.059638 O -2.035169 -0.113187 0.071087 H 2.330327 0.154552 -0.341543 H -0.166676 -1.228290 0.257159 H 0.413340 1.412213 0.889972 H -2.649172 -0.259126 -0.665964 H -1.363358 0.516635 -0.263578	9 FW_TS3_F C 1.274883 -0.027064 -0.152545 O 0.495850 1.130357 -0.004843 N 0.905899 -1.207106 0.107875 O -2.124432 -0.104098 0.040721 H 2.258730 0.181379 -0.591835 H -0.060337 -1.216033 0.477229 H 0.507622 1.411498 0.930033 H -2.316548 -0.459033 -0.843536 H -1.351399 0.484242 -0.098768
	9 FW_M4_G C -1.284104 -0.093070 0.019678 H -2.370143 0.074258 0.064905 N -0.795793 -1.252797 -0.003009 O -0.537693 1.082138 -0.004291 H 0.237778 -1.235852 -0.053452 H -1.134810 1.851345 -0.016296 O 2.112792 -0.077761 -0.092960 H 2.513092 -0.016176 0.789203 H 1.428465 0.619409 -0.103362	9 FW_M4_F C -1.306081 -0.029455 0.018497 H -2.373935 0.220351 0.064485 N -0.905457 -1.232238 -0.007503 O -0.468724 1.058868 -0.008357 H 0.126788 -1.273355 -0.051516 H -0.983676 1.887102 0.016827 O 2.161854 -0.107030 -0.097228 H 2.442342 -0.175734 0.830946 H 1.418120 0.529327 -0.074530
	9 FW_TS4_G C -1.236618 -0.235307 0.016672 H -2.244569 0.171880 0.006442 N -0.616810 -1.263943 0.015138 O -0.263332 1.296448 -0.100799 H 0.664590 -0.953458 -0.022025 H -0.461825 1.848578 0.677631 O 1.608956 -0.201888 -0.091022 H 2.169255 -0.278314 0.700128 H 0.844940 0.714273 -0.033602	9 FW_TS4_F C -1.222779 -0.230118 0.026991 H -2.239116 0.159111 0.072915 N -0.605930 -1.266651 -0.000370 O -0.290908 1.265445 -0.112446 H 0.703037 -0.922373 -0.028324 H -0.498657 1.815916 0.666969 O 1.622875 -0.177079 -0.085404 H 2.133167 -0.235555 0.743019 H 0.824017 0.723231 -0.031127

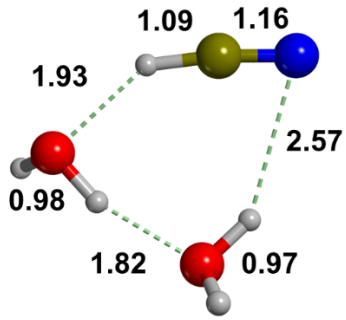
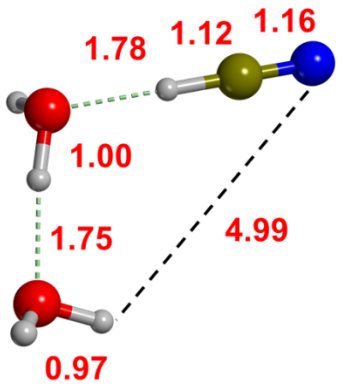
	9 FW_M5_G C -1.326161 -0.677828 0.026302 O 1.518862 -1.172576 0.085794 N -2.209746 0.075264 -0.019875 O 0.890196 1.536344 -0.084132 H -0.411492 -1.282610 0.053589 H 2.145768 -1.469564 -0.591952 H 1.487436 -0.186623 0.011805 H -0.075047 1.489058 -0.217955 H 1.006060 2.079707 0.712533	
		9 FW_M5_F C -1.887455 0.051252 0.018811 O 0.683484 -1.276547 0.094510 N -2.920268 0.583821 -0.012137 O 2.513184 0.768125 -0.080905 H -0.896379 -0.460973 0.047756 H 0.823088 -1.838514 -0.684623 H 1.402938 -0.576904 0.044901 H 1.968605 1.532983 -0.324073 H 2.895014 1.016531 0.779299

Figure S3: PBE-D2/TZVP optimized geometries for the H_2O assisted formamide dehydration reaction. In the first column the optimized structures with the most representative bond lengths (in Å) in gas phase (black), and in PCM (F) (red) are shown. In the second and third columns the cartesian coordinates of the optimized structures in gas phase, and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue.

Formamide + H_2O decarbonylation reaction

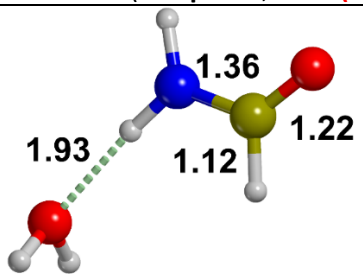
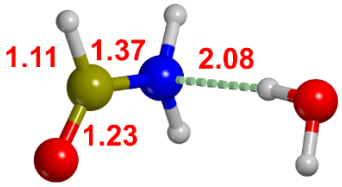
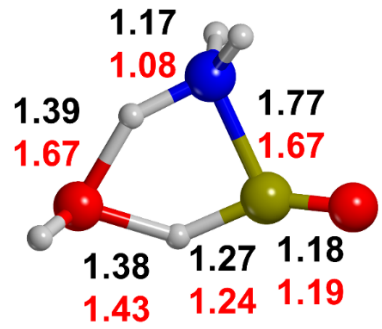
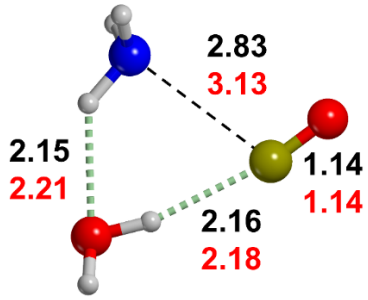
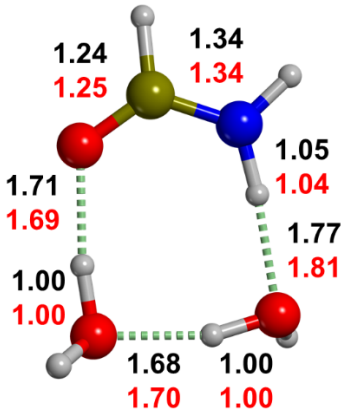
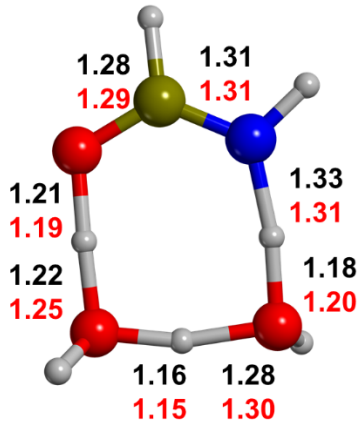
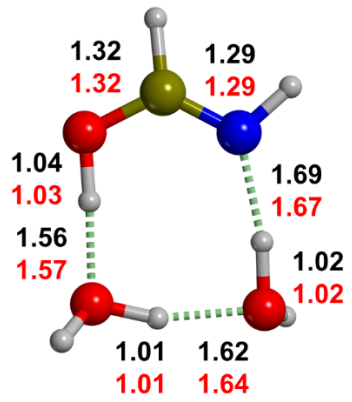
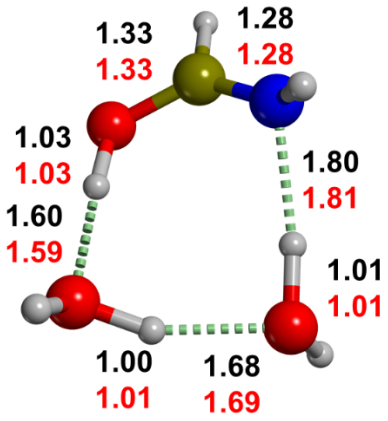
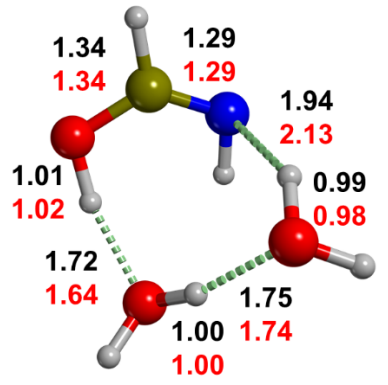
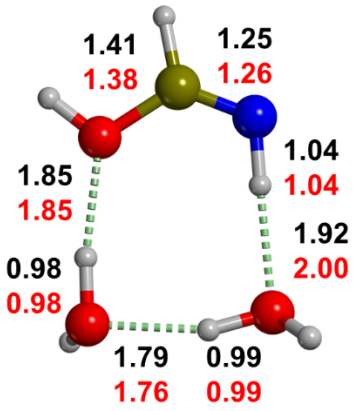
Structures (**Gas phase**, **PCM (F)**)	**Gas phase** coordinates	**PCM (F)** coordinates
	9 FW_R_G 6 1.120983 -0.334431 -0.000253 1 0.630009 -1.339402 -0.000910 8 2.337524 -0.194568 0.000176 7 0.201841 0.666102 -0.000072 1 0.528717 1.628449 0.000565 1 -0.801942 0.461608 -0.000161 8 -2.647918 -0.091570 0.000176 1 -3.005214 -0.560128 0.771953 1 -3.007207 -0.557547 -0.772236	
		9 FW_R_F 6 1.281914 -0.579637 -0.052204 1 -0.785441 -1.273164 -0.103812 8 2.308453 -0.100310 0.050219 7 -0.822875 1.735584 0.040201 1 -1.374427 2.395094 0.594759 1 -0.786519 2.116717 -0.908432 8 -1.763123 -1.307329 -0.095821 1 -1.363042 0.864329 -0.014191 1 -1.984568 -1.513137 0.828303
	9 FW_TS_G 6 0.670208 -0.401112 -0.176021 1 -0.495201 -0.906635 -0.234261 8 1.809884 -0.525479 0.093976 7 -0.068848 1.197004 0.019646 1 0.330738 1.720245 0.804359 1 0.009811 1.749782 -0.838913 8 -1.805737 -0.509899 -0.047910 1 -1.107328 0.675993 0.151885 1 -2.310506 -0.928718 0.667007	9 FW_TS_F 6 0.620045 -0.383612 -0.193811 1 -0.534803 -0.837003 -0.290156 8 1.742102 -0.634921 0.098894 7 0.074209 1.199011 0.022522 1 0.487253 1.665269 0.837860 1 0.229466 1.770084 -0.815743 8 -1.894494 -0.458945 -0.053229 1 -0.961869 0.914306 0.142673 1 -2.240643 -0.853133 0.765261
	9 FW_P_G 6 1.140070 -0.693605 -0.013736 1 -0.992491 -1.012335 -0.080545 8 2.220696 -0.331070 0.008154 7 -0.473043 1.635252 0.011402 1 -0.403403 2.290999 0.791525 1 -0.535431 2.186413 -0.846490 8 -1.969031 -0.943891 -0.069326 1 -1.346843 1.107682 0.110916 1 -2.264263 -1.658202 0.516577	9 FW_P_F 6 -1.093093 0.050227 0.376307 1 -1.225649 0.215340 1.467266 8 -1.542651 -0.931368 -0.208233 7 -0.340041 1.027365 -0.210640 1 -0.305537 1.068016 -1.228927 1 -0.189189 1.900289 0.290709 8 2.396549 -0.297063 0.103206 1 1.549772 0.191743 0.038780 1 2.278266 -1.040860 -0.510975

Figure S4: PBE-D2/TZVP optimized geometries for the H_2O assisted formamide decarbonylation reaction. In the first column the optimized structures with the most representative bond lengths (in Å) in gas phase (black), and in PCM (F) (red) are shown. In the second and third columns the cartesian coordinates of the optimized structures in gas phase, and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue.

Formamide + $2H_2O$ dehydration reaction

Structures (**Gas phase, PCM (F)**)	**Gas phase** coordinates	**PCM (F)** coordinates
	12 F2W_M1_G C -1.718822 -0.102301 0.001318 H -2.830281 -0.088169 0.044230 O -1.111849 -1.178497 -0.091506 N -1.163317 1.120406 0.057330 N -1.772517 1.926507 0.151606 N -0.127361 1.266891 0.033602 O 1.637557 1.348194 0.047520 H 1.792554 0.356492 0.067709 O 1.585981 -1.311884 -0.030774 H 0.586378 -1.348582 -0.082099 H 1.829579 -1.861477 0.730254 H 2.084289 1.656803 -0.756449	12 F2W_M1_F 6 1.728160 -0.073592 0.004106 1 2.835972 -0.042237 -0.022317 8 1.132978 -1.165521 0.104534 7 1.150680 1.130270 -0.080124 1 1.744015 1.951238 -0.158520 1 0.115818 1.256694 -0.056181 8 -1.695174 1.330191 -0.040743 1 -1.806838 0.333784 -0.017861 8 -1.556656 -1.351621 0.027879 1 -0.553238 -1.334732 0.050303 1 -1.787614 -1.781082 -0.812778 1 -2.021015 1.641604 0.820218
	12 F2W_TS1_G C 1.598440 0.065354 -0.001347 H 2.702047 0.124142 -0.018833 O 1.123827 -1.124941 0.073926 N 0.900037 1.173805 -0.056342 H 1.479729 2.009835 -0.126421 H -0.428184 1.239453 -0.033594 O -1.607014 1.116105 -0.053081 H -1.601438 -0.160602 -0.005355 O -1.308419 -1.283589 0.045024 H -0.084299 -1.227782 0.051368 H -1.629731 -1.753146 -0.741973 H -1.996173 1.498740 0.750328	12 F2W_TS1_F 6 1.601324 0.074303 0.002883 1 2.701658 0.139776 0.003103 8 1.126918 -1.125371 0.083073 7 0.893625 1.169935 -0.075231 1 1.463909 2.014309 -0.132064 1 -0.416982 1.228703 -0.038705 8 -1.614247 1.118823 -0.043229 1 -1.597253 -0.177298 0.001297 8 -1.308913 -1.290997 0.038058 1 -0.062584 -1.218884 0.042533 1 -1.615608 -1.724906 -0.777130 1 -1.966520 1.483301 0.787062
	12 F2W_M2_G C 1.668764 0.205542 -0.005012 H 2.766142 0.305796 -0.018985 O 1.304088 -1.058228 0.068013 N 0.867912 1.215744 -0.053608 H 1.394118 2.090442 -0.116075 H -0.820344 1.253952 -0.054819 O -1.829422 1.097116 -0.057797 H -1.662704 -0.517358 0.016482 O -1.260990 -1.448528 0.051988 H 0.276229 -1.186530 0.059806 H -1.583654 -1.916225 -0.734711 H -2.167163 1.503582 0.756006	12 F2W_M2_F 6 -1.672656 -0.202836 0.002529 1 -2.767972 -0.303768 0.018109 8 -1.296789 1.065264 0.076116 7 -0.870726 -1.207267 -0.076754 1 -1.395957 -2.084143 -0.123100 1 0.803088 -1.250164 -0.046541 8 1.819165 -1.118022 -0.048591 1 1.661817 0.515486 0.011315 8 1.277666 1.453005 0.046590 1 -0.268845 1.181219 0.047328 1 1.564261 1.890940 -0.773021 1 2.134295 -1.483664 0.795090

	12 F2W_TS2_G C -1.646362 -0.123199 0.079261 H -2.681673 -0.176530 0.473249 O -1.153512 1.076563 0.369471 N -1.053468 -1.131600 -0.431560 H -0.802253 -1.432870 -1.358835 H 0.653158 -1.272887 0.110137 O 1.648216 -1.214528 0.250750 H 1.710324 0.444170 -0.018753 O 1.387536 1.375928 -0.211447 H -0.182300 1.188970 0.049476 H 1.675651 1.582142 -1.114652 H 1.821624 -1.576303 1.134544	12 F2W_TS2_F 6 1.650859 -0.115322 -0.076625 1 2.695272 -0.146617 -0.447311 8 1.131361 1.070286 -0.392415 7 1.063942 -1.124860 0.436922 1 0.826574 -1.427652 1.369555 1 -0.663329 -1.269175 -0.091713 8 -1.654666 -1.227516 -0.258438 1 -1.705148 0.432023 0.053954 8 -1.391689 1.372389 0.227650 1 0.154393 1.167739 -0.068842 1 -1.569877 1.540852 1.168802 1 -1.770682 -1.452485 -1.197529
	12 F2W_M3_G C -1.415737 -0.582589 -0.150770 H -2.057549 -1.202167 -0.790052 O -1.563362 0.723363 -0.420807 N -0.645892 -1.145817 0.712044 H -0.177217 -0.428940 1.286915 H 1.078295 -1.335811 -0.165881 O 1.892004 -0.847705 -0.450990 H 1.396878 0.768332 0.010856 O 0.875894 1.556809 0.335366 H -0.762024 1.205801 -0.043104 H 1.269423 2.338224 -0.083762 H 2.631576 -1.288926 -0.003209	12 F2W_M3_F 6 -1.498660 -0.472481 -0.153748 1 -2.247013 -0.995476 -0.763250 8 -1.414355 0.824570 -0.485357 7 -0.838743 -1.125950 0.736837 1 -0.227709 -0.491301 1.272720 1 1.045008 -1.438509 -0.213386 8 1.852685 -0.943429 -0.473403 1 1.469231 0.671897 0.056506 8 0.986601 1.479100 0.397602 1 -0.559687 1.211121 -0.085158 1 1.405205 2.246787 -0.027436 1 2.578670 -1.369909 0.013905
	12 F2W_M4_G C -1.809770 -0.103595 -0.020197 O -1.078846 1.097682 0.009520 N -1.321773 -1.255033 0.037413 H -2.893881 0.070408 -0.096146 H -0.282048 -1.302183 0.098237 H -1.691974 1.848104 -0.091464 O 1.734391 1.324061 -0.094680 H 2.011426 1.705548 0.753868 H 0.749765 1.336211 -0.073573 O 1.637536 -1.412573 0.084219 H 2.005041 -1.868645 -0.688940 H 1.868059 -0.456005 -0.035171	12 F2W_M4_F 6 1.801027 -0.153562 -0.068295 8 1.132656 1.001946 0.292714 7 1.250706 -1.276604 -0.246514 1 2.883858 -0.012102 -0.186086 1 0.220739 -1.262062 -0.098962 1 1.762677 1.744383 0.358709 8 -1.629716 1.376648 -0.111297 1 -1.790112 1.712346 -1.009502 1 -0.649596 1.375436 -0.009785 8 -1.772561 -1.352436 0.077335 1 -1.971808 -1.545738 1.008559 1 -1.859889 -0.363932 0.002419

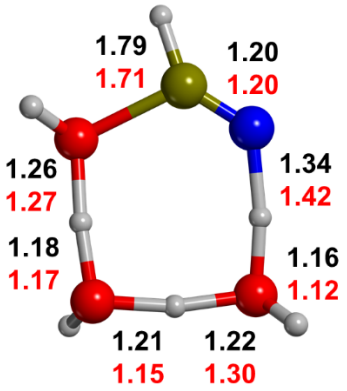
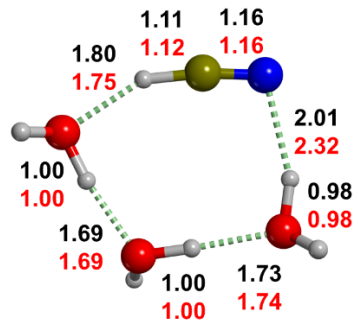
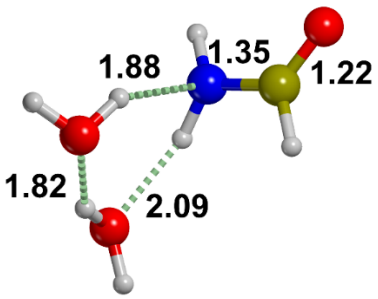
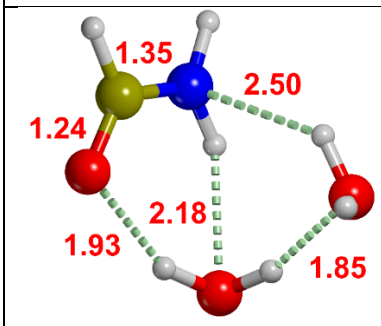
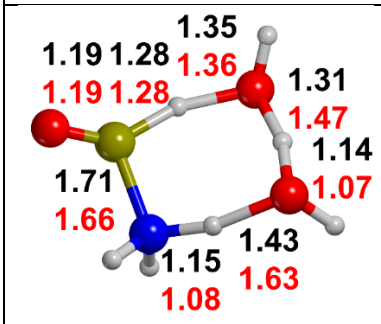
	12 F2W_TS4_G C 1.662325 -0.474134 0.019470 O 1.085874 1.221215 -0.092222 N 0.904197 -1.397497 -0.026989 H 2.730845 -0.268001 0.064124 H -0.436232 -1.349910 -0.061768 H 1.554703 1.751393 0.578096 O -1.341358 1.272483 0.102360 H -1.724028 1.738063 -0.659493 H -0.165238 1.307467 0.024521 O -1.579881 -1.128218 -0.082114 H -2.002777 -1.565474 0.675641 H -1.577682 0.089906 0.026793	12 F2W_TS4_F 6 1.659996 -0.411844 0.071778 8 1.060873 1.165081 -0.184339 7 0.944394 -1.380319 0.020500 1 2.721636 -0.191536 0.215317 1 -0.470254 -1.328388 -0.085068 1 1.601900 1.788533 0.337653 8 -1.347119 1.259511 0.186521 1 -1.780497 1.775606 -0.516342 1 -0.189874 1.286576 0.026333 8 -1.572991 -1.140436 -0.149486 1 -1.997888 -1.615790 0.586194 1 -1.581864 0.145047 0.040171
	12 F2W_M5_G C -0.289685 -1.733415 -0.048411 O 2.284773 -0.551172 0.010398 N -1.451289 -1.727354 -0.063196 H 0.809403 -1.583031 -0.013939 H -1.971621 0.211568 -0.066489 H 2.903045 -0.514214 0.756646 H 0.817629 1.717667 -0.029984 H 0.926061 2.271998 -0.818686 H 1.816183 0.333452 0.000619 O -1.858367 1.183330 0.023970 H -2.375718 1.429905 0.807267 H -0.162493 1.543690 0.032352	12 F2W_M5_F 6 -1.386885 -1.159165 -0.048939 8 1.399606 -1.758293 0.027213 7 -2.430751 -0.649494 -0.093786 1 -0.343397 -1.561303 0.002142 1 -1.317387 1.383612 -0.009919 1 1.728275 -2.088785 0.880046 8 1.859417 0.891574 -0.059656 1 2.251484 1.181152 -0.900419 1 1.653185 -0.786453 0.002304 8 -0.613071 2.057651 0.045599 1 -0.769369 2.511366 0.891817 1 0.966164 1.334410 -0.021080

Figure S5: PBE-D2/TZVP optimized geometries for the $2H_2O$ assisted formamide dehydration reaction. In the first column the optimized structures with the most representative bond lengths (in Å) in gas phase (black), in PCM (W) (blue), and in PCM (F) (red) are shown, in the second, third, and fourth columns the cartesian coordinates of the optimized structures in gas phase, in PCM (W) and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue.

Formamide + $2H_2O$ decarbonylation reaction

Structures (**Gas phase**, **PCM (F)**)	**Gas phase** coordinates	**PCM (F)** coordinates
	12 F2W_R_G 6 1.551184 0.191290 -0.344265 1 1.153821 0.392818 -1.367531 8 2.697470 -0.172377 -0.136936 7 0.581577 0.353529 0.617396 1 0.904890 0.361429 1.584121 1 -0.266804 0.900516 0.387995 8 -2.075031 1.201352 -0.052548 1 -2.219931 0.228670 -0.160078 1 -2.413334 1.615165 -0.861712 8 -1.606948 -1.489465 -0.125196 1 -0.731328 -1.227737 0.238657 1 -1.929383 -2.209372 0.439799	
		12 F2W_R_F 6 -1.560836 0.369182 0.213868 1 -2.341635 1.093125 0.523701 8 -1.342425 -0.669611 0.854150 7 -0.881936 0.746657 -0.890629 1 -0.200106 0.096877 -1.296270 1 -1.173903 1.564620 -1.417302 8 1.011014 -1.534010 -0.507214 1 1.542429 -0.774299 -0.165755 1 0.206377 -1.501233 0.061373 8 2.084884 0.913597 0.368456 1 1.270969 1.421137 0.190813 1 2.206651 0.978265 1.331489
	12 F2W_TS_G 6 -1.161250 0.353362 -0.103270 1 -0.126370 1.092266 -0.269377 8 -2.241704 0.385795 0.383762 7 -0.537857 -1.216341 -0.352499 1 -1.126511 -1.904750 0.131391 1 -0.557816 -1.410816 -1.359925 8 1.176029 1.443999 -0.289644 1 1.692921 0.315546 0.139009 1 1.376396 2.209112 0.273927 8 1.852922 -0.778368 0.433568 1 0.555686 -1.191275 -0.002960 1 2.620212 -1.127278 -0.046438	12 F2W_TS_F 6 1.142718 0.318289 0.107073 1 0.103311 1.050982 0.267884 8 2.244427 0.433133 -0.335022 7 0.614953 -1.242668 0.279540 1 1.186895 -1.894402 -0.272679 1 0.680713 -1.506949 1.270760 8 -1.177711 1.505090 0.272200 1 -1.759319 0.221380 -0.132285 1 -1.282360 2.184664 -0.415849 8 -1.949658 -0.798840 -0.383742 1 -0.429946 -1.254176 -0.006668 1 -2.596727 -1.127616 0.262125

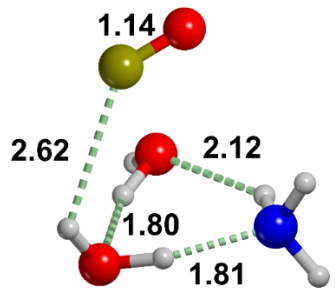
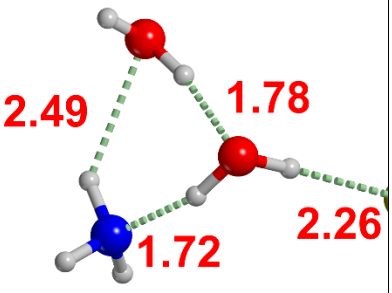
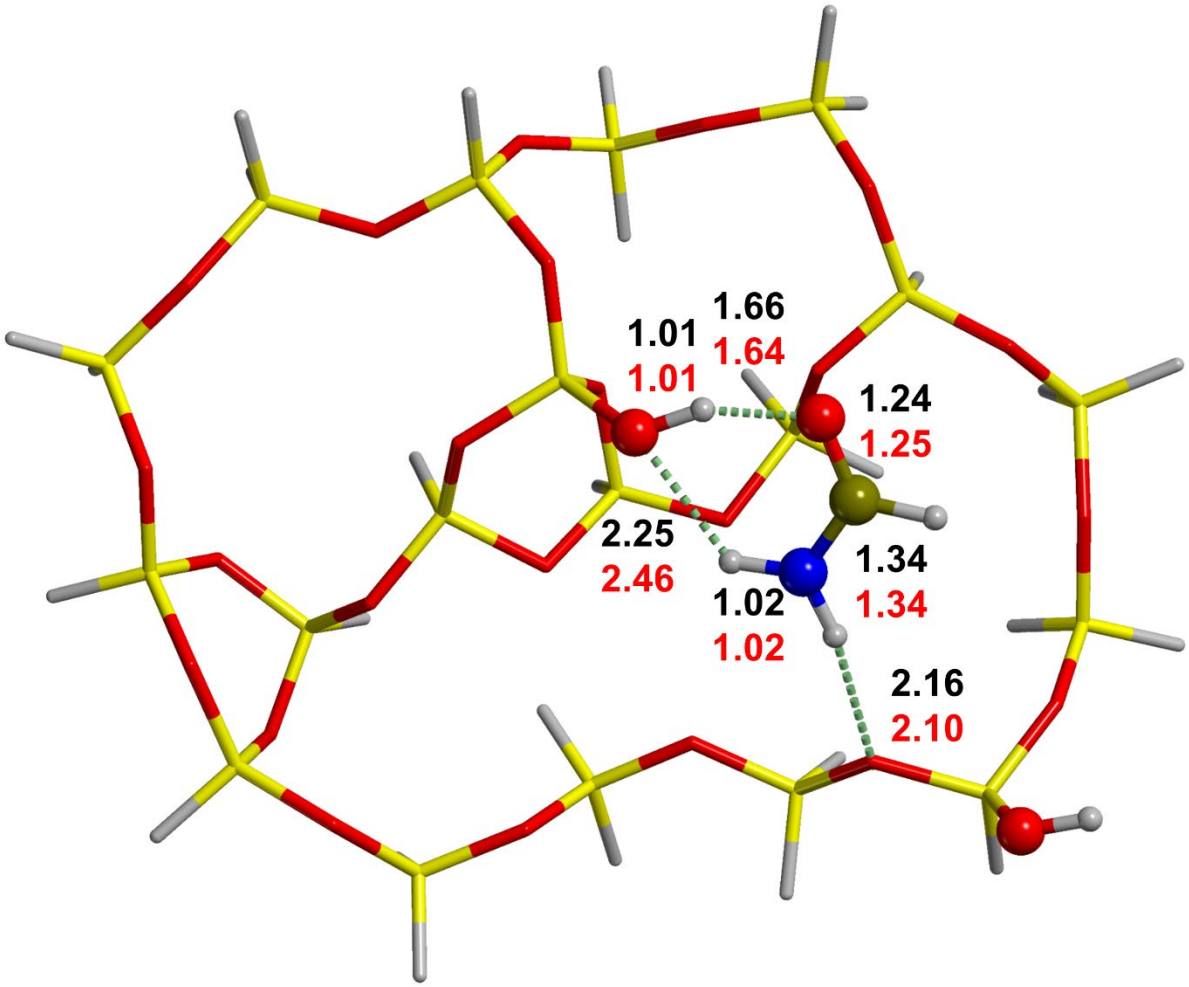
	12 F2W_P_G 6 -1.767280 -0.384181 0.646307 1 1.172942 0.394847 0.959282 8 -2.209658 0.276525 -0.168372 7 0.910972 1.645539 -0.319399 1 0.071433 2.226749 -0.347878 1 1.710735 2.247817 -0.522057 8 1.310077 -0.525887 1.341420 1 0.945417 -1.164201 -0.299329 1 0.519646 -0.693970 1.881025 8 0.632537 -1.161104 -1.243469 1 0.835816 0.942633 -1.068230 1 1.107243 -1.883838 -1.681492	
		12 F2W_P_F 6 -2.597139 -0.068408 0.044007 1 0.878012 0.649501 0.705301 8 -3.636919 0.013592 -0.407193 7 1.894774 1.634717 -0.278811 1 1.436817 2.217940 -0.982651 1 2.609059 2.210630 0.172071 8 0.445003 -0.154345 1.153806 1 1.445236 -1.187745 0.097815 1 -0.483677 -0.147993 0.856186 8 2.090468 -1.591223 -0.544701 1 2.375218 0.875308 -0.773778 1 2.870330 -1.794403 -0.002609

Figure S6: PBE-D2/TZVP optimized geometries for the $2H_2O$ assisted formamide decarbonylation reaction. In the first column the optimized structures with the most representative bond lengths (in Å) in gas phase (black), in PCM (W) (blue), and in PCM (F) (red) are shown, in the second, third, and fourth columns the cartesian coordinates of the optimized structures in gas phase, in PCM (W) and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue.

Formamide + Silica 1.5 dehydration reaction



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H 6.530458 -4.360668 2.673857	H 6.520304 -4.630810 2.640186
O 6.390676 -2.954255 0.313246	O 6.393587 -2.948001 0.312295
C 3.375475 -0.054921 2.537463	C 3.386847 -0.083155 2.596997
H 4.436243 -0.294653 2.756931	H 4.375137 -0.352908 3.015094
N 2.712688 -1.046165 1.918161	N 2.880662 -0.996719 1.761835
H 1.735364 -0.906563 1.656849	H 1.999596 -0.819903 1.279491
H 3.165841 -1.926057 1.675386	H 3.377830 -1.859978 1.538333
O 2.895094 1.046626 2.848566	O 2.833431 0.991576 2.909192
Si -2.311954 -0.259588 -0.294708	Si -2.315627 -0.264790 -0.303260
O -0.091551 1.550262 -0.631550	O -0.109354 1.554183 -0.627674
H -2.773403 0.554885 -1.459464	H -2.773562 0.553363 -1.459913
Si -4.805334 4.191442 0.427527	Si -4.808600 4.187993 0.427443
O -3.223817 3.741868 0.471749	O -3.226694 3.739784 0.471592
Si -1.769996 4.463301 0.750364	Si -1.773493 4.462450 0.750241
H -5.112790 4.709234 -0.943620	H -5.116532 4.705640 -0.943652
O -2.041810 0.737222 1.008293	O -2.062615 0.732892 1.014987
Si -0.598805 1.628619 0.991123	Si -0.615934 1.624863 0.985345

O -1.217891 5.121595 -0.654812	O -1.221987 5.121346 -0.654889
O -0.789897 3.237502 1.316422	O -0.795898 3.232865 1.330722
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Si 2.768391 -4.242326 -0.578731	Si 2.772400 -4.239128 -0.579720
O 0.406286 0.866047 2.024904	O 0.366312 0.858009 2.044645
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O -0.853519 -1.014649 -0.677531	O -0.846546 -1.008089 -0.655358
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H -0.906123 -3.191360 -1.963534	H -0.903051 -3.191220 -1.964354
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Si 3.034719 5.629903 -0.310210	Si 3.030189 5.633304 -0.310330
Si 4.296006 2.893453 -0.032903	Si 4.293850 2.897923 -0.033292
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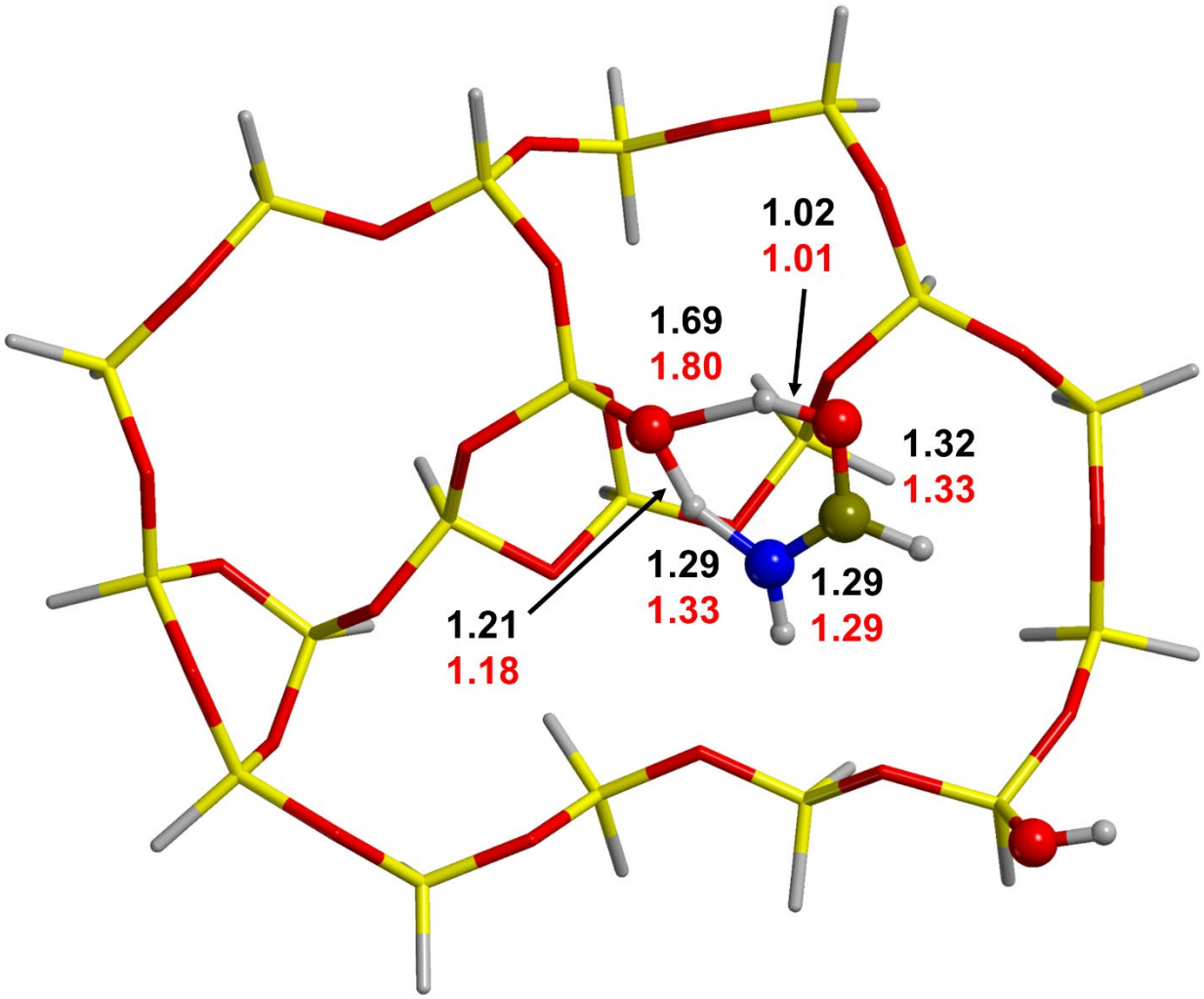

Gas phase coordinates	**PCM** coordinates
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H 6.541382 -4.408028 2.669274	H 6.510935 -4.676307 2.641942
O 6.390914 -2.975234 0.321710	O 6.383481 -2.988255 0.319521
C 3.109488 -0.201932 2.486721	C 3.185442 -0.139446 2.482590
H 4.111067 -0.623724 2.632354	H 4.190683 -0.553625 2.614262
N 2.133735 -0.844804 1.938201	N 2.203731 -0.776824 1.946969
H 1.105081 -0.072694 1.854602	H 1.131591 0.005737 1.872661
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Si -4.786199 4.200282 0.415562	Si -4.781964 4.205407 0.412975
O -3.205935 3.746558 0.462064	O -3.202414 3.749163 0.459086
Si -1.750518 4.464433 0.741545	Si -1.745705 4.464904 0.737303
H -5.090728 4.717399 -0.956492	H -5.086311 4.721923 -0.959345
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O 1.260862 -3.574957 -0.622879	O 1.252016 -3.580430 -0.622148
O -5.781385 -2.348500 1.007285	O -5.787459 -2.341284 1.010391
H 0.314463 3.891158 -2.369427	H 0.316861 3.885814 -2.374194
H 0.033773 6.339967 -2.503513	H 0.040068 6.334967 -2.510098
Si 0.167133 5.159026 -1.598569	Si 0.171950 5.154532 -1.604277
O -5.653280 -0.916673 -1.337909	O -5.653379 -0.908967 -1.333563
O -6.413968 0.396203 0.896487	O -6.415655 0.404350 0.897707
H -7.394979 1.859771 -1.014631	H -7.395209 1.867981 -1.014110
Si -7.030762 1.880742 0.435856	Si -7.030265 1.889518 0.436185
O -5.838439 2.983318 0.731609	O -5.836021 2.990399 0.730492
Si -6.456426 -1.071847 0.137515	Si -6.460849 -1.064233 0.139924
Si -5.202691 -3.811291 0.419245	Si -5.211412 -3.805477 0.423240
H 6.069993 -1.955159 -2.018762	H 6.063094 -1.969526 -2.021609
O -4.878248 -3.479708 -1.211567	O -4.888545 -3.474090 -1.206381
H 4.040941 0.337473 -1.876334	H 4.037821 0.326497 -1.880043
Si 2.788341 0.925965 -1.406228	Si 2.793364 0.922611 -1.412228
H 2.154159 1.795715 -2.452485	H 2.153125 1.787332 -2.456459
O 3.061826 1.772005 0.015706	O 3.050886 1.773261 0.015294
O -3.806908 -4.591233 0.911960	O -3.816658 -4.587283 0.915913
Si -0.188545 -4.223337 -1.163491	Si -0.198696 -4.226895 -1.161554
Si -2.663632 -5.379614 -0.053622	Si -2.675120 -5.378282 -0.049585
H -3.049090 -5.328292 -1.495199	H -3.061182 -5.327484 -1.491018
Si -4.332538 -1.926999 -1.471296	Si -4.335941 -1.924876 -1.473867
H 0.152346 -5.409708 -2.016177	H 0.139868 -5.414494 -2.013454
O -1.132186 -4.753205 0.115188	O -1.142582 -4.754216 0.117997
H -3.615699 -1.844958 -2.751273	H -3.622756 -1.844240 -2.749598
O -3.345220 -1.526870 -0.160438	O -3.351042 -1.525079 -0.151689
H -0.903910 -3.195437 -1.963083	H -0.912779 -3.198476 -1.961622
O 3.733476 4.340447 0.554919	O 3.737991 4.331898 0.548164
O 1.476284 5.359914 -0.614020	O 1.481894 5.354085 -0.620512
Si 3.058476 5.617122 -0.314843	Si 3.064643 5.608971 -0.322292

Si 4.312177 2.877635 -0.033145	Si 4.314045 2.867685 -0.039008
H 4.604861 3.187551 -1.477145	H 4.606541 3.175976 -1.483395
Si 6.926793 -1.873566 -0.794675	Si 6.920609 -1.888345 -0.797996
O 5.707967 2.097752 0.459581	O 5.708806 2.085937 0.453674
Si 6.851195 1.309325 -0.505970	Si 6.850298 1.294894 -0.511792
H 6.531315 1.539226 -1.947665	H 6.530102 1.524163 -1.953517
O 6.860864 -0.325817 -0.180684	O 6.857476 -0.340003 -0.185208
H 8.183421 1.852083 -0.118090	H 8.183583 1.835803 -0.124978
H 3.799442 5.771272 -1.607148	H 3.805240 5.760893 -1.615073
H 3.194841 6.812123 0.563037	H 3.203359 6.804448 0.554570
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H -8.201423 2.205287 1.300089	H -8.199989 2.216644 1.300716
H -1.845895 5.522435 1.774856	H -1.838878 5.523883 1.769815
H -6.309274 -4.785764 0.572947	H -6.319497 -4.778036 0.578247
H -2.619725 -6.778131 0.462091	H -2.633229 -6.776457 0.467221
H 2.606093 -5.739286 -0.454921	H 2.593824 -5.746798 -0.453105
H 8.353803 -2.201980 -1.083517	H 8.346948 -2.219297 -1.087255
H -7.873624 -1.419750 -0.145485	H -7.878743 -1.410069 -0.142124
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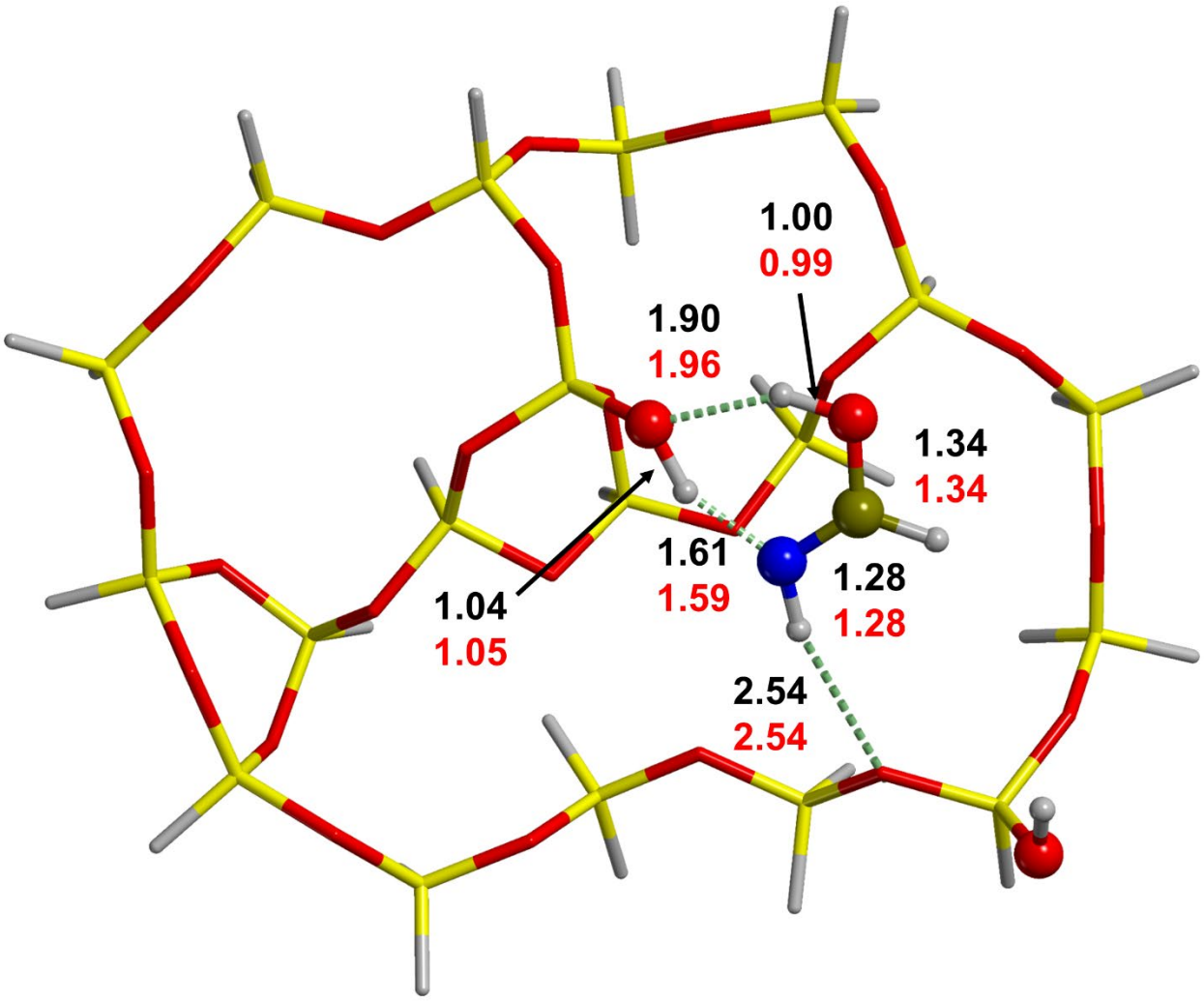

Gas phase coordinates	**PCM** coordinates

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O 5.716756 -4.715974 2.295661	O 5.585964 -4.573395 2.357959
H 5.677385 -4.057813 3.006706	H 6.512954 -4.661849 2.636359
O 6.379426 -2.982801 0.322113	O 6.381743 -2.978644 0.313893
C 3.291810 -0.134211 2.407828	C 3.273854 -0.228995 2.449157
H 4.326630 -0.499602 2.466706	H 4.281218 -0.654165 2.539575
N 2.294522 -0.796767 1.951448	N 2.253526 -0.838653 1.971033
H 0.992666 0.148049 1.925565	H 1.000323 0.142285 1.917699
H 2.539480 -1.730618 1.612888	H 2.474261 -1.782900 1.642494
O 3.188098 1.115797 2.867438	O 3.218912 1.030503 2.901824
Si -2.305507 -0.261999 -0.297526	Si -2.303133 -0.262367 -0.307281
O -0.055929 1.516288 -0.617691	O -0.069159 1.523069 -0.620187
H -2.771273 0.555362 -1.461992	H -2.770770 0.558383 -1.463145
Si -4.790675 4.203627 0.415829	Si -4.790718 4.203952 0.419317
O -3.210813 3.748433 0.461656	O -3.210688 3.749237 0.464090
Si -1.754486 4.465245 0.739111	Si -1.754500 4.466235 0.741796
H -5.095779 4.719341 -0.956625	H -5.096483 4.721040 -0.952474
O -2.012752 0.721999 1.013235	O -2.022458 0.719647 1.018914
Si -0.575341 1.628655 0.994094	Si -0.579798 1.625709 0.986271
O -1.199513 5.118268 -0.667395	O -1.200247 5.120955 -0.664204
O -0.785511 3.234844 1.306389	O -0.786291 3.230946 1.319766
H 3.453643 -3.904290 -1.844272	H 3.455496 -3.898779 -1.852438
Si 2.752809 -4.259820 -0.568156	Si 2.755235 -4.255915 -0.576454
O 0.502851 1.052430 2.085030	O 0.490734 1.041193 2.086470
O 1.775428 -0.392690 -1.143433	O 1.774779 -0.377735 -1.127328
Si 0.193550 0.041716 -1.386820	Si 0.196820 0.047165 -1.394092
O -0.853289 -1.029781 -0.679409	O -0.842399 -1.021808 -0.662577
H -0.099845 0.135212 -2.824298	H -0.099688 0.140587 -2.826854
O 3.745422 -3.757048 0.672083	O 3.748122 -3.754145 0.663970
H 2.254012 1.425543 2.711090	H 2.310314 1.386745 2.716074
O 1.248059 -3.578733 -0.617721	O 1.250241 -3.575276 -0.624751
O -5.791721 -2.343455 1.016434	O -5.789367 -2.344104 1.013239
H 0.307504 3.886128 -2.372764	H 0.306571 3.891153 -2.371434
H 0.029073 6.335039 -2.509661	H 0.027276 6.340116 -2.505598
Si 0.162002 5.155089 -1.603361	Si 0.160921 5.159237 -1.600615
O -5.662857 -0.913150 -1.330359	O -5.657904 -0.910146 -1.329856
O -6.421741 0.401719 0.902735	O -6.420342 0.400980 0.902716
H -7.402834 1.863871 -1.009425	H -7.402605 1.864859 -1.007521
Si -7.037458 1.886282 0.440750	Si -7.036720 1.885833 0.442545
O -5.843841 2.988071 0.734205	O -5.843365 2.987704 0.736760
Si -6.466208 -1.067226 0.145613	Si -6.464591 -1.067165 0.144031
Si -5.214900 -3.807529 0.429751	Si -5.212268 -3.807355 0.424777
H 6.057658 -1.965311 -2.019367	H 6.058801 -1.958745 -2.026376
O -4.894913 -3.479658 -1.203219	O -4.892829 -3.476235 -1.205778
H 4.030934 0.329455 -1.878189	H 4.031362 0.335192 -1.882009
Si 2.781404 0.918944 -1.410946	Si 2.787924 0.929960 -1.413683
H 2.145109 1.788805 -2.454670	H 2.144847 1.794532 -2.456249
O 3.045052 1.777250 0.003155	O 3.041019 1.782611 0.012493
O -3.819486 -4.588210 0.922341	O -3.816418 -4.588100 0.916029
Si -0.202396 -4.226379 -1.156396	Si -0.200191 -4.222828 -1.163606

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Si -4.348009 -1.929788 -1.466651	Si -4.342494 -1.927159 -1.473921
H 0.136681 -5.414134 -2.007878	H 0.138978 -5.409553 -2.016485
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O -3.355978 -1.530013 -0.156919	O -3.354374 -1.528819 -0.152079
H -0.917395 -3.198780 -1.956698	H -0.915817 -3.194606 -1.962548
O 3.729237 4.335726 0.548348	O 3.729197 4.338752 0.548941
O 1.472116 5.355929 -0.620085	O 1.471320 5.359458 -0.617591
Si 3.054789 5.611977 -0.322465	Si 3.054014 5.615714 -0.320260
Si 4.306065 2.871632 -0.038358	Si 4.306303 2.875481 -0.039545
H 4.597917 3.179478 -1.482969	H 4.597537 3.184977 -1.483928
Si 6.915495 -1.883034 -0.796054	Si 6.917047 -1.877497 -0.803281
O 5.701487 2.091009 0.454241	O 5.702161 2.094795 0.451717
Si 6.843197 1.300285 -0.511228	Si 6.843790 1.305490 -0.515008
H 6.522409 1.528710 -1.952955	H 6.522412 1.535357 -1.956374
O 6.851541 -0.334463 -0.183927	O 6.852795 -0.329606 -0.189467
H 8.176249 1.842231 -0.125063	H 8.176799 1.847467 -0.128735
H 3.794892 5.763814 -1.615539	H 3.793604 5.769187 -1.613433
H 3.192996 6.807931 0.553829	H 3.192135 6.810770 0.557270
H -5.002953 5.260471 1.453809	H -5.002977 5.259610 1.458507
H -8.207130 2.213028 1.305496	H -8.206192 2.211258 1.308060
H -1.848032 5.524616 1.771186	H -1.848031 5.524465 1.775043
H -6.322302 -4.780742 0.585525	H -6.319291 -4.781104 0.579899
H -2.634768 -6.776810 0.474248	H -2.631131 -6.775822 0.465162
H 2.591330 -5.744152 -0.448137	H 2.594294 -5.740428 -0.457974
H 8.341959 -2.213184 -1.085604	H 8.343518 -2.206858 -1.093695
H -7.883963 -1.414110 -0.135847	H -7.882331 -1.414218 -0.137296
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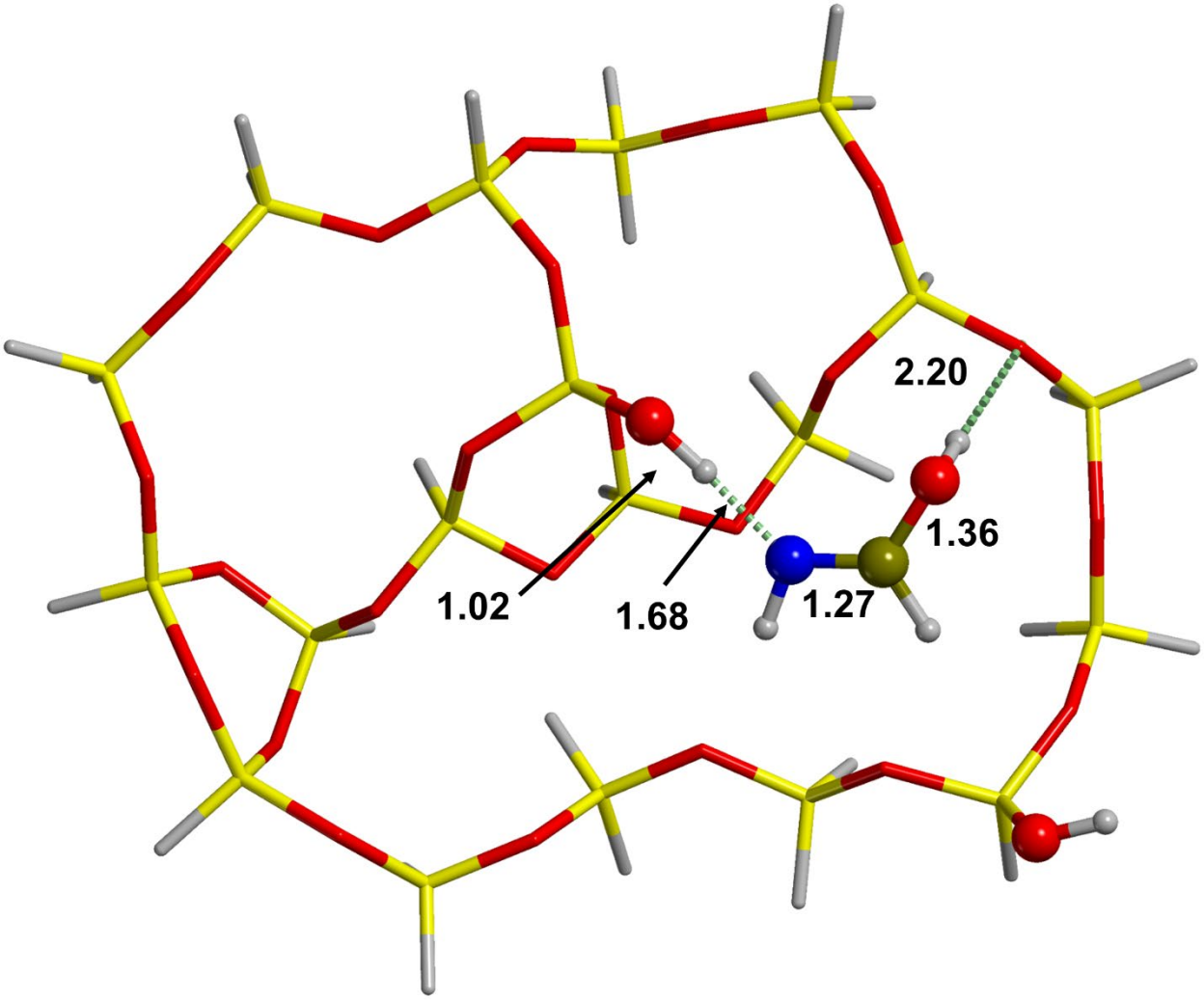

Gas phase coordinates	**PCM** coordinates
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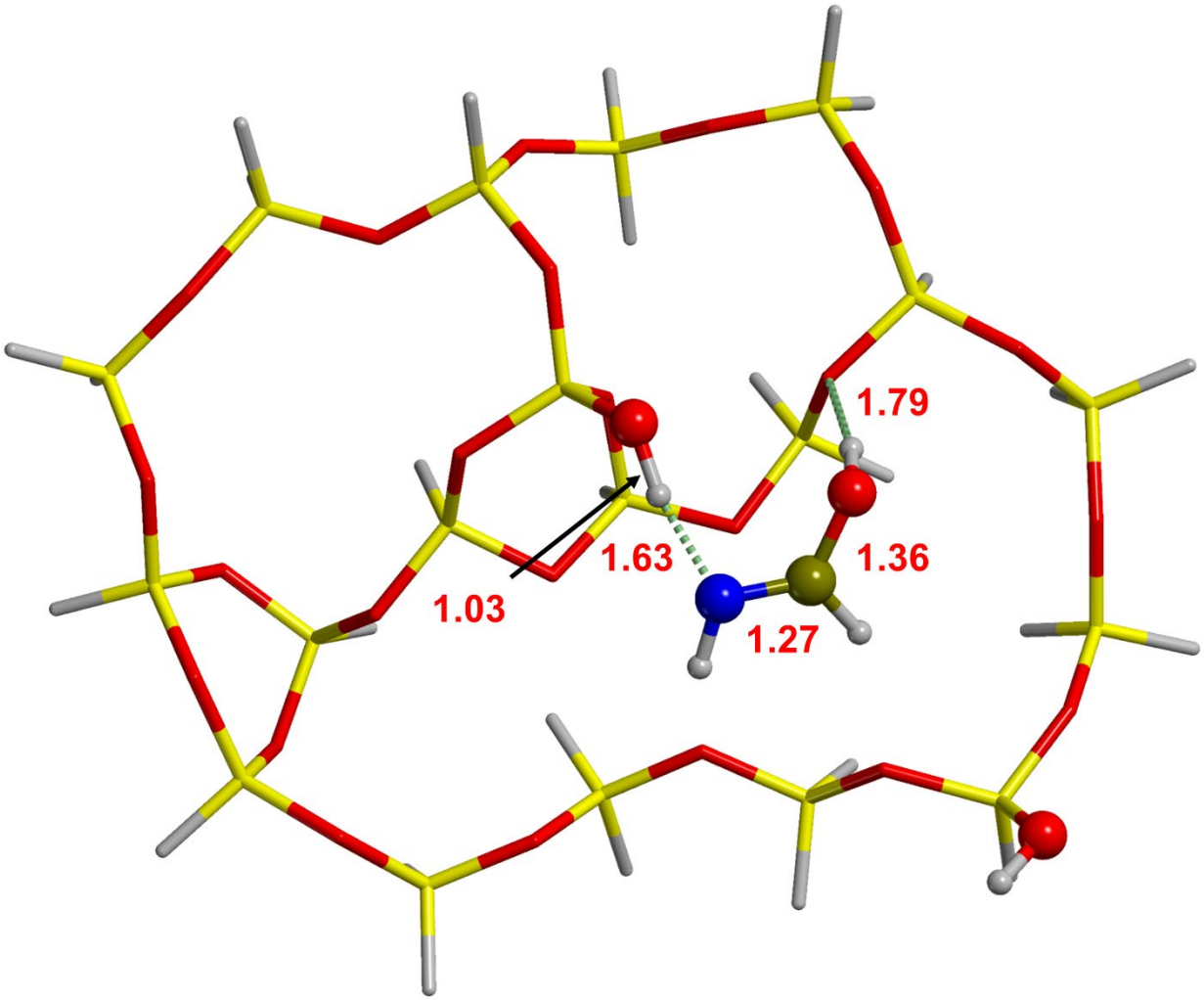
O -1.284290 5.132093 -0.624053 O -0.844251 3.245080 1.321093 H 3.458810 -3.834546 -1.867691 Si 2.764455 -4.205271 -0.592326 O 0.475999 1.105460 2.142754 O 1.752724 -0.360640 -1.157170 Si 0.162038 0.073356 -1.376994 O -0.874257 -1.012391 -0.679704 H -0.138208 0.174241 -2.814643 O 3.754674 -3.699903 0.648724 H 4.644021 0.823674 1.877557 O 1.252722 -3.539389 -0.634407 O -5.795767 -2.386968 1.022642 H 0.231534 3.926236 -2.340384 H -0.072370 6.372960 -2.461266 Si 0.074693 5.188784 -1.562700 O -5.686225 -0.941083 -1.314612 O -6.454240 0.352230 0.927583 H -7.454555 1.816164 -0.973220 Si -7.086217 1.833241 0.476278 O -5.903350 2.945402 0.774097 Si -6.485275 -1.112319 0.161321 Si -5.205218 -3.841320 0.425504 H 6.042333 -1.867771 -2.036192 O -4.883835 -3.495513 -1.202818 H 3.992432 0.405064 -1.876220 Si 2.735398 0.970684 -1.399416 H 2.090426 1.848503 -2.439437 O 3.033539 1.796509 0.035605 O -3.800762 -4.610660 0.910175 Si -0.192202 -4.198571 -1.174018 Si -2.653079 -5.383471 -0.062736 H -3.043301 -5.328497 -1.502897 Si -4.354775 -1.935866 -1.455098 H 0.157185 -5.377396 -2.033699 O -1.127040 -4.743651 0.104733 H -3.646109 -1.844338 -2.739666 O -3.368054 -1.528148 -0.144633 H -0.919501 -3.173380 -1.966286 O 3.654929 4.392719 0.576132 O 1.384848 5.396933 -0.580999 Si 2.965461 5.667394 -0.285178 Si 4.245481 2.938344 -0.021021 H 4.530952 3.258245 -1.464288 Si 6.901996 -1.784352 -0.814240 O 5.649949 2.169070 0.463651 Si 6.797586 1.396217 -0.509229 H 6.471272 1.630364 -1.948797 O 6.823471 -0.240377 -0.192238 H 8.125848 1.949429 -0.122531 H 3.701096 5.834952 -1.578858 H 3.093300 6.859187 0.598330	

H -5.084285 5.221783 1.506180 H -8.257269 2.142490 1.345578 H -1.931559 5.516428 1.818421 H -6.302209 -4.826838 0.577541 H -2.594594 -6.784089 0.445765 H 2.618532 -5.691919 -0.481339 H 8.331125 -2.097954 -1.108933 H -7.900006 -1.472012 -0.119262 H 5.606098 -5.268134 -0.191911	



Gas phase coordinates	**PCM** coordinates
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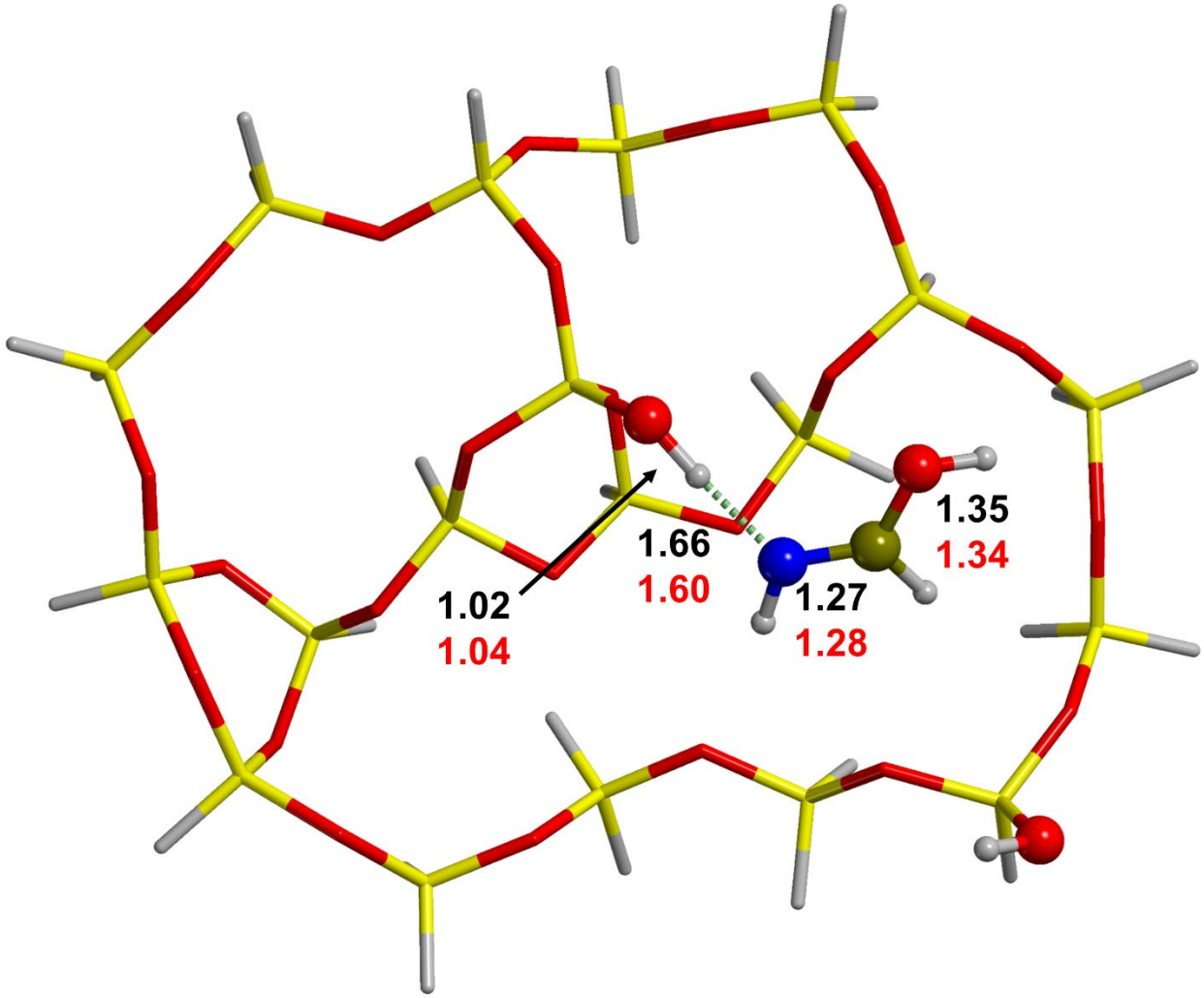
	O 3.254118 0.173057 2.328501 Si -2.291011 -0.259248 -0.316231 O -0.045086 1.535310 -0.525850 H -2.741315 0.574282 -1.465174 Si -4.815830 4.181013 0.432707 O -3.230893 3.744460 0.484115 Si -1.784976 4.476087 0.776859 H -5.118903 4.705319 -0.936934 O -2.069378 0.719208 1.017699 Si -0.633915 1.635610 1.061773 O -1.229536 5.148456 -0.620385 O -0.819556 3.251961 1.352373 H 3.539183 -3.806641 -1.849121 Si 2.835008 -4.182010 -0.580516 O 0.321056 1.109407 2.274064 O 1.807551 -0.314920 -1.096243 Si 0.217661 0.095553 -1.362684 O -0.815967 -0.997824 -0.662490 H -0.056878 0.198530 -2.814827 O 3.814110 -3.678312 0.669996 H 3.300104 0.772419 1.538967 O 1.322520 -3.518607 -0.633239 O -5.741346 -2.382756 0.968861 H 0.302442 3.949854 -2.327429 H -0.004704 6.396371 -2.444212 Si 0.137020 5.210019 -1.547662 O -5.618543 -0.932763 -1.366596 O -6.403768 0.355558 0.875772 H -7.390957 1.822921 -1.029244 Si -7.034581 1.836701 0.423277 O -5.856135 2.950075 0.733814 Si -6.425960 -1.106960 0.105335 Si -5.143384 -3.834471 0.372684 H 6.120588 -1.834994 -1.991057 O -4.827582 -3.494028 -1.257357 H 4.065499 0.433885 -1.841831 Si 2.806693 0.996375 -1.388427 H 2.165688 1.875584 -2.416785 O 3.074981 1.804836 0.087614 O -3.741629 -4.602714 0.866818 Si -0.116773 -4.178799 -1.186495 Si -2.584644 -5.370919 -0.098696 H -2.963105 -5.312712 -1.541865 Si -4.294257 -1.937514 -1.513573 H 0.241717 -5.354689 -2.046446 O -1.061147 -4.728942 0.083048 H -3.561769 -1.826250 -2.774156 O -3.321115 -1.543111 -0.181490 H -0.839310 -3.152711 -1.981954 O 3.700923 4.414295 0.618401 O 1.438694 5.417751 -0.554656 Si 3.016351 5.690116 -0.245112

	Si 4.298887 2.962557 0.022210 H 4.595662 3.286857 -1.417792 Si 6.970026 -1.753414 -0.761853 O 5.700656 2.194379 0.516346 Si 6.857594 1.426134 -0.449139 H 6.542723 1.663621 -1.890707 O 6.883710 -0.211267 -0.136359 H 8.181669 1.980570 -0.050035 H 3.762306 5.862440 -1.532240 H 3.134852 6.879728 0.642626 H -5.047069 5.225864 1.478745 H -8.213277 2.141587 1.283742 H -1.897533 5.525062 1.817708 H -6.239876 -4.822275 0.513033 H -2.527913 -6.772808 0.406491 H 2.690757 -5.669201 -0.474741 H 8.402074 -2.063768 -1.045622 H -7.837709 -1.468315 -0.187847 H 5.675102 -5.241084 -0.159600



Gas phase coordinates	**PCM** coordinates
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O 6.376594 -2.924994 0.326038	O 6.385204 -2.914690 0.324931
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H -0.917333 -3.177081 -1.958149	H -0.908028 -3.175925 -1.960512
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H 2.606705 -5.706922 -0.459206	H 2.619267 -5.701509 -0.462044
H 8.335011 -2.136325 -1.076869	H 8.342732 -2.122751 -1.077363
H -7.896233 -1.445421 -0.133354	H -7.889599 -1.454641 -0.136107
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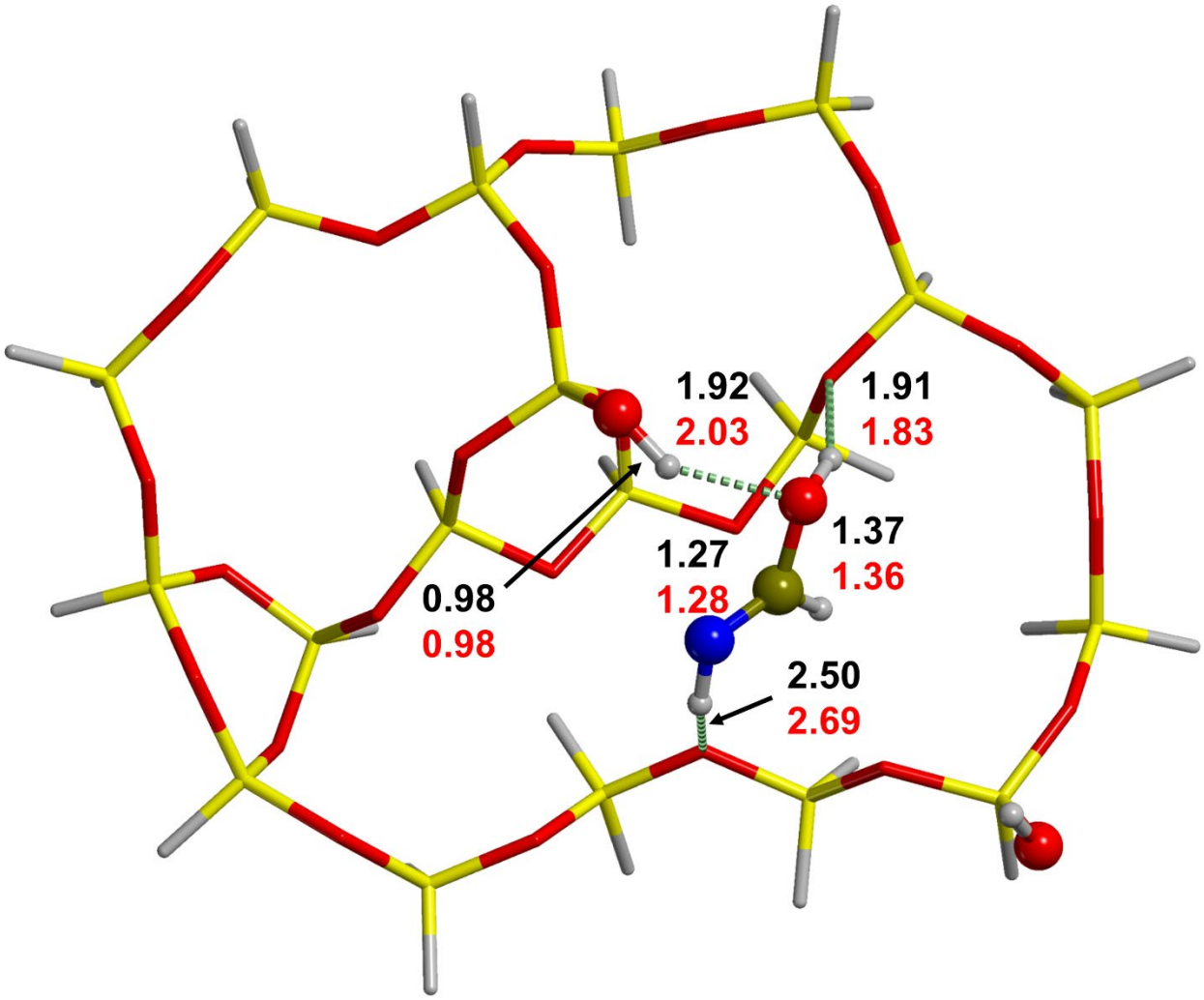

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O 6.465258 -2.842356 0.359389	O 6.455833 -2.838631 0.346818
C 2.309369 -1.148179 1.724640	C 2.660873 -1.054246 1.832477
H 2.936957 -1.434010 0.870529	H 3.411964 -1.385443 1.097644
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Si -4.813023 4.173601 0.399341	Si -4.832573 4.160755 0.420048
O -3.226982 3.741918 0.457573	O -3.245771 3.731337 0.474163
Si -1.784609 4.478178 0.756175	Si -1.803787 4.469407 0.770164
H -5.111916 4.696599 -0.971720	H -5.135412 4.684700 -0.949785
O -2.035913 0.707089 1.008613	O -2.063382 0.693519 1.009087
Si -0.637536 1.641793 1.232403	Si -0.662455 1.636339 1.141398

O -1.225305 5.151741 -0.638882	O -1.248709 5.145198 -0.625503
O -0.851118 3.269277 1.371924	O -0.872881 3.250856 1.394076
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O 1.837212 -0.319161 -1.208910	O 1.809595 -0.294182 -1.152445
Si 0.257341 0.204414 -1.297512	Si 0.236453 0.199669 -1.343710
O -0.799727 -0.949044 -0.774058	O -0.796635 -0.948088 -0.753080
H -0.053527 0.654346 -2.679819	H -0.055978 0.554029 -2.749323
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H 0.003381 6.402931 -2.457880	H -0.026079 6.400024 -2.446076
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O -5.850808 2.939560 0.696408	O -5.867860 2.924896 0.718270
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Si -5.115716 -3.842865 0.340270	Si -5.123679 -3.856082 0.353550
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Si 3.017279 5.706567 -0.245842	Si 2.993960 5.705840 -0.241743
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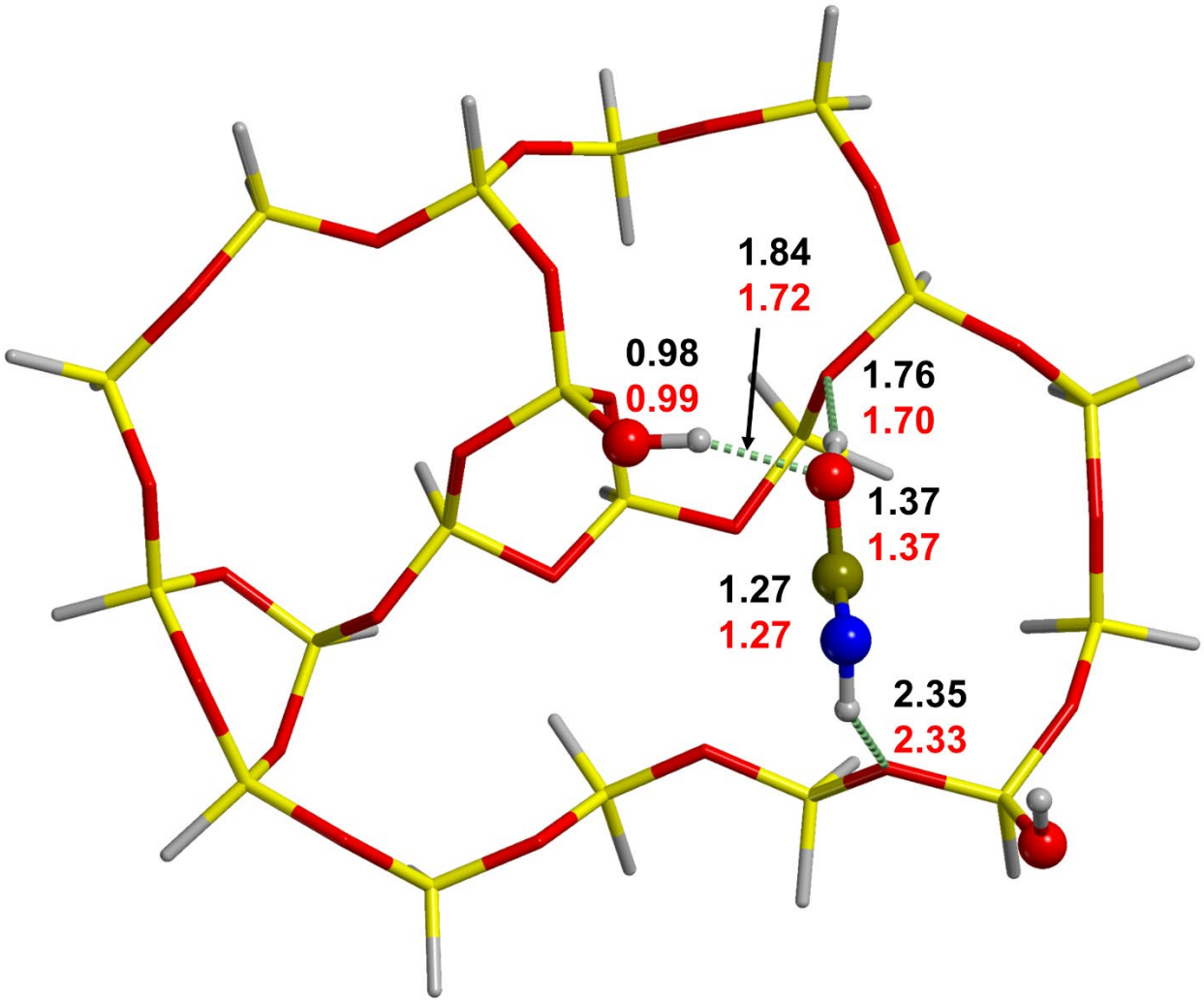

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H 5.668104 -3.905660 2.946263	H 5.819747 -3.893413 2.947023
O 6.445405 -2.810917 0.277095	O 6.452836 -2.810398 0.294323
C 3.048263 -0.939029 2.113057	C 3.043152 -0.950237 2.071691
H 3.080929 -1.184797 1.037719	H 3.561692 -1.166072 1.125224
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H 1.158247 0.895772 2.380227	H 1.133143 0.811670 2.298904
H 3.139135 -2.710097 2.655773	H 2.944178 -2.736989 2.580415

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H 3.538623 -3.763283 -1.901495	H 3.550705 -3.762766 -1.890455
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H 4.029151 0.481464 -1.879243	H 4.042009 0.481914 -1.868217
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Si -0.109926 -4.169130 -1.218184	Si -0.099426 -4.167726 -1.215128
Si -2.560955 -5.386644 -0.120459	Si -2.553122 -5.384481 -0.122519
H -2.948726 -5.325575 -1.561041	H -2.937686 -5.323710 -1.563973
Si -4.315739 -1.962453 -1.507715	Si -4.301415 -1.962663 -1.520544
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O 1.368441 5.437467 -0.554962	O 1.379333 5.438754 -0.551123
Si 2.945690 5.721848 -0.253877	Si 2.955972 5.722905 -0.246610

Si 4.252224 3.004330 -0.006050	Si 4.261422 3.005185 0.004836
H 4.538029 3.336924 -1.446401	H 4.550457 3.337375 -1.434977
Si 6.958641 -1.685721 -0.826383	Si 6.968736 -1.685589 -0.808308
O 5.663974 2.245774 0.476351	O 5.671954 2.246490 0.490522
Si 6.821396 1.491367 -0.499495	Si 6.831388 1.491607 -0.482550
H 6.495665 1.732282 -1.938076	H 6.508891 1.732214 -1.921911
O 6.863202 -0.147023 -0.193833	O 6.872197 -0.146707 -0.176371
H 8.143144 2.055334 -0.106088	H 8.152367 2.055424 -0.086363
H 3.682175 5.905889 -1.544798	H 3.695347 5.906467 -1.535949
H 3.059507 6.908680 0.638155	H 3.068041 6.909950 0.645354
H -5.102913 5.182221 1.517035	H -5.096643 5.185302 1.506598
H -8.244133 2.072124 1.328186	H -8.238044 2.075767 1.311589
H -1.954120 5.506639 1.838081	H -1.948491 5.509190 1.834528
H -6.216869 -4.871512 0.515855	H -6.210334 -4.868469 0.505557
H -2.489313 -6.790115 0.378401	H -2.482858 -6.787835 0.376861
H 2.716391 -5.638724 -0.529881	H 2.725070 -5.637689 -0.520182
H 8.391496 -1.982778 -1.120188	H 8.402181 -1.983000 -1.098858
H -7.847186 -1.528250 -0.161017	H -7.838493 -1.525069 -0.175794
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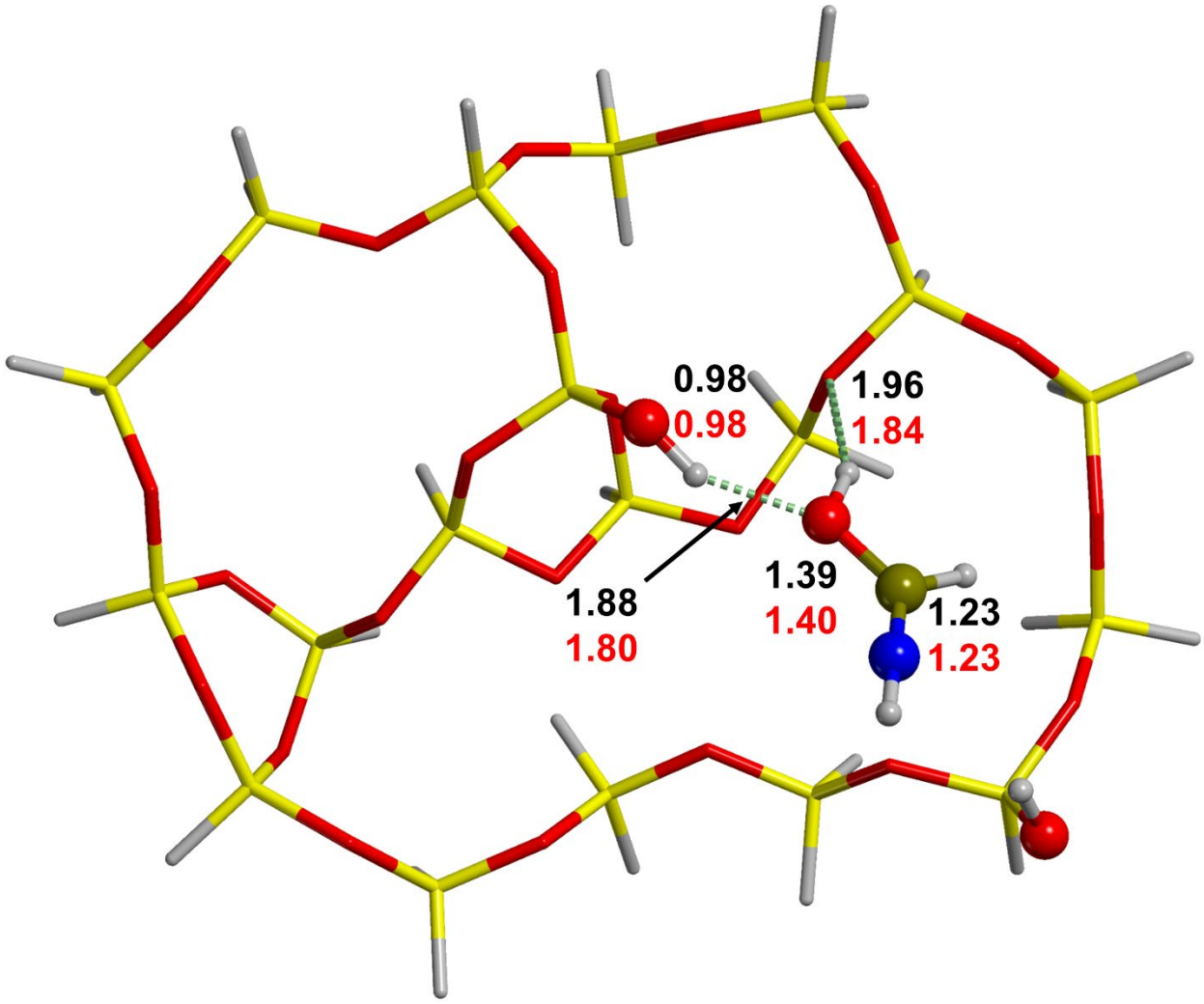

Gas phase coordinates	**PCM** coordinates

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H 5.392166 -3.770810 2.827213	H 5.426973 -3.847457 2.870412
O 6.439867 -2.749414 0.223221	O 6.434802 -2.774841 0.230073
C 3.832981 -1.088793 2.418923	C 3.791943 -0.963254 2.373362
H 4.747292 -0.919763 1.813346	H 4.623571 -0.888755 1.644619
N 3.674635 -1.964076 3.265648	N 3.677844 -1.778246 3.285328
H 1.074477 0.453358 2.155180	H 1.122062 0.546346 2.156729
H 3.546392 -2.672958 3.951396	H 3.623103 -2.484180 3.987528
O 2.848644 -0.159968 2.095134	O 2.844881 0.034664 2.134637
Si -2.325432 -0.269690 -0.301948	Si -2.327337 -0.274368 -0.313683
O -0.065702 1.549621 -0.552663	O -0.066395 1.538070 -0.535801
H -2.817977 0.556411 -1.450356	H -2.812394 0.555319 -1.454095
Si -4.930432 4.110805 0.503575	Si -4.914863 4.120205 0.491474
O -3.337973 3.700360 0.533197	O -3.323661 3.705024 0.522583
Si -1.901222 4.453531 0.816330	Si -1.884753 4.454459 0.804674
H -5.257744 4.642212 -0.857727	H -5.240053 4.649706 -0.871079
O -2.043287 0.696245 1.022436	O -2.076705 0.700222 1.021783
Si -0.631755 1.640136 1.046168	Si -0.653253 1.628490 1.042465
O -1.372933 5.147455 -0.580837	O -1.353843 5.143820 -0.593756
O -0.899191 3.239567 1.342153	O -0.893522 3.232102 1.356331
H 3.529670 -3.715239 -1.944864	H 3.522532 -3.736487 -1.937085
Si 2.846357 -4.113679 -0.671924	Si 2.837537 -4.130162 -0.663568
O 0.393654 1.156639 2.220263	O 0.306739 1.089997 2.261232
O 1.765812 -0.282687 -1.175875	O 1.766325 -0.290751 -1.158560
Si 0.164092 0.109907 -1.392344	Si 0.169595 0.102020 -1.395354
O -0.858342 -0.995565 -0.713514	O -0.850590 -0.995662 -0.687216
H -0.143218 0.237689 -2.833466	H -0.138081 0.225601 -2.835492
O 3.831045 -3.605081 0.572248	O 3.823279 -3.621896 0.579903
H 3.179150 0.478839 1.422772	H 3.129402 0.612923 1.383252
O 1.322502 -3.475245 -0.701552	O 1.315624 -3.487202 -0.695139
O -5.740563 -2.472059 0.990074	O -5.745028 -2.459140 0.991620
H 0.159231 3.989993 -2.315860	H 0.175485 3.978066 -2.325729
H -0.189847 6.431980 -2.406818	H -0.166193 6.420896 -2.421999
Si -0.018227 5.240179 -1.522797	Si 0.001496 5.230462 -1.535386
O -5.667635 -0.996717 -1.332370	O -5.664305 -0.989641 -1.332591
O -6.449424 0.255518 0.929459	O -6.445637 0.270427 0.924946
H -7.482481 1.723162 -0.950861	H -7.473547 1.737185 -0.958882
Si -7.109877 1.729897 0.497632	Si -7.101476 1.745871 0.489737
O -5.946640 2.859998 0.805079	O -5.934954 2.873111 0.795237
Si -6.456070 -1.200210 0.145991	Si -6.456374 -1.186934 0.144564
Si -5.125379 -3.908176 0.373985	Si -5.133941 -3.898409 0.378817
H 6.076182 -1.699528 -2.097737	H 6.075168 -1.728791 -2.093247
O -4.825682 -3.541966 -1.254992	O -4.834204 -3.538061 -1.249549
H 3.985503 0.533242 -1.904707	H 3.991159 0.510676 -1.905762
Si 2.719735 1.064739 -1.430570	Si 2.732136 1.051330 -1.441675
H 2.055567 1.948057 -2.445093	H 2.065704 1.930152 -2.449895
O 3.007111 1.860519 0.037813	O 3.002495 1.852719 0.034692
O -3.705514 -4.657260 0.845297	O -3.716521 -4.650769 0.852266
Si -0.111805 -4.154412 -1.244631	Si -0.120517 -4.163193 -1.237332

Si -2.546980 -5.397333 -0.140130	Si -2.559851 -5.396420 -0.131140
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Si -4.325809 -1.973234 -1.493707	Si -4.325940 -1.972173 -1.498878
H 0.256372 -5.316408 -2.119254	H 0.244486 -5.328147 -2.109347
O -1.032393 -4.731613 0.030356	O -1.043327 -4.734908 0.038519
H -3.613268 -1.845695 -2.771945	H -3.614420 -1.847177 -2.770894
O -3.341450 -1.564770 -0.179345	O -3.344306 -1.567803 -0.173431
H -0.860304 -3.133483 -2.022526	H -0.865638 -3.141665 -2.017679
O 3.582827 4.484814 0.595745	O 3.599449 4.468743 0.586146
O 1.291031 5.460756 -0.542615	O 1.311040 5.449171 -0.555167
Si 2.867362 5.756689 -0.248329	Si 2.888144 5.740974 -0.260900
Si 4.198017 3.048684 -0.020367	Si 4.210540 3.029459 -0.026680
H 4.472951 3.390767 -1.460586	H 4.487052 3.367656 -1.467515
Si 6.938072 -1.614743 -0.877446	Si 6.936846 -1.644016 -0.872805
O 5.617890 2.299655 0.450957	O 5.627968 2.277155 0.446782
Si 6.776378 1.559537 -0.534441	Si 6.784594 1.531458 -0.536596
H 6.441218 1.804622 -1.970150	H 6.450721 1.774505 -1.972952
O 6.833264 -0.079933 -0.236959	O 6.836422 -0.107541 -0.235615
H 8.095509 2.132447 -0.145177	H 8.105298 2.101213 -0.148037
H 3.595653 5.952978 -1.542124	H 3.617517 5.932320 -1.554827
H 2.976169 6.940121 0.648858	H 3.000178 6.925974 0.633816
H -5.167087 5.142242 1.561649	H -5.148811 5.154593 1.547266
H -8.283608 2.007314 1.374030	H -8.274699 2.028684 1.365091
H -2.019301 5.491006 1.867948	H -2.000105 5.494515 1.854043
H -6.203629 -4.915399 0.517594	H -6.215279 -4.902070 0.524144
H -2.461212 -6.802546 0.351556	H -2.478507 -6.800839 0.363559
H 2.728046 -5.603952 -0.578100	H 2.714695 -5.619870 -0.566629
H 8.371768 -1.898569 -1.180104	H 8.369794 -1.932804 -1.174305
H -7.864864 -1.582486 -0.134616	H -7.866207 -1.565555 -0.135776
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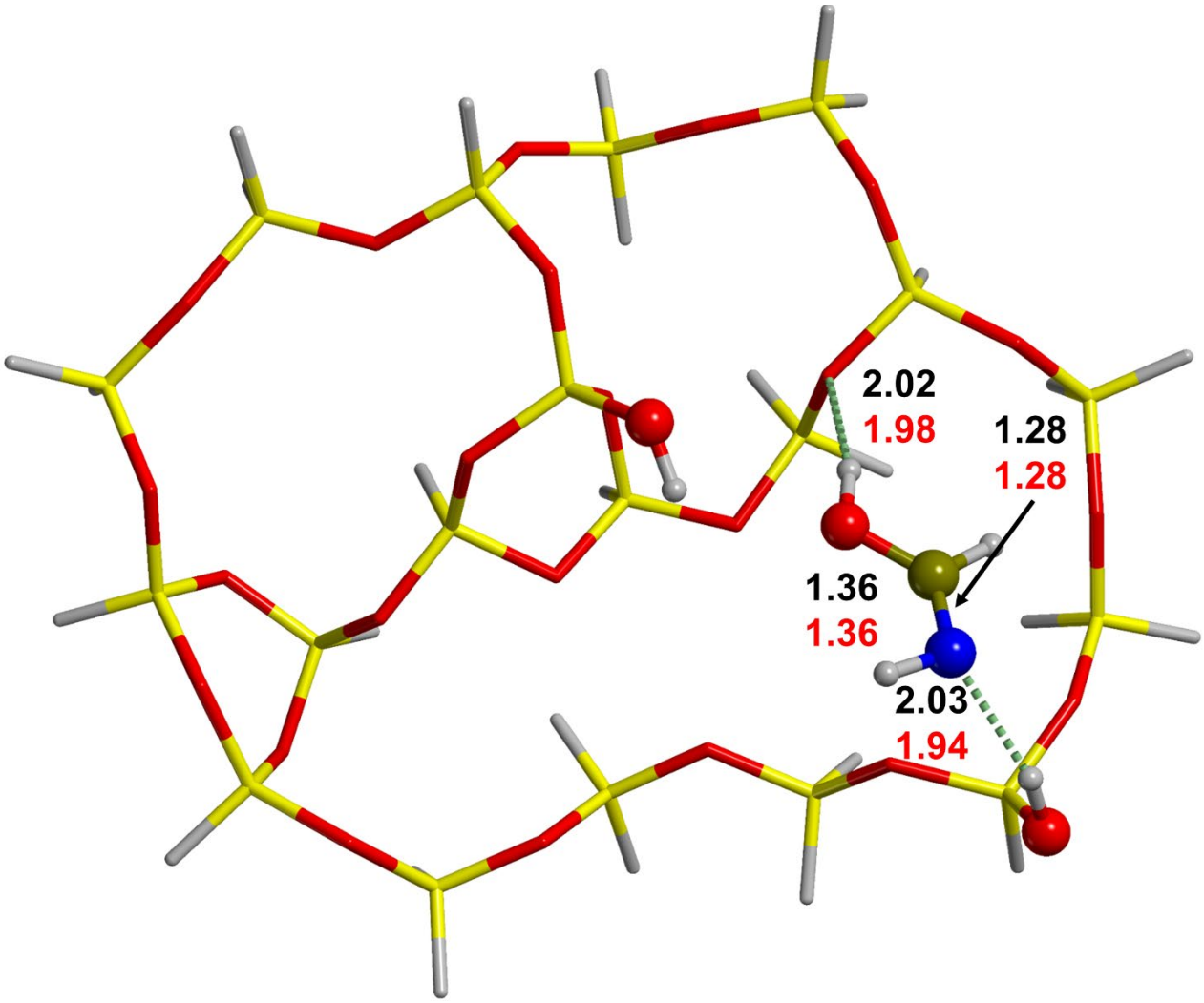

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H 5.512593 -3.628262 2.770634	H 5.453225 -3.544677 2.742948
O 6.426575 -2.740815 0.218118	O 6.419680 -2.752224 0.214436
C 4.263065 -0.918942 2.301202	C 4.329466 -0.925076 2.251337
H 5.106883 -0.524668 1.718337	H 5.118272 -0.649061 1.539925
N 4.420771 -1.935209 3.050322	N 4.509037 -1.885977 3.073619
H 0.777100 0.235779 2.102798	H 0.758847 0.242872 2.100781
H 3.536702 -2.194990 3.509899	H 3.677278 -2.031605 3.663125
O 3.084868 -0.253677 2.146993	O 3.192734 -0.190106 2.178016
Si -2.348526 -0.284307 -0.292493	Si -2.349449 -0.287252 -0.302066
O -0.148482 1.573875 -0.594290	O -0.151660 1.564437 -0.582513
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O -3.362325 3.691401 0.543497	O -3.360079 3.693822 0.540971
Si -1.926275 4.447579 0.822134	Si -1.922814 4.448206 0.818211
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O -2.063106 0.679426 1.039901	O -2.079158 0.676678 1.043760
Si -0.673096 1.647999 1.014908	Si -0.686254 1.643158 1.012655

O -1.402672 5.140632 -0.577226	O -1.399081 5.139519 -0.581960
O -0.915368 3.237508 1.355459	O -0.916577 3.233592 1.368189
H 3.512882 -3.714834 -1.941591	H 3.503355 -3.723751 -1.942840
Si 2.833410 -4.112851 -0.666465	Si 2.824087 -4.119904 -0.667024
O 0.444947 1.149353 2.115878	O 0.410816 1.149909 2.149493
O 1.730137 -0.261621 -1.140158	O 1.727914 -0.265707 -1.131271
Si 0.132995 0.117404 -1.390649	Si 0.134233 0.112338 -1.397078
O -0.870922 -0.993913 -0.690343	O -0.868537 -0.995722 -0.678443
H -0.169424 0.230174 -2.826409	H -0.173991 0.225730 -2.828326
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H 3.183270 0.503778 1.525936	H 3.263429 0.503762 1.478150
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O -5.752439 -2.484813 1.014328	O -5.758491 -2.478722 1.017683
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H -0.226404 6.424924 -2.407771	H -0.222118 6.420854 -2.414130
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Si -5.136118 -3.920607 0.398625	Si -5.144531 -3.915816 0.402652
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O -4.844949 -3.557894 -1.233154	O -4.852308 -3.555012 -1.227029
H 3.960999 0.534526 -1.908116	H 3.957394 0.525005 -1.912703
Si 2.698546 1.069496 -1.422779	Si 2.701130 1.067607 -1.430749
H 2.027152 1.945084 -2.445646	H 2.025189 1.937860 -2.450104
O 2.986016 1.862025 0.046979	O 2.982542 1.852379 0.050486
O -3.713733 -4.666462 0.867452	O -3.722906 -4.663308 0.871175
Si -0.126060 -4.159770 -1.231898	Si -0.135780 -4.163117 -1.230668
Si -2.556247 -5.405703 -0.119828	Si -2.567034 -5.404869 -0.116256
H -2.955647 -5.343540 -1.557178	H -2.967200 -5.343189 -1.553415
Si -4.347877 -1.990850 -1.476566	Si -4.349723 -1.988129 -1.478177
H 0.242120 -5.322237 -2.105892	H 0.230265 -5.326726 -2.104040
O -1.042475 -4.736980 0.046087	O -1.052236 -4.738132 0.048277
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H -0.878330 -3.141240 -2.009301	H -0.887096 -3.144105 -2.008360
O 3.557153 4.488640 0.588127	O 3.560526 4.481476 0.580922
O 1.260799 5.458875 -0.545915	O 1.264848 5.454083 -0.552460
Si 2.837294 5.758087 -0.255866	Si 2.841929 5.751313 -0.263561
Si 4.173478 3.052832 -0.027601	Si 4.174490 3.044369 -0.034134
H 4.444271 3.393524 -1.468936	H 4.444899 3.383645 -1.475874
Si 6.920008 -1.606681 -0.885248	Si 6.914033 -1.619573 -0.890042
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Si 6.753314 1.567745 -0.546011	Si 6.751951 1.555326 -0.553001
H 6.414204 1.810326 -1.981219	H 6.412326 1.797341 -1.988182
O 6.813940 -0.071224 -0.246520	O 6.810477 -0.083511 -0.252361
H 8.072334 2.143587 -0.160720	H 8.071998 2.129612 -0.168908
H 3.562068 5.954009 -1.551691	H 3.566205 5.945293 -1.559958
H 2.946112 6.942897 0.639501	H 2.952925 6.936616 0.630884

H -5.191575 5.131274 1.574517	H -5.186714 5.136979 1.572036
H -8.302773 1.990387 1.398615	H -8.302377 2.000293 1.400249
H -2.043698 5.486219 1.872676	H -2.038171 5.487764 1.868070
H -6.212160 -4.929619 0.546184	H -6.221887 -4.923224 0.551578
H -2.466696 -6.810109 0.373490	H -2.479141 -6.809042 0.378022
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H -7.881107 -1.600621 -0.106340	H -7.886593 -1.592383 -0.102360
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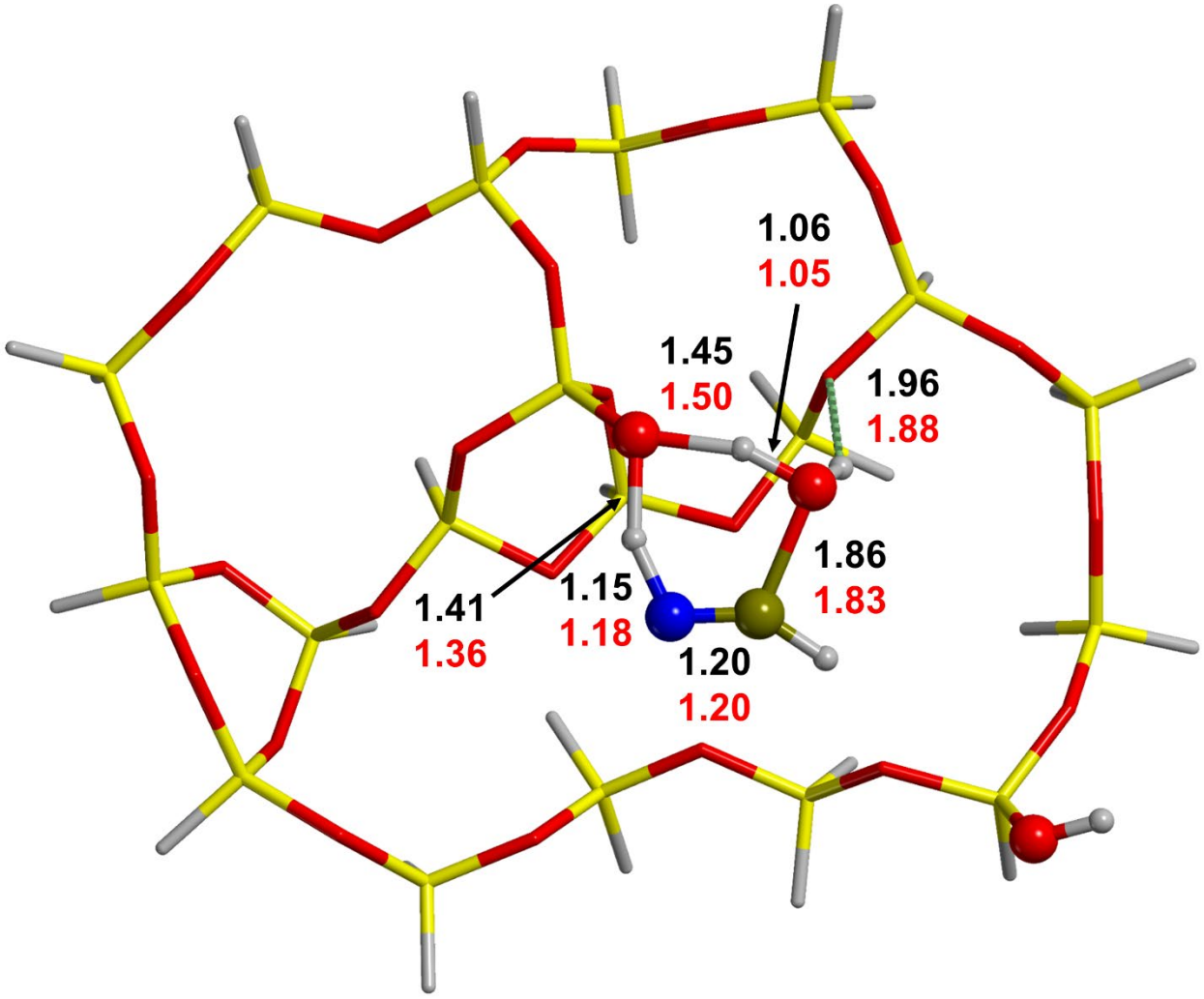

Gas phase coordinates	**PCM** coordinates
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O 6.460707 -2.875687 0.341771	O 6.457166 -2.884179 0.341584
C 2.033377 -1.477591 2.269473	C 2.119807 -1.382346 2.260781
H 2.933109 -2.082191 2.203833	H 3.037866 -1.955857 2.157634
N 0.837329 -1.515196 2.313136	N 0.924356 -1.461874 2.331841
H 1.810340 0.743436 2.317811	H 1.840537 0.814509 2.326889
H 0.349090 -0.468477 2.277896	H 0.407890 -0.402930 2.300755

O 2.743626 0.234336 2.384523	O 2.769001 0.328939 2.377495
Si -2.273205 -0.235277 -0.311990	Si -2.271976 -0.243662 -0.323284
O -0.026421 1.573061 -0.566078	O -0.043803 1.560454 -0.552269
H -2.712399 0.586765 -1.475519	H -2.713278 0.584346 -1.477554
Si -4.785713 4.190806 0.428763	Si -4.783173 4.192043 0.423523
O -3.201516 3.751796 0.482195	O -3.199344 3.751726 0.477118
Si -1.755207 4.480572 0.780121	Si -1.752359 4.479556 0.774077
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O -1.195832 5.156181 -0.613917	O -1.192644 5.153308 -0.620723
O -0.780492 3.257527 1.341861	O -0.788214 3.249334 1.356280
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Si 2.855227 -4.180189 -0.593432	Si 2.850410 -4.186510 -0.591713
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O 1.825999 -0.307658 -1.101453	O 1.821947 -0.303541 -1.086779
Si 0.230516 0.120590 -1.361275	Si 0.234851 0.113887 -1.367943
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H -0.025696 0.211153 -2.820681	H -0.027129 0.205101 -2.822804
O 3.832344 -3.681826 0.660810	O 3.828168 -3.687747 0.661869
H 3.183251 0.501243 1.546065	H 3.190275 0.603647 1.525716
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H 0.034621 6.407788 -2.431436	H 0.038569 6.402063 -2.439687
Si 0.172759 5.218557 -1.538137	Si 0.175841 5.213596 -1.545238
O -5.597863 -0.917651 -1.390737	O -5.595274 -0.916336 -1.388112
O -6.380082 0.366345 0.857069	O -6.380748 0.369374 0.855878
H -7.361158 1.840813 -1.045619	H -7.360886 1.842805 -1.048097
Si -7.007812 1.849743 0.407679	Si -7.007283 1.852867 0.405132
O -5.828419 2.960481 0.724010	O -5.826883 2.962905 0.720163
Si -6.402760 -1.093833 0.082229	Si -6.404812 -1.091547 0.082485
Si -5.124676 -3.823980 0.344122	Si -5.129024 -3.822530 0.346855
H 6.147107 -1.833739 -1.990044	H 6.144060 -1.844264 -1.991204
O -4.802135 -3.477537 -1.285217	O -4.807739 -3.478003 -1.281160
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Si 2.826301 0.996051 -1.384011	Si 2.834268 0.994053 -1.392366
H 2.198454 1.883808 -2.412972	H 2.198525 1.876249 -2.417127
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O -3.725067 -4.595719 0.838889	O -3.729992 -4.594980 0.842143
Si -0.095297 -4.170907 -1.205549	Si -0.100211 -4.175301 -1.203333
Si -2.567161 -5.362707 -0.126491	Si -2.572910 -5.363914 -0.122676
H -2.942507 -5.299651 -1.570271	H -2.948451 -5.301962 -1.566454
Si -4.270467 -1.918513 -1.527638	Si -4.270237 -1.921450 -1.532189
H 0.263305 -5.344753 -2.068247	H 0.257235 -5.350306 -2.064934
O -1.043124 -4.723469 0.060364	O -1.048294 -4.725800 0.063286
H -3.533561 -1.808664 -2.793398	H -3.536721 -1.811678 -2.792926
O -3.300114 -1.525152 -0.203197	O -3.302600 -1.529803 -0.196470
H -0.814689 -3.141419 -1.999464	H -0.818856 -3.145980 -1.998142
O 3.730956 4.411227 0.633002	O 3.733718 4.405359 0.626087
O 1.472642 5.421446 -0.541792	O 1.476069 5.416355 -0.549317
Si 3.050034 5.690608 -0.228130	Si 3.053744 5.684473 -0.236191

Si 4.328083 2.960422 0.033731	Si 4.329497 2.953451 0.028147
H 4.628344 3.288577 -1.404672	H 4.629792 3.279928 -1.410631
Si 6.994071 -1.757037 -0.758817	Si 6.991300 -1.767073 -0.760199
O 5.727702 2.188739 0.528508	O 5.728538 2.181057 0.523447
Si 6.885561 1.421707 -0.436842	Si 6.885573 1.412078 -0.441344
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H 3.798937 5.865694 -1.513172	H 3.802577 5.857647 -1.521533
H 3.168384 6.877394 0.663402	H 3.173266 6.872036 0.654149
H -5.017646 5.232867 1.477430	H -5.014031 5.235336 1.471201
H -8.187872 2.153764 1.266580	H -8.186934 2.158748 1.263934
H -1.868397 5.526484 1.823888	H -1.864472 5.526594 1.816830
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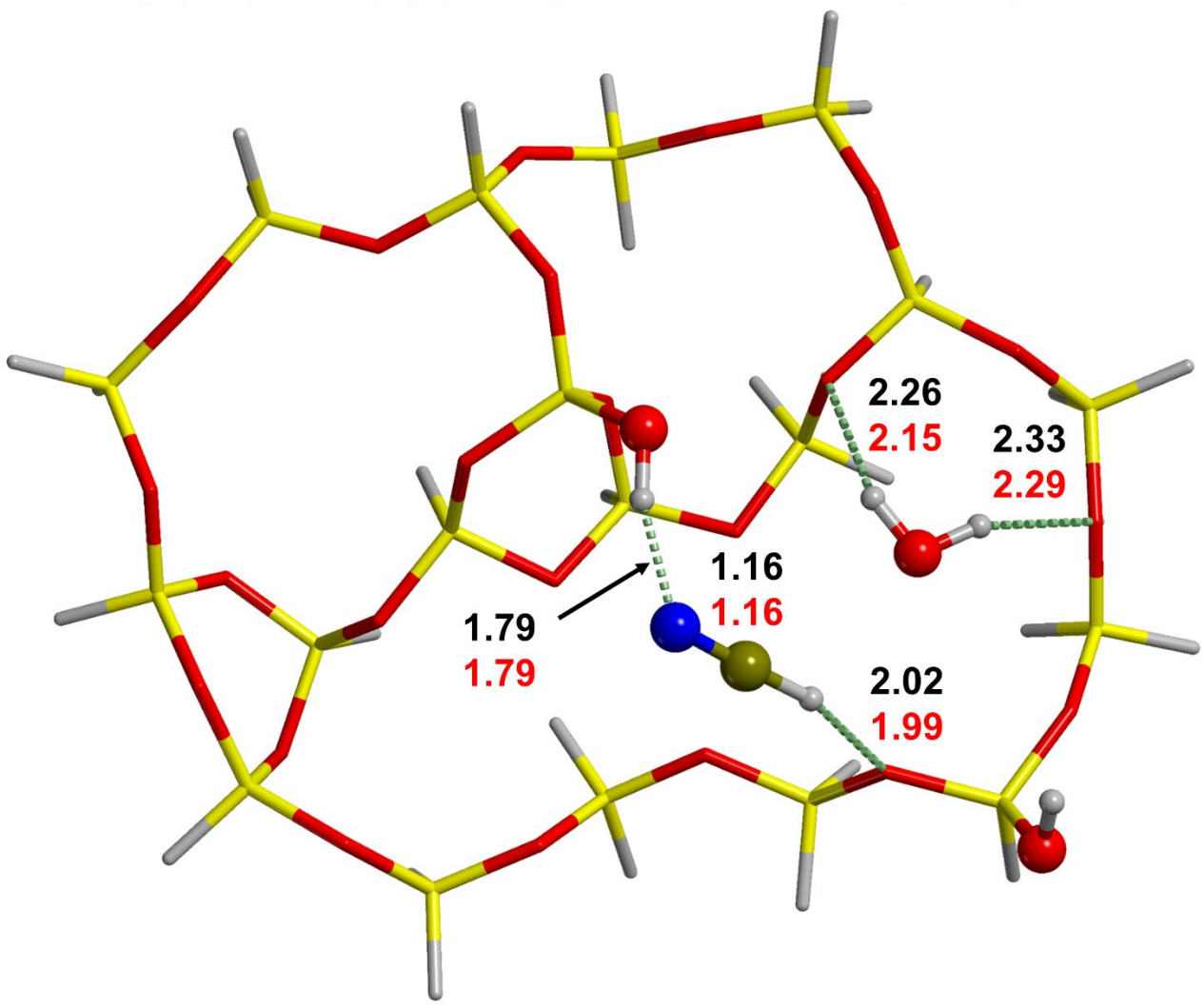
H -7.814409 -1.452271 -0.214994	H -7.816819 -1.449067 -0.214143
H 5.692857 -5.244610 -0.169685	H 5.687196 -5.252945 -0.167399



Gas phase coordinates	**PCM** coordinates

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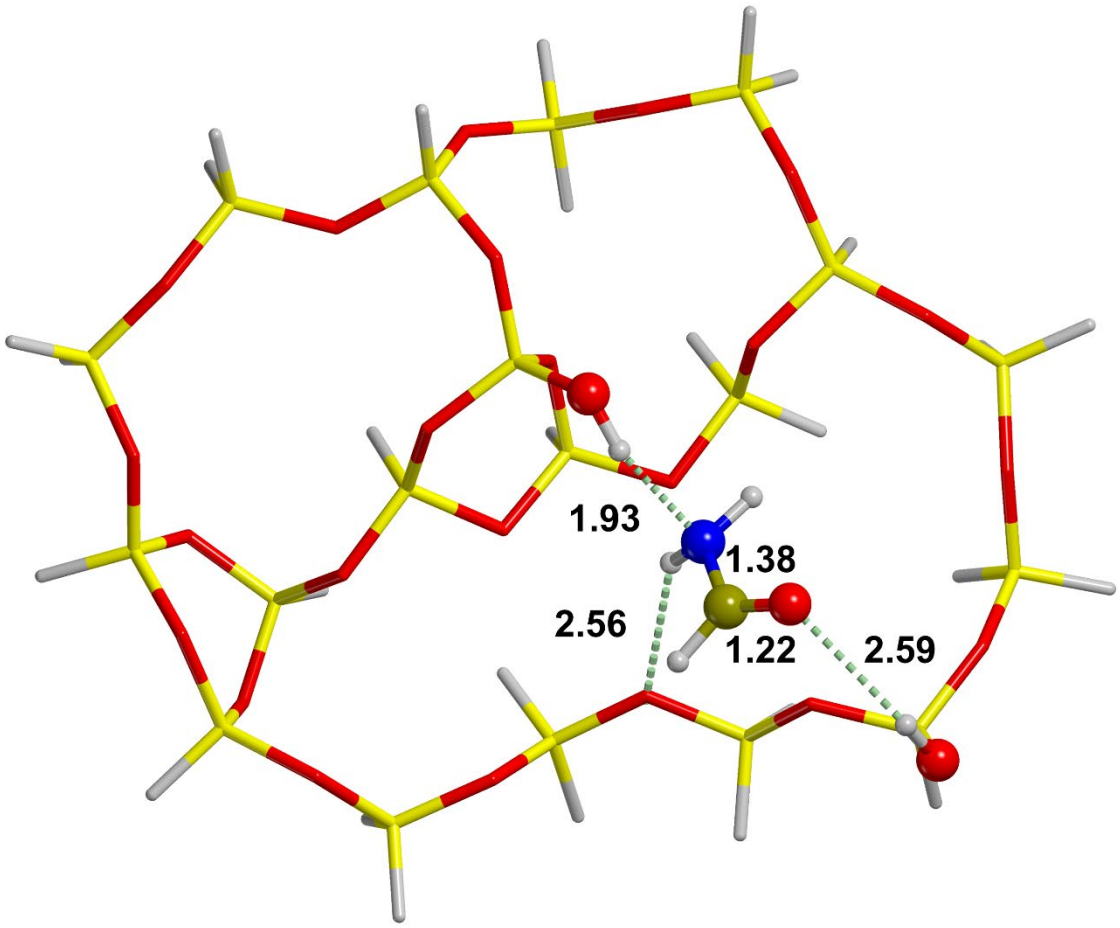
O 5.811258 -4.548096 2.281140	O 5.804494 -4.566597 2.268261
H 5.861345 -3.855468 2.959295	H 5.748742 -3.900773 2.974653
O 6.458199 -2.789251 0.334119	O 6.454247 -2.792793 0.319983
C 1.811036 -2.072566 2.320432	C 1.910321 -2.071723 2.352695
H 2.713628 -2.535422 1.932528	H 2.797476 -2.579335 1.979454
N 0.855028 -1.535712 2.693678	N 0.958202 -1.512641 2.703798
H 3.588093 0.201725 1.513657	H 3.791669 0.341296 1.414659
H 0.408457 0.177993 2.432610	H 0.454542 0.178391 2.396156
O 4.197788 -0.556461 1.578198	O 4.285814 -0.412929 1.789591
Si -2.285195 -0.246777 -0.308233	Si -2.289360 -0.254080 -0.321736
O -0.068705 1.587551 -0.555292	O -0.077517 1.577204 -0.545734
H -2.751027 0.587974 -1.460743	H -2.756259 0.586923 -1.462548
Si -4.860154 4.160800 0.462931	Si -4.861521 4.160923 0.463198
O -3.271500 3.737821 0.513299	O -3.272930 3.737456 0.511420
Si -1.832581 4.479888 0.814175	Si -1.833337 4.479085 0.810045
H -5.160795 4.693518 -0.902913	H -5.163928 4.693379 -0.902339
O -2.030734 0.713149 1.028736	O -2.048328 0.702596 1.032128
Si -0.623284 1.662611 1.049903	Si -0.643638 1.656727 1.043419
O -1.280974 5.168291 -0.576698	O -1.283490 5.167000 -0.581777
O -0.840903 3.266345 1.355705	O -0.846512 3.260220 1.368080
H 3.568455 -3.734137 -1.870246	H 3.561225 -3.737312 -1.879980
Si 2.865773 -4.125955 -0.605826	Si 2.860237 -4.128596 -0.614476
O 0.435334 1.134330 2.178779	O 0.387673 1.149897 2.218745
O 1.802944 -0.268222 -1.105530	O 1.799716 -0.264375 -1.094979
Si 0.213927 0.141291 -1.363248	Si 0.212964 0.134802 -1.372934
O -0.815466 -0.972417 -0.699891	O -0.810810 -0.973774 -0.682071
H -0.066465 0.256772 -2.809139	H -0.073713 0.254485 -2.814705
O 3.838439 -3.623959 0.650427	O 3.834888 -3.626595 0.640288
H 5.065581 -0.182343 1.346666	H 5.158720 -0.350780 1.359947
O 1.347515 -3.475536 -0.655514	O 1.342102 -3.477700 -0.662144
O -5.728476 -2.414997 0.944629	O -5.731257 -2.414473 0.947812
H 0.259080 3.997067 -2.290957	H 0.253733 3.994841 -2.297935
H -0.069485 6.441646 -2.388462	H -0.074179 6.439496 -2.395594
Si 0.086373 5.249417 -1.501305	Si 0.082560 5.247447 -1.508369
O -5.615850 -0.944255 -1.379044	O -5.617611 -0.944004 -1.374205
O -6.414911 0.318033 0.872607	O -6.416925 0.318741 0.876069
H -7.412171 1.791994 -1.022043	H -7.416409 1.792553 -1.017523
Si -7.058101 1.797168 0.431097	Si -7.060255 1.797989 0.435110
O -5.889996 2.918343 0.752459	O -5.891345 2.918860 0.754518
Si -6.423037 -1.138344 0.090361	Si -6.426625 -1.137824 0.094217
Si -5.116828 -3.856512 0.337695	Si -5.120937 -3.856351 0.340360
H 6.132576 -1.738744 -1.992200	H 6.125960 -1.742716 -2.006145
O -4.797497 -3.497741 -1.289526	O -4.805215 -3.498740 -1.285828
H 4.057316 0.510648 -1.827874	H 4.051605 0.507410 -1.839455
Si 2.790769 1.056153 -1.354189	Si 2.791274 1.060334 -1.371356
H 2.145751 1.935144 -2.394179	H 2.139479 1.932180 -2.403184
O 3.048021 1.880763 0.093084	O 3.048555 1.864166 0.096261
O -3.709084 -4.616335 0.827799	O -3.712742 -4.616485 0.828655
Si -0.085043 -4.143875 -1.216345	Si -0.091458 -4.145716 -1.220773

Si -2.543917 -5.366475 -0.142073	Si -2.549202 -5.367265 -0.142670
H -2.920719 -5.299941 -1.585317	H -2.928036 -5.300965 -1.585403
Si -4.281098 -1.933180 -1.523865	Si -4.284966 -1.935978 -1.528877
H 0.285101 -5.309576 -2.085191	H 0.277061 -5.311757 -2.089847
O -1.026418 -4.712570 0.047234	O -1.031219 -4.713785 0.044285
H -3.548297 -1.809038 -2.790361	H -3.556237 -1.810166 -2.790447
O -3.308421 -1.537996 -0.199237	O -3.313130 -1.542909 -0.193595
H -0.815427 -3.117809 -2.004637	H -0.822645 -3.119623 -2.008279
O 3.653921 4.467661 0.663841	O 3.652920 4.465106 0.651810
O 1.384675 5.460584 -0.504620	O 1.382346 5.458442 -0.513576
Si 2.959402 5.744340 -0.190415	Si 2.957617 5.741773 -0.201690
Si 4.265571 3.026132 0.056883	Si 4.263105 3.023322 0.044493
H 4.566578 3.369704 -1.379964	H 4.562370 3.366217 -1.392910
Si 6.979414 -1.659601 -0.761041	Si 6.974135 -1.663665 -0.776102
O 5.673326 2.266366 0.547001	O 5.671416 2.263180 0.532785
Si 6.838448 1.516182 -0.422843	Si 6.835353 1.512280 -0.438556
H 6.523646 1.762537 -1.862938	H 6.518149 1.758365 -1.878269
O 6.878555 -0.123400 -0.123258	O 6.874926 -0.127180 -0.139051
H 8.156976 2.079030 -0.017201	H 8.154186 2.074857 -0.034938
H 3.705727 5.933638 -1.474941	H 3.702167 5.930497 -1.487323
H 3.066065 6.927733 0.707081	H 3.065942 6.925349 0.695352
H -5.097172 5.195122 1.517000	H -5.096690 5.195574 1.517347
H -8.240728 2.084682 1.292151	H -8.241567 2.086094 1.297772
H -1.950856 5.514286 1.868276	H -1.949778 5.513834 1.864050
H -6.204760 -4.855055 0.468338	H -6.208996 -4.854499 0.472819
H -2.475563 -6.771851 0.351869	H -2.480591 -6.772526 0.351515
H 2.734487 -5.615156 -0.512252	H 2.728596 -5.617715 -0.520327
H 8.414580 -1.955027 -1.045064	H 8.409138 -1.959600 -1.062023
H -7.831100 -1.509752 -0.207942	H -7.835230 -1.508849 -0.201991
H 5.714427 -5.163306 -0.188978	H 5.709152 -5.166744 -0.201445

Figure S7: PBE-D2/TZVP optimized geometries for the formamide dehydration reaction catalysed by hydrophobic silica. In the figures the most representative bond lengths (in Å) in gas phase (black) and in PCM (F) (red) are reported. In the left and the right columns the cartesian coordinates of the optimized structures in gas phase and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue, silicons in yellow.

Formamide + Silica 1.5 decarbonylation reaction



Gas phase coordinates	**PCM (F)** coordinates
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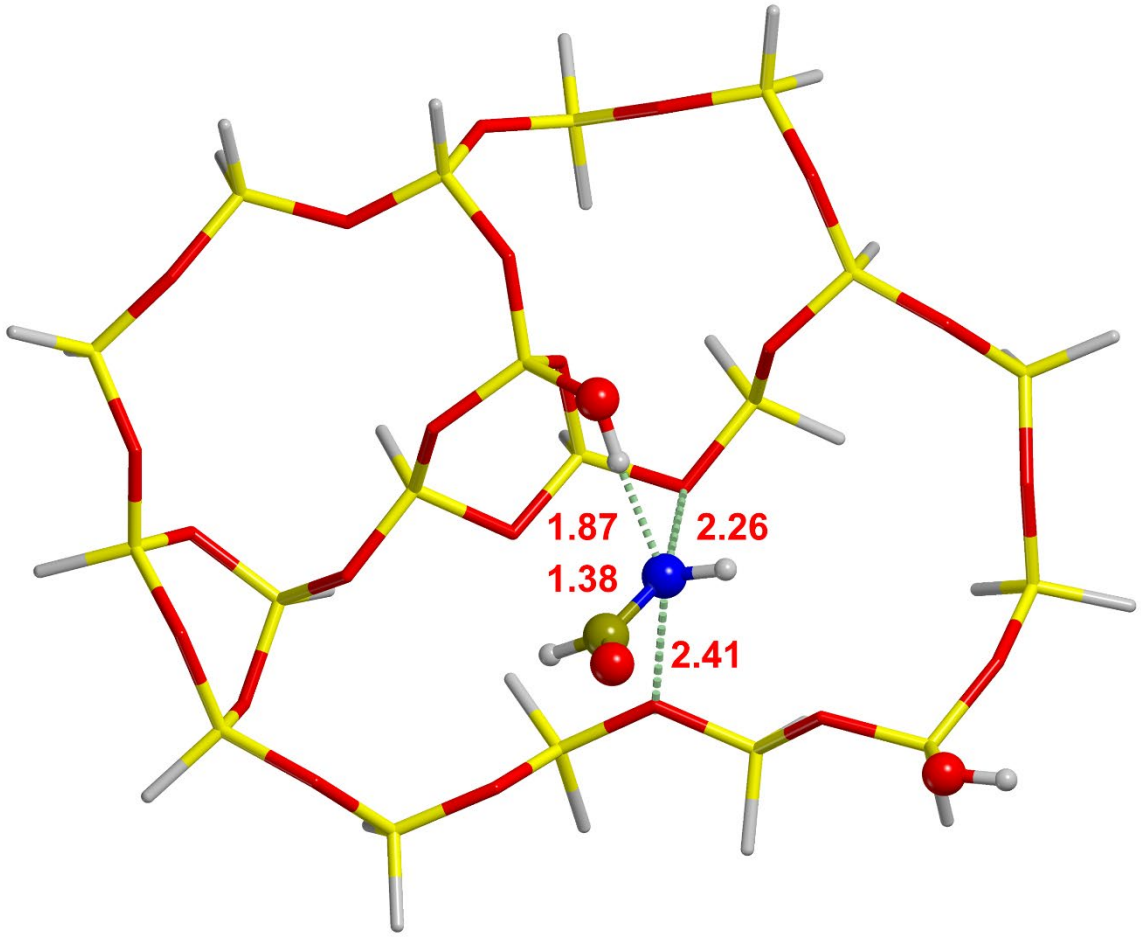
O -0.8957140349 3.2423082771 1.3895521124 H 3.6139069651 -3.6480967229 -1.9555028876 Si 2.9264009651 -4.0619857229 -0.6897728876 O 0.5107749651 1.1672622771 2.1342751124 O 1.7755989651 -0.1816147229 -1.2087618876 Si 0.2015739651 0.2882032771 -1.5024298876 O -0.7817650349 -0.9028117229 -0.9007248876 H -0.0427000349 0.5739272771 -2.9371248876 O 3.9005219651 -3.5568597229 0.5640961124 H 0.9835569651 0.3054812771 2.0396771124 O 1.3982249651 -3.4341257229 -0.7226258876 O -5.6810720349 -2.4951017229 0.9376841124 H 0.1907999651 4.0359352771 -2.2812418876 H -0.1751460349 6.4760662771 -2.3538268876 Si 0.0000379651 5.2781252771 -1.4788308876 O -5.5798450349 -0.9955647229 -1.3557758876 O -6.4089900349 0.2278012771 0.8957991124 H -7.4420280349 1.7037722771 -0.9780008876 Si -7.0775210349 1.7010302771 0.4725631124 O -5.9240810349 2.8367212771 0.7959161124 Si -6.4009260349 -1.2213357229 0.1002161124 Si -5.0522750349 -3.9216307229 0.3131201124 H 6.1468109651 -1.6132157229 -2.0773228876 O -4.7435720349 -3.5417117229 -1.3101408876 H 4.0392199651 0.6030302771 -1.8775098876 Si 2.7812929651 1.1495432771 -1.4014998876 H 2.1022599651 2.0086442771 -2.4167578876 O 3.0236029651 1.9284572771 0.0627801124 O -3.6297450349 -4.6645657229 0.7861321124 Si -0.0281750349 -4.1188567229 -1.2793678876 Si -2.4605270349 -5.3881627229 -0.1989148876 H -2.8487740349 -5.3141567229 -1.6387558876 Si -4.2406190349 -1.9719957229 -1.5300328876 H 0.3531089651 -5.2708637229 -2.1615558876 O -0.9516880349 -4.7131957229 -0.0144078876 H -3.5374660349 -1.8222677229 -2.8070158876 O -3.2255690349 -1.5899837229 -0.2283598876 H -0.7796020349 -3.0967777229 -2.0529198876 O 3.5945779651 4.5306172771 0.6534671124 O 1.3022499651 5.4997882771 -0.4895028876 Si 2.8747679651 5.8043862771 -0.1839348876 Si 4.2234719651 3.1040052771 0.0289821124 H 4.5038599651 3.4601022771 -1.4068288876 Si 7.0012949651 -1.5325467229 -0.8515598876 O 5.6459159651 2.3611682771 0.5019961124 Si 6.8151079651 1.6375412771 -0.4830578876 H 6.4861749651 1.8922392771 -1.9185328876 O 6.8820109651 -0.0039227229 -0.1989158876 H 8.1279439651 2.2164852771 -0.0816518876 H 3.6088149651 6.0166382771 -1.4719488876 H 2.9701799651 6.9810202771 0.7236651124 H -5.1650050349 5.1180142771 1.5758111124	

H -8.2580380349 1.9628002771 1.3446481124 H -2.0215260349 5.4864512771 1.9026511124 H -6.1241060349 -4.9376227229 0.4422951124 H -2.3674840349 -6.7967967229 0.2815341124 H 2.8181839651 -5.5537937229 -0.6090198876 H 8.4386319651 -1.8036807229 -1.1485268876 H -7.8053860349 -1.6112057229 -0.1914518876 H 5.7932909651 -5.0599967229 -0.3028628876	



Gas phase coordinates	**PCM (F)** coordinates
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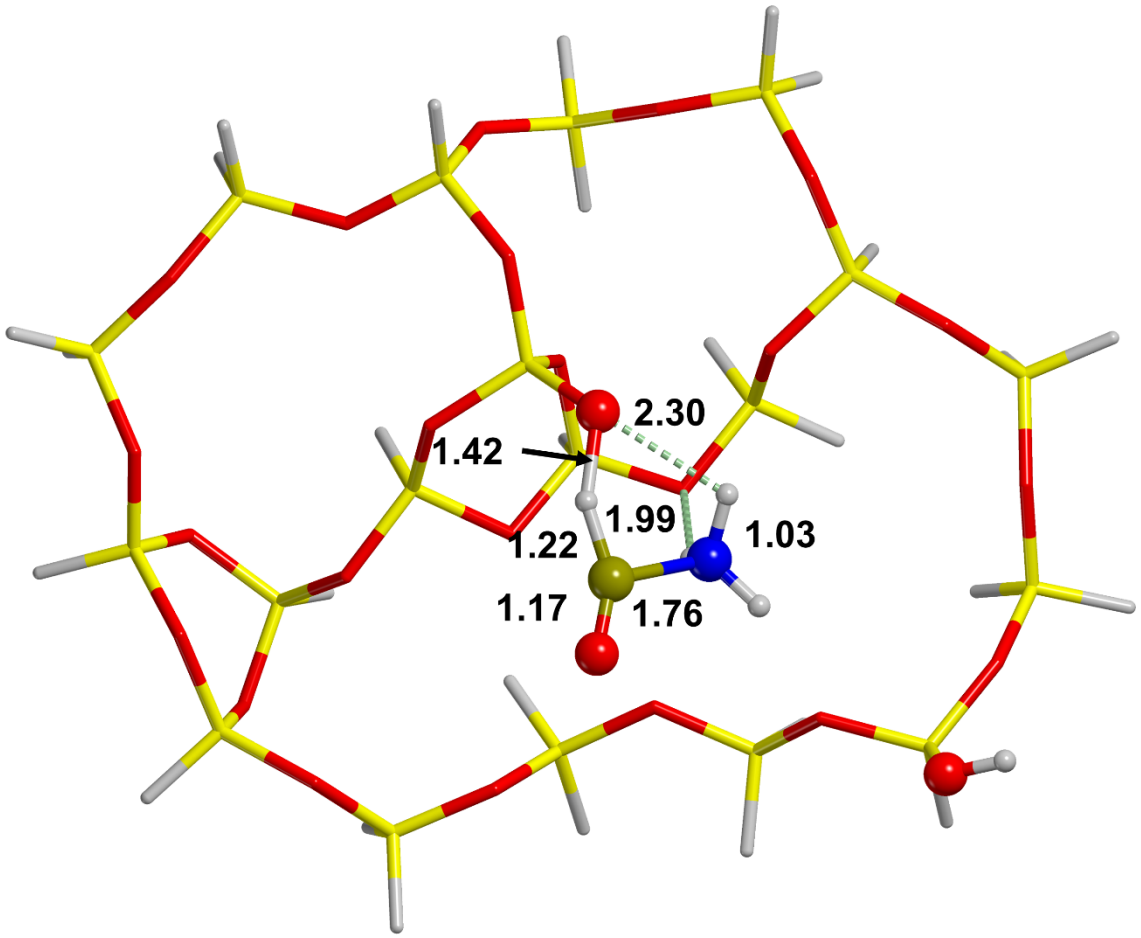

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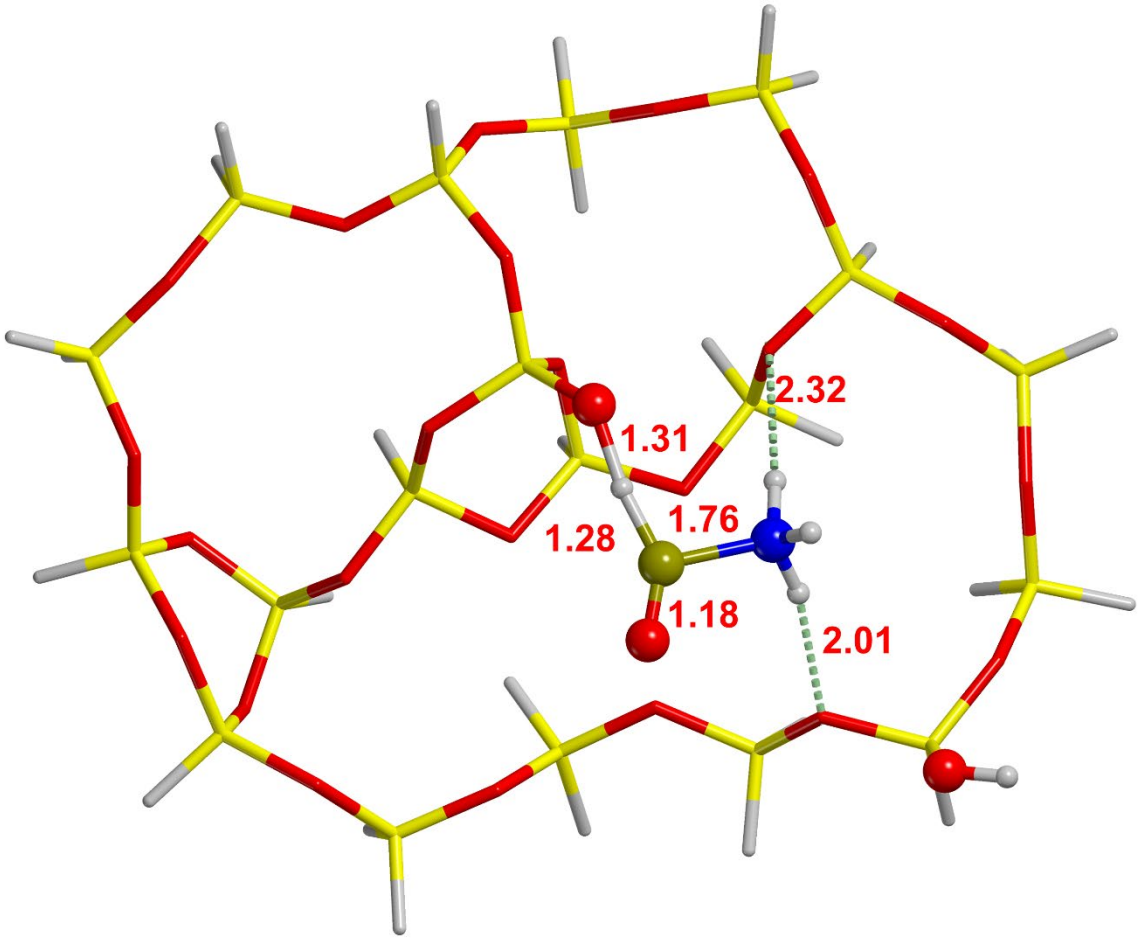

Gas phase coordinates	**PCM (F)** coordinates
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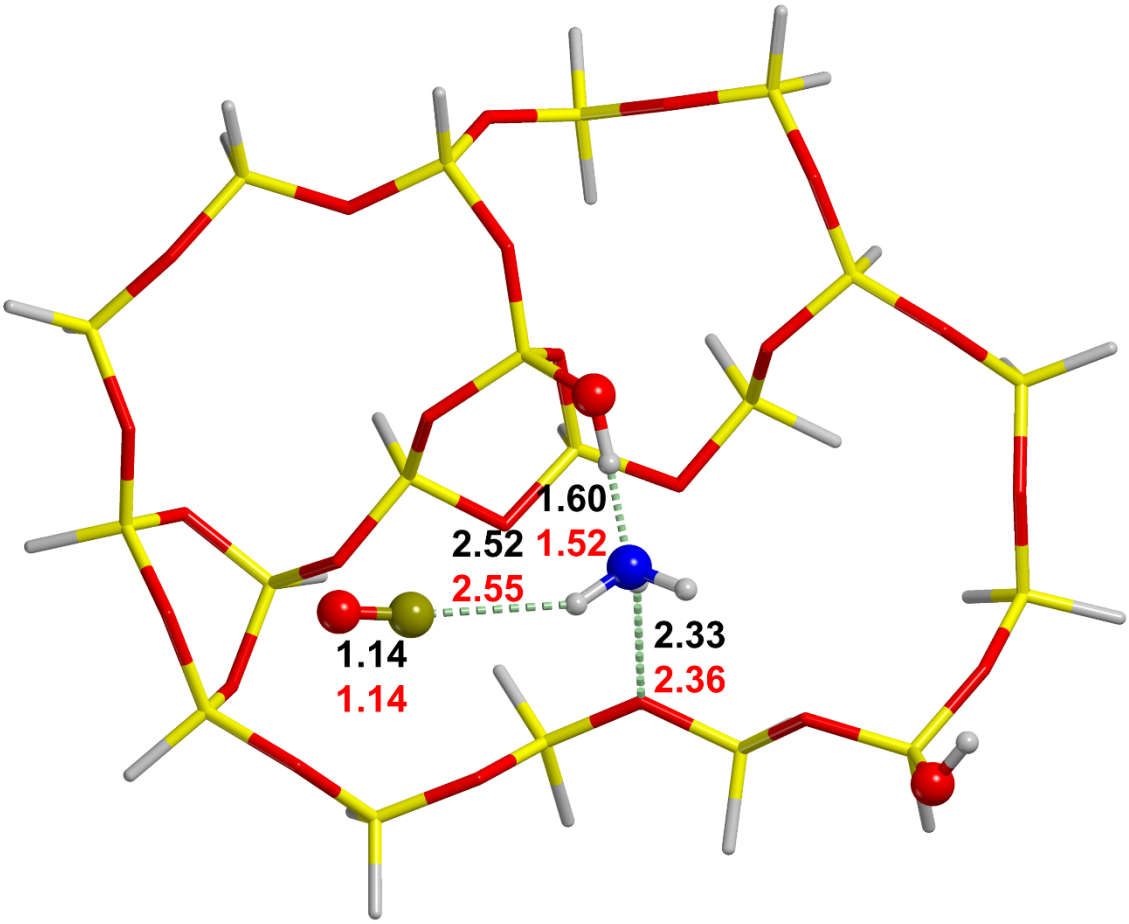

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H 0.6554783962 4.0257597224 -2.2586128448	H 0.6614848931 4.0257384883 -2.2604863941
H 0.4235473962 6.4821017224 -2.3361928448	H 0.4305538931 6.4821994883 -2.3372833941
Si 0.5065643962 5.2756597224 -1.4592888448	Si 0.5129508931 5.2754484883 -1.4607583941
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H 6.2902043962 -1.9355612776 -1.8830178448	H 6.2937508931 -1.9379745117 -1.8859803941
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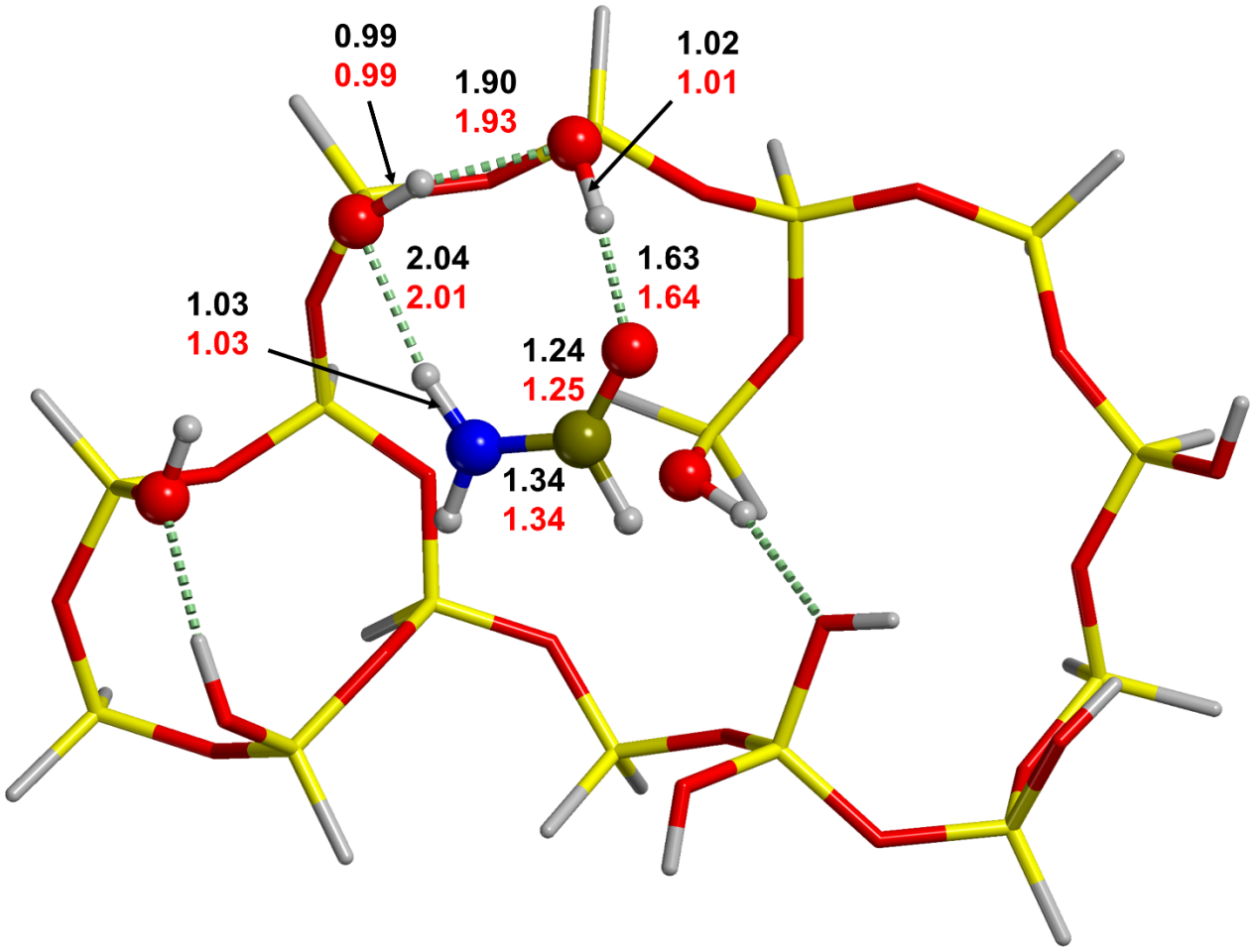
H -3.3635756038 -1.6230502776 -2.9163898448	H -3.3597551069 -1.6212735117 -2.9208563941
O -3.1197696038 -1.4077662776 -0.3244308448	O -3.1287961069 -1.4062655117 -0.3228643941
H -0.7032146038 -3.0446952776 -2.0796378448	H -0.7000811069 -3.0442295117 -2.0840923941
O 3.9870423962 4.3340277224 0.7825961552	O 3.9926068931 4.3315804883 0.7814556059
O 1.7870443962 5.4260517224 -0.4290608448	O 1.7933198931 5.4249624883 -0.4302853941
Si 3.3632523962 5.6453877224 -0.0735518448	Si 3.3695788931 5.6435554883 -0.0744513941
Si 4.5575553962 2.8764667224 0.1743601552	Si 4.5627358931 2.8738494883 0.1727366059
H 4.9017803962 3.2181587224 -1.2509478448	H 4.9072938931 3.2160334883 -1.2524253941
Si 7.1088353962 -1.9021132776 -0.6308718448	Si 7.1121858931 -1.9052635117 -0.6336863941
O 5.9226773962 2.0576307224 0.6897191552	O 5.9273488931 2.0544244883 0.6880826059
Si 7.0816013962 1.2730047224 -0.2600148448	Si 7.0862068931 1.2697774883 -0.2617803941
H 6.8121443962 1.5464317224 -1.7044208448	H 6.8170628931 1.5437484883 -1.7061353941
O 7.0513333962 -0.3698992776 0.0217491552	O 7.0552048931 -0.3732555117 0.0194326059
H 8.4103923962 1.7802167224 0.1838641552	H 8.4151008931 1.7762594883 0.1824846059
H 4.1477803962 5.8191047224 -1.3373618448	H 4.1543598931 5.8173704883 -1.3380763941
H 3.4931363962 6.8143327224 0.8396931552	H 3.4997658931 6.8121344883 0.8392066059
H -4.7531116038 5.3904917224 1.4315201552	H -4.7471491069 5.3914134883 1.4292326059
H -8.0023026038 2.4063157224 1.0952001552	H -7.9974871069 2.4086574883 1.0913936059
H -1.6062136038 5.5891277224 1.8576861552	H -1.6002121069 5.5886654883 1.8559496059

H -6.2146556038 -4.5979752776 0.2419681552	H -6.2125221069 -4.5960625117 0.2361126059
H -2.5600876038 -6.6562302776 0.1941291552	H -2.5587721069 -6.6557765117 0.1881676059
H 2.7105493962 -5.6929622776 -0.5303588448	H 2.7120928931 -5.6943415117 -0.5349623941
H 8.5381563962 -2.2498222776 -0.8833508448	H 8.5414168931 -2.2534745117 -0.8860573941
H -7.6941436038 -1.1853932776 -0.4353698448	H -7.6905221069 -1.1826645117 -0.4403413941
H 5.6964903962 -5.3600652776 -0.1295858448	H 5.6983928931 -5.3628015117 -0.1338133941

Figure S8: PBE-D2/TZVP optimized geometries for the formamide decarbonylation reaction catalysed by hydrophobic silica. In the figures the most representative bond lengths (in Å) in gas phase (black) and in PCM (F) (red) are reported. In the left and the right columns the cartesian coordinates of the optimized structures in gas phase and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue, silicons in yellow.

Formamide + Silica 4.5 dehydration reaction



Gas phase coordinates	**PCM** coordinates
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N -1.781261 0.677055 2.073703	N -1.829250 0.699671 2.105786
H -2.362448 1.521011 2.026341	H -2.400824 1.553402 2.075320
H -2.118305 -0.181205 1.640830	H -2.211618 -0.161578 1.717280
O 0.064265 1.802217 2.864498	O 0.061403 1.777017 2.853937
O -3.193808 3.379256 1.985742	O -3.179051 3.401524 1.989825
O -0.585968 4.286824 2.239738	O -0.545595 4.287565 2.246402
H -2.408325 3.790638 2.428293	H -2.411438 3.836900 2.433829
H -0.285631 3.360621 2.529098	H -0.299329 3.338737 2.510171
O 2.425643 -1.448314 1.221845	O 2.435781 -1.454540 1.237061
O 5.192685 -2.828538 2.011118	O 5.135526 -2.825606 2.025412
H 5.875407 -2.170668 1.792039	H 6.001964 -2.386423 1.978423
O 7.199072 0.405662 1.276548	O 7.205667 0.420364 1.278997
H 7.394069 1.205267 1.789410	H 7.545755 1.231350 1.692787
H 3.201209 -1.391799 1.808197	H 3.298963 -1.413212 1.691671
O 0.701787 -3.378156 2.005856	O 0.698265 -3.341849 2.016117
H 0.543238 -4.321244 2.165359	H 0.297934 -4.226210 1.967084
O -4.757237 -2.577810 2.009861	O -4.759672 -2.558149 2.009609

H -5.065230 -1.643466 2.049536	H -5.058069 -1.614141 2.017845
O -5.567408 0.077703 1.522407	O -5.593979 0.040439 1.525469
H -5.216661 0.899135 1.907290	H -5.307785 0.853170 1.976015
O 0.767809 0.362237 -0.204987	O 0.794287 0.370954 -0.194958
H 1.483359 -0.124338 0.260149	H 1.493563 -0.163704 0.245506
O 3.691272 3.956187 -0.398278	O 3.697004 3.952094 -0.399403
H 5.353293 3.356622 -2.284911	H 5.359316 3.350451 -2.285118
Si -0.357815 4.618672 0.621958	Si -0.351920 4.618671 0.618813
H 1.965948 4.685334 -2.125399	H 1.973152 4.682398 -2.127506
Si 2.189309 3.693529 -1.035092	Si 2.195083 3.690679 -1.036829
Si -3.221878 3.818302 0.364311	Si -3.216619 3.820931 0.360081
O -1.694411 4.060670 -0.205048	O -1.688666 4.061705 -0.208649
O 1.001646 3.884197 0.086311	O 1.007091 3.882770 0.083983
O 5.068716 -3.383614 -0.675061	O 5.067655 -3.389077 -0.673571
O 5.742621 -0.788686 -0.501240	O 5.743926 -0.794738 -0.500147
O 3.111589 -4.102452 0.981888	O 3.109099 -4.105620 0.982683
Si 6.098735 -2.236629 -1.238071	Si 6.099010 -2.243216 -1.236424
H 5.901241 -2.132508 -2.712970	H 5.902284 -2.139309 -2.711440
Si 5.192327 3.414446 -0.796635	Si 5.197728 3.408830 -0.796931
Si 4.740419 -3.955049 0.848434	Si 4.738127 -3.959789 0.849929
O 5.455733 1.900303 -0.171625	O 5.459423 1.894610 -0.171391
Si 6.490554 0.639123 -0.226963	Si 6.493080 0.632440 -0.225917
Si -2.470344 -1.269435 -1.349769	Si -2.469102 -1.267977 -1.352278
Si 1.887998 -2.999343 0.904436	Si 1.886583 -3.001380 0.904376
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O -0.941268 -1.780576 -1.642258	O -0.940376 -1.780638 -1.643934
Si -6.725384 -2.663907 -0.990613	Si -6.725617 -2.658341 -0.994678
H -6.831961 -2.507406 -2.472845	H -6.831373 -2.502142 -2.477001
O -2.985089 -1.866514 0.109469	O -2.985072 -1.864175 0.106887
H -3.361161 -1.713901 -2.454232	H -3.359836 -1.711903 -2.457026
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Si -4.078475 -3.016625 0.563090	Si -4.079748 -3.013132 0.560323
O -5.214370 0.386102 -1.175923	O -5.211645 0.390192 -1.180128
H -0.150569 1.431848 -2.326551	H -0.146339 1.430853 -2.328738
O -2.508792 0.372261 -1.201849	O -2.506070 0.373794 -1.204821
Si -6.333522 0.211956 0.020409	Si -6.331504 0.217426 0.015742
H -3.882469 1.770606 -2.843377	H -3.877683 1.772988 -2.847352
Si -3.856140 1.290188 -1.439125	Si -3.852444 1.292926 -1.442958
Si 1.122414 0.927387 -1.734548	Si 1.125899 0.925353 -1.736020
H 1.789750 -0.108434 -2.586018	H 1.792645 -0.111327 -2.586906
O 1.299824 -2.936684 -0.633134	O 1.299167 -2.938584 -0.633478
H 0.220352 -3.750681 -2.760144	H 0.219894 -3.752141 -2.760758
O 2.225420 2.177723 -1.651014	O 2.230045 2.174672 -1.652323
Si -0.112173 -3.191592 -1.418428	Si -0.112713 -3.192374 -1.419345
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H 5.355805 -5.297403 1.016209	H 5.352172 -5.302676 1.018348
H -0.964061 -4.131439 -0.611584	H -0.965853 -4.131199 -0.612633
H -3.417208 -4.331477 0.757795	H -3.419809 -4.328553 0.755685
H -7.698814 -3.659821 -0.452807	H -7.700230 -3.653191 -0.457045

H -7.295845 1.342834 0.047514	H -7.292773 1.349217 0.042103
H -4.072590 5.011171 0.109104	H -4.066090 5.014532 0.104164
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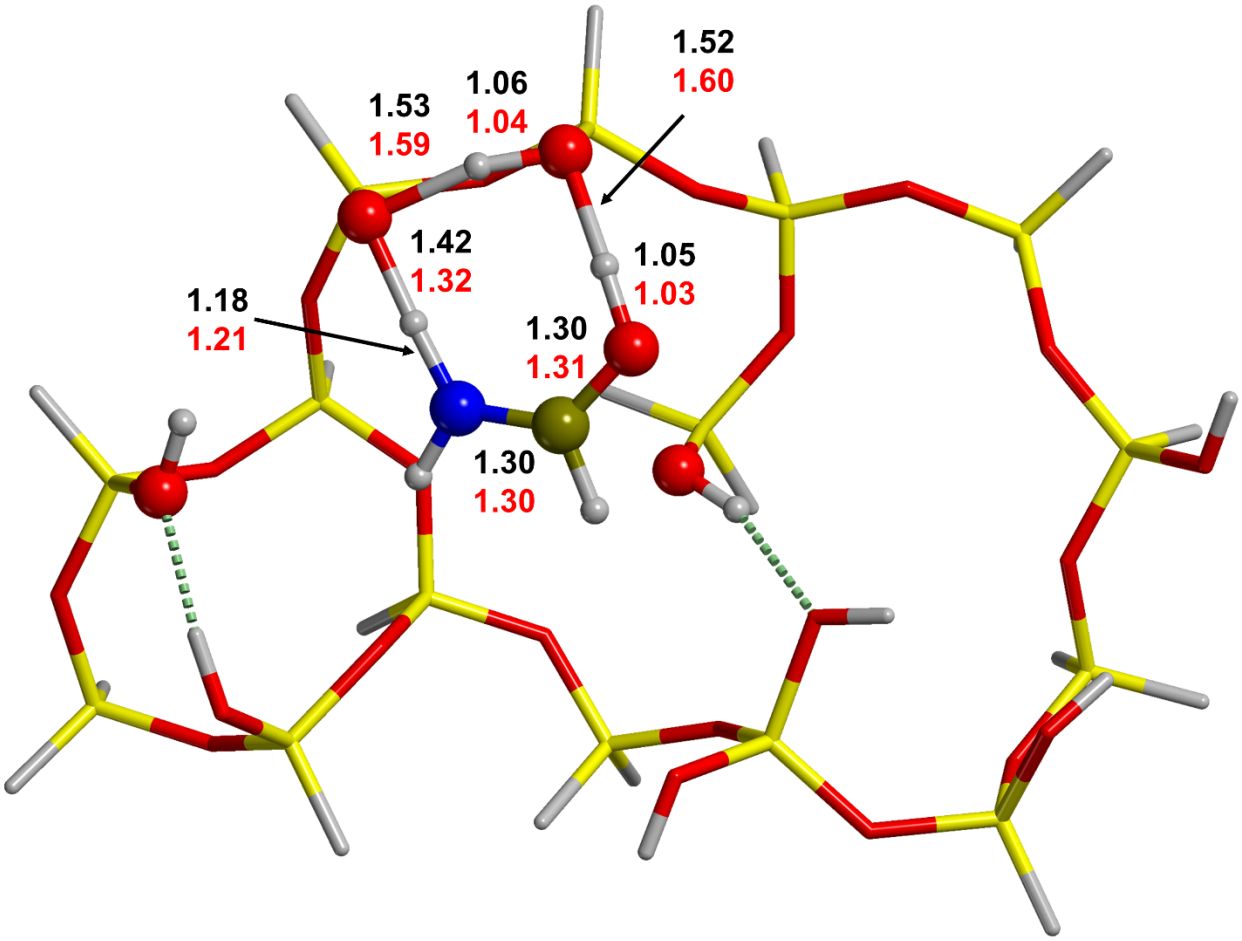

Gas phase coordinates	**PCM** coordinates
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C -0.674340 0.876043 2.334449	C -0.860504 0.833988 2.459056
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N -1.917855 1.085378 2.008086	N -2.091233 1.122953 2.173057
H -2.449431 2.113478 2.004980	H -2.580237 2.228646 2.096294
H -2.410959 0.267195 1.644237	H -2.670201 0.313986 1.935509
O 0.169178 1.772566 2.742501	O 0.077650 1.694925 2.756808
O -3.040212 3.401576 1.957015	O -3.062805 3.453223 1.961723
O -0.622579 4.161600 2.228104	O -0.597623 4.175099 2.226130
H -1.667599 3.977314 2.297818	H -1.623784 4.026711 2.315278
H -0.147368 2.760948 2.599068	H -0.190575 2.676634 2.603177
O 2.433456 -1.460248 1.249183	O 2.444988 -1.454305 1.240035
O 5.180978 -2.820468 2.014645	O 5.147026 -2.818672 2.037135
H 5.906024 -2.201256 1.820859	H 6.013315 -2.379096 1.991452
O 7.199978 0.401163 1.279392	O 7.210160 0.430658 1.287738
H 7.412947 1.201193 1.784384	H 7.555188 1.241678 1.697370
H 3.260217 -1.422246 1.764222	H 3.305909 -1.410149 1.698540
O 0.698547 -3.358165 2.017900	O 0.710919 -3.347188 2.022751

H 0.349793 -4.263087 2.017852	H 0.325592 -4.238659 1.982638
O -4.753387 -2.584661 2.021810	O -4.755687 -2.576016 2.007569
H -5.066218 -1.651660 2.058670	H -5.056129 -1.633866 2.020375
O -5.557339 0.078175 1.529084	O -5.558399 0.042625 1.509048
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O 0.777825 0.356018 -0.190975	O 0.789157 0.375612 -0.190428
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O 3.689450 3.949467 -0.397783	O 3.696037 3.952177 -0.400863
H 5.351079 3.348612 -2.284351	H 5.361980 3.351149 -2.283567
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H 1.963145 4.675851 -2.125088	H 1.972664 4.675788 -2.132255
Si 2.187384 3.685369 -1.033760	Si 2.195480 3.686361 -1.039679
Si -3.223355 3.809065 0.367468	Si -3.218194 3.806823 0.350450
O -1.696213 4.051542 -0.202715	O -1.690092 4.050073 -0.216822
O 1.000035 3.876706 0.087862	O 1.005700 3.877640 0.079374
O 5.070370 -3.389966 -0.666898	O 5.083397 -3.386355 -0.661283
O 5.743074 -0.794518 -0.496209	O 5.753667 -0.790231 -0.491309
O 3.114194 -4.107912 0.991560	O 3.124431 -4.104548 0.993772
Si 6.099626 -2.243107 -1.231557	Si 6.112877 -2.239121 -1.224769
H 5.901547 -2.140723 -2.706500	H 5.917715 -2.138077 -2.700193
Si 5.190624 3.408014 -0.796082	Si 5.198452 3.411614 -0.795676
Si 4.742904 -3.959864 0.857351	Si 4.753291 -3.955296 0.862754
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Si 6.490410 0.633959 -0.223793	Si 6.499300 0.639065 -0.218521
Si -2.469963 -1.280211 -1.341222	Si -2.457242 -1.283211 -1.352622
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Si -6.724192 -2.676354 -0.978970	Si -6.711076 -2.682487 -0.997897
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O -5.174110 -3.144046 -0.649084	O -5.161293 -3.148667 -0.664486
O -3.917050 2.538697 -0.400478	O -3.909306 2.535283 -0.417885
Si -4.076549 -3.026053 0.574164	Si -4.066316 -3.028812 0.560895
O -5.214732 0.374182 -1.168222	O -5.203685 0.369110 -1.186528
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O -2.509157 0.361630 -1.195115	O -2.498052 0.358714 -1.207912
Si -6.333366 0.200824 0.028709	Si -6.324611 0.195810 0.008266
H -3.884111 1.757478 -2.837700	H -3.870785 1.752140 -2.854407
Si -3.857039 1.278637 -1.432923	Si -3.846184 1.274446 -1.449194
Si 1.121584 0.917931 -1.729749	Si 1.133320 0.917510 -1.735612
H 1.789117 -0.118512 -2.580309	H 1.803413 -0.119076 -2.583982
O 1.301276 -2.944825 -0.624100	O 1.313867 -2.944214 -0.626502
H 0.221430 -3.761714 -2.749812	H 0.239001 -3.763674 -2.753748
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H 7.490732 0.866691 -1.310832	H 7.501643 0.871732 -1.303711
H 7.511007 -2.615237 -0.876806	H 7.523832 -2.609830 -0.866852
H 5.359004 -5.301732 1.026397	H 5.370123 -5.296532 1.034128
H -0.962018 -4.140657 -0.600399	H -0.948509 -4.141848 -0.606441

H -3.414571 -4.340365 0.770091	H -3.403682 -4.342433 0.759221
H -7.696942 -3.672143 -0.439703	H -7.684120 -3.678627 -0.459809
H -7.296230 1.331262 0.054904	H -7.288434 1.325493 0.031597
H -4.074741 5.001234 0.111242	H -4.070015 4.998101 0.091538
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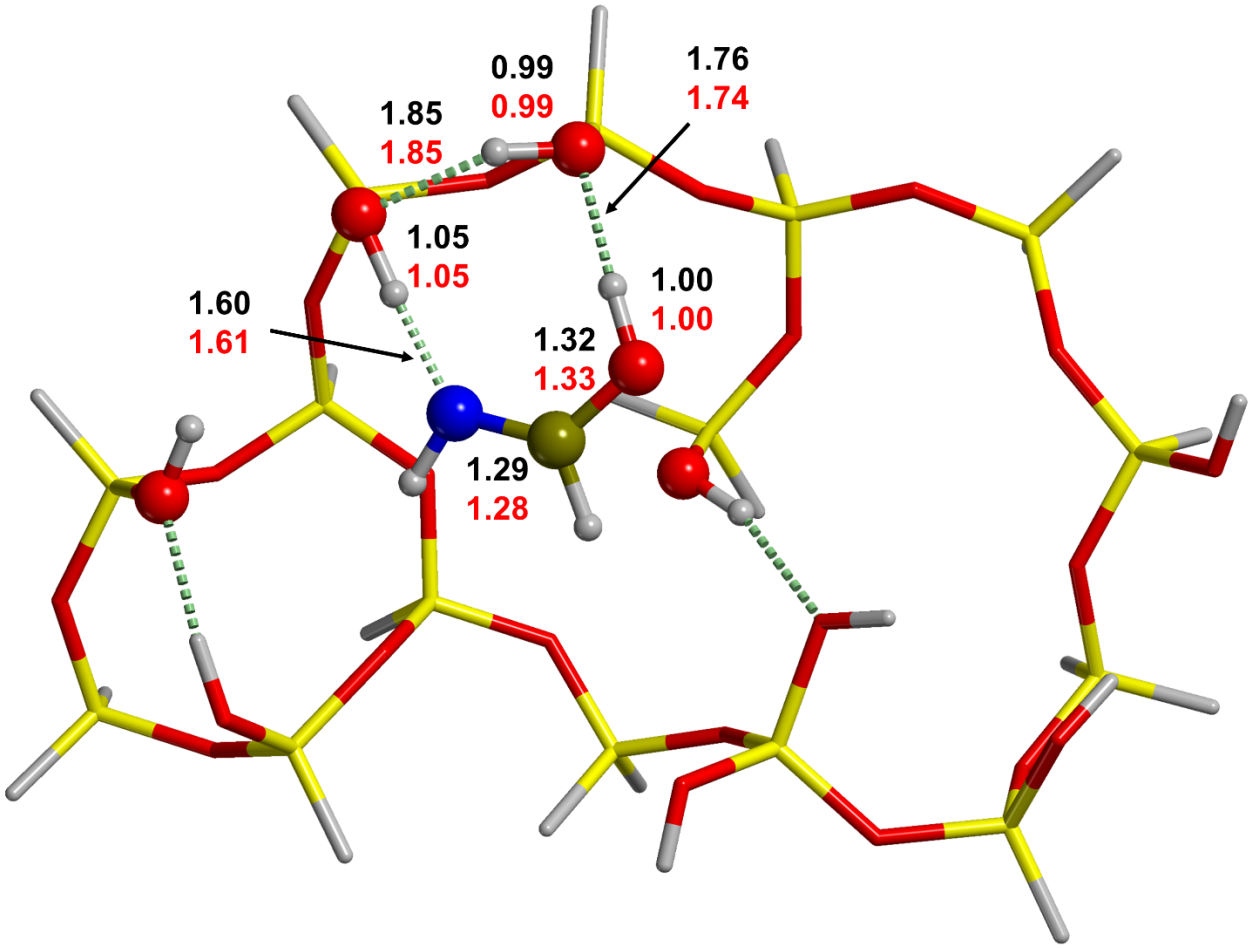

Gas phase coordinates	**PCM** coordinates
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H -0.404371 -0.285554 2.317686	H -0.455760 -0.287824 2.471949
N -1.995401 1.068680 2.089831	N -2.025004 1.083048 2.183411
H -2.720736 2.496751 2.101582	H -2.738436 2.525349 2.127237
H -2.516136 0.245399 1.771043	H -2.579768 0.261329 1.924192
O 0.165797 1.587808 2.753755	O 0.145847 1.602834 2.802632
O -3.146749 3.451789 1.992305	O -3.138639 3.482935 1.988872
O -0.529244 4.209333 2.248916	O -0.514353 4.202088 2.240489
H -1.496818 4.151381 2.472046	H -1.482712 4.165980 2.468075
H -0.113506 2.544466 2.644151	H -0.135211 2.557336 2.658899
O 2.431707 -1.448826 1.220439	O 2.443108 -1.454423 1.237011
O 5.209469 -2.830735 2.017917	O 5.142434 -2.819653 2.032366
H 5.864617 -2.150996 1.781906	H 6.009011 -2.380683 1.986081
O 7.200613 0.411078 1.282393	O 7.207594 0.428232 1.282458
H 7.405316 1.211064 1.790761	H 7.551697 1.239409 1.692569

H 3.181201 -1.384931 1.838265	H 3.305011 -1.412481 1.693951
O 0.712602 -3.372665 2.017330	O 0.705676 -3.342941 2.020337
H 0.504540 -4.312442 2.134372	H 0.311259 -4.230177 1.975130
O -4.756456 -2.591091 2.010976	O -4.758934 -2.571907 2.007841
H -5.067487 -1.657810 2.048310	H -5.057195 -1.628543 2.017433
O -5.562498 0.068870 1.521433	O -5.581465 0.034817 1.516370
H -5.178850 0.886932 1.882297	H -5.320363 0.853569 1.971447
O 0.767815 0.369656 -0.200128	O 0.788197 0.373775 -0.196176
H 1.476098 -0.116718 0.276095	H 1.482805 -0.156870 0.255879
O 3.690231 3.956125 -0.396374	O 3.695170 3.952155 -0.404423
H 5.353941 3.357599 -2.281848	H 5.359910 3.350111 -2.287868
Si -0.360178 4.614208 0.621458	Si -0.355582 4.614114 0.609521
H 1.964898 4.682264 -2.124753	H 1.971583 4.677107 -2.135041
Si 2.188913 3.691303 -1.033813	Si 2.194162 3.687438 -1.042635
Si -3.223132 3.810213 0.362776	Si -3.218847 3.811576 0.349757
O -1.695673 4.054145 -0.205934	O -1.690811 4.053803 -0.218132
O 1.000449 3.881111 0.086887	O 1.004982 3.879463 0.076928
O 5.076760 -3.382135 -0.668610	O 5.077291 -3.387324 -0.665995
O 5.747413 -0.786297 -0.495807	O 5.749446 -0.791683 -0.496098
O 3.119668 -4.102491 0.987722	O 3.118513 -4.104278 0.989819
Si 6.105666 -2.234190 -1.231698	Si 6.107338 -2.240765 -1.229821
H 5.908795 -2.131083 -2.706751	H 5.911632 -2.139471 -2.705154
Si 5.192148 3.416006 -0.793684	Si 5.197044 3.410573 -0.799903
Si 4.748385 -3.953172 0.855018	Si 4.747422 -3.956155 0.858135
O 5.457081 1.902512 -0.167747	O 5.460559 1.897736 -0.171783
Si 6.493466 0.642566 -0.221898	Si 6.496192 0.637070 -0.223507
Si -2.464527 -1.277501 -1.348255	Si -2.462163 -1.278854 -1.354031
Si 1.894773 -3.000915 0.909070	Si 1.894369 -3.002038 0.908807
O -7.076134 -1.228979 -0.254672	O -7.074553 -1.226004 -0.263955
O -0.934681 -1.786931 -1.639699	O -0.932420 -1.789626 -1.643664
Si -6.718047 -2.676970 -0.990529	Si -6.716827 -2.675184 -0.997644
H -6.824061 -2.521375 -2.472896	H -6.821638 -2.521468 -2.480293
O -2.979286 -1.874443 0.111035	O -2.978385 -1.873557 0.105657
H -3.354240 -1.723631 -2.452937	H -3.351332 -1.725875 -2.458790
O -5.167910 -3.143723 -0.659569	O -5.167231 -3.142474 -0.664915
O -3.915228 2.539791 -0.406522	O -3.911167 2.540580 -0.418390
Si -4.071500 -3.025648 0.564703	Si -4.071660 -3.023480 0.560019
O -5.210657 0.374781 -1.176670	O -5.207381 0.375374 -1.186664
H -0.147550 1.426096 -2.325274	H -0.142760 1.422004 -2.332866
O -2.505051 0.364224 -1.201215	O -2.501765 0.363088 -1.209175
Si -6.330204 0.199897 0.019185	Si -6.327930 0.202762 0.008584
H -3.879596 1.760034 -2.844173	H -3.874207 1.757602 -2.854989
Si -3.853396 1.280384 -1.439656	Si -3.849356 1.279779 -1.449824
Si 1.125746 0.923497 -1.732360	Si 1.129778 0.919385 -1.738343
H 1.794777 -0.111955 -2.582948	H 1.798792 -0.117602 -2.587072
O 1.307305 -2.939778 -0.628831	O 1.308087 -2.942551 -0.629611
H 0.229907 -3.756203 -2.755962	H 0.231762 -3.761091 -2.756472
O 2.227185 2.175220 -1.648922	O 2.231940 2.170526 -1.655725
Si -0.103981 -3.196818 -1.414708	Si -0.102774 -3.199737 -1.416203
H 6.171108 4.355609 -0.164482	H 6.176124 4.350387 -0.171204
H 7.494562 0.876671 -1.307928	H 7.498245 0.869121 -1.309096
H 7.517010 -2.605497 -0.875936	H 7.518183 -2.612490 -0.872519

H 5.365321 -5.294687 1.023809	H 5.363389 -5.297834 1.029146
H -0.955133 -4.137280 -0.607805	H -0.955118 -4.138605 -0.608702
H -3.408731 -4.339591 0.760433	H -3.409863 -4.337581 0.757968
H -7.690536 -3.673788 -0.452695	H -7.690343 -3.670685 -0.459229
H -7.293918 1.329615 0.045208	H -7.290953 1.333118 0.032405
H -4.075168 5.001910 0.106512	H -4.069943 5.003470 0.091293
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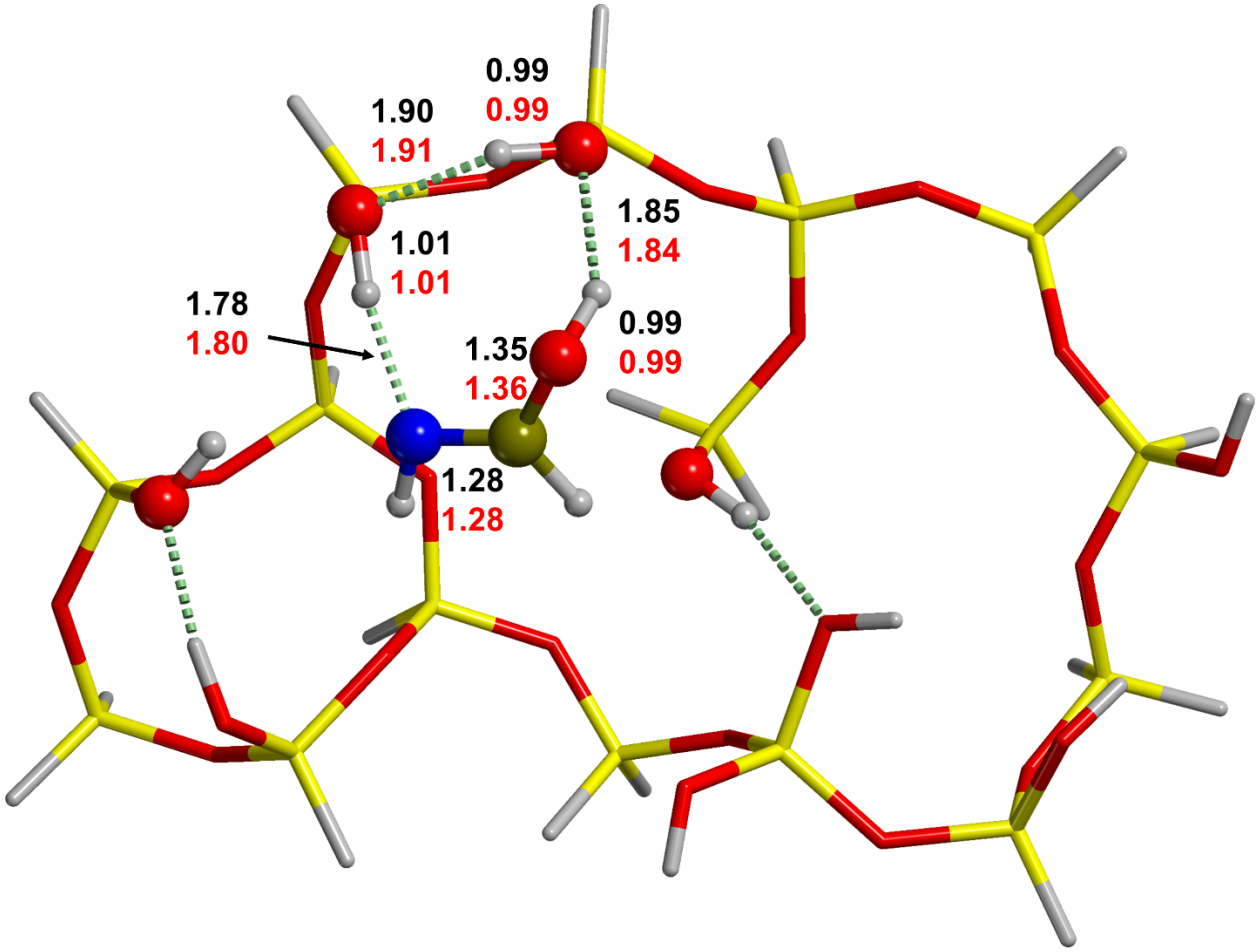

Gas phase coordinates	**PCM** coordinates
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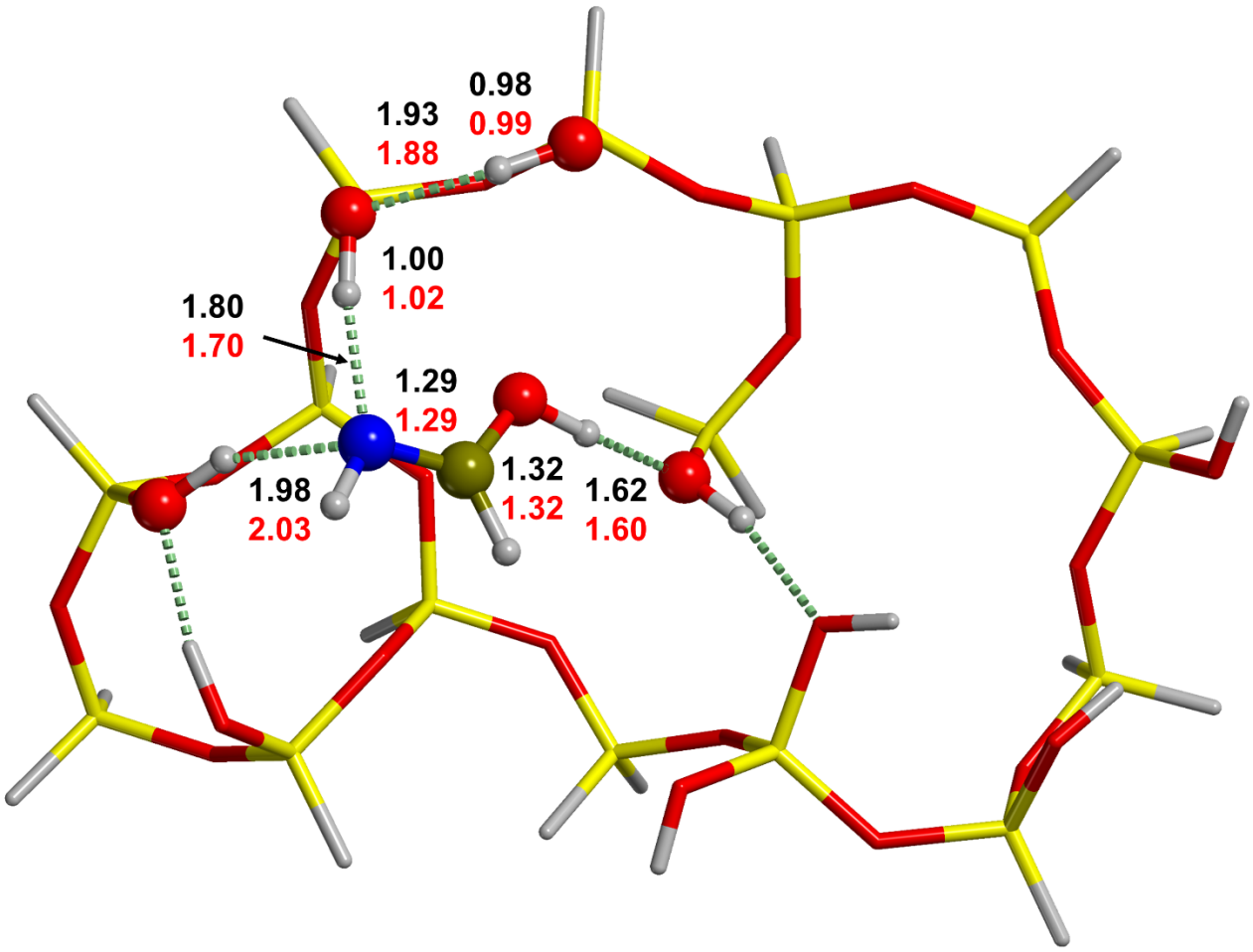
N -2.467555 0.807976 2.044137	N -2.484973 0.789396 2.102321
H -3.034050 2.497080 2.145892	H -3.044342 2.495008 2.149380
H -2.667739 0.013158 1.422167	H -2.709693 0.008992 1.469826
O -0.740377 1.692152 3.252502	O -0.723230 1.679596 3.250789
O -3.177048 3.484046 1.970455	O -3.170930 3.482264 1.974002
O -0.499836 4.208816 2.221828	O -0.487698 4.195500 2.223719
H -1.455448 4.125385 2.471620	H -1.445411 4.123881 2.469304
H -0.300358 2.462695 2.808776	H -0.294863 2.450644 2.792094
O 2.467335 -1.436247 1.221813	O 2.468997 -1.441472 1.242176
O 5.222318 -2.799482 2.042930	O 5.168649 -2.800051 2.056009

H 5.922543 -2.156267 1.836633	H 6.035224 -2.360508 2.016057
O 7.223152 0.436776 1.311553	O 7.229015 0.452454 1.312848
H 7.438806 1.238032 1.813384	H 7.574188 1.263740 1.721836
H 3.245937 -1.379476 1.804340	H 3.326827 -1.394288 1.706194
O 0.741949 -3.364758 2.017301	O 0.734791 -3.338546 2.022095
H 0.570970 -4.306397 2.172214	H 0.361243 -4.235300 1.988678
O -4.727626 -2.602770 1.983038	O -4.729181 -2.582346 1.984374
H -5.068462 -1.677136 2.004693	H -5.057124 -1.647704 1.979943
O -5.535975 0.028225 1.475469	O -5.551396 0.008289 1.481175
H -4.902376 0.714428 1.757317	H -5.010667 0.742835 1.824694
O 0.808829 0.383722 -0.193202	O 0.823232 0.384534 -0.189373
H 1.511340 -0.133478 0.261048	H 1.518566 -0.155068 0.252788
O 3.711000 3.968451 -0.393904	O 3.715383 3.965696 -0.394167
H 5.386448 3.370446 -2.269122	H 5.390801 3.366467 -2.269021
Si -0.346682 4.616858 0.600911	Si -0.341990 4.617547 0.599658
H 1.992705 4.685373 -2.133108	H 1.998183 4.684368 -2.133730
Si 2.213874 3.697656 -1.038652	Si 2.218190 3.696309 -1.039349
Si -3.205826 3.803728 0.328986	Si -3.201777 3.806976 0.326863
O -1.676105 4.050870 -0.232208	O -1.671690 4.052845 -0.233891
O 1.018929 3.886561 0.075289	O 1.023116 3.886117 0.074300
O 5.120721 -3.366265 -0.641398	O 5.118700 -3.370227 -0.642279
O 5.782743 -0.768040 -0.471203	O 5.782968 -0.772610 -0.471556
O 3.157024 -4.088547 1.006255	O 3.153929 -4.090999 1.004755
Si 6.149186 -2.216589 -1.201753	Si 6.148328 -2.221383 -1.202205
H 5.959831 -2.117543 -2.678067	H 5.959452 -2.121971 -2.678556
Si 5.216597 3.431876 -0.781977	Si 5.220609 3.427846 -0.781913
Si 4.785971 -3.934687 0.881820	Si 4.783044 -3.938559 0.880773
O 5.482699 1.920657 -0.151060	O 5.485211 1.916307 -0.151129
Si 6.523090 0.663681 -0.196738	Si 6.524505 0.658420 -0.196701
Si -2.423069 -1.285719 -1.365938	Si -2.423059 -1.282930 -1.368542
Si 1.929300 -2.990814 0.918510	Si 1.927197 -2.992172 0.916832
O -7.040531 -1.248363 -0.296897	O -7.040770 -1.241646 -0.300722
O -0.890196 -1.791273 -1.648071	O -0.890558 -1.789798 -1.650336
Si -6.674255 -2.697011 -1.027413	Si -6.675578 -2.690518 -1.031337
H -6.772871 -2.545224 -2.510686	H -6.773666 -2.538444 -2.514616
O -2.943783 -1.880753 0.092019	O -2.944685 -1.877702 0.089197
H -3.305588 -1.737098 -2.474252	H -3.305681 -1.733381 -2.477151
O -5.124516 -3.158361 -0.687147	O -5.126337 -3.153281 -0.690722
O -3.890063 2.529440 -0.440950	O -3.886933 2.533396 -0.443427
Si -4.034965 -3.034136 0.542627	Si -4.037004 -3.030183 0.539359
O -5.174962 0.358772 -1.212808	O -5.173541 0.363967 -1.215920
H -0.108979 1.422462 -2.337086	H -0.106323 1.423340 -2.338708
O -2.469244 0.356220 -1.223007	O -2.467824 0.359029 -1.225401
Si -6.300307 0.183370 -0.022485	Si -6.299357 0.189396 -0.025920
H -3.839197 1.744054 -2.876523	H -3.836113 1.748295 -2.879093
Si -3.819019 1.267794 -1.470753	Si -3.816728 1.271827 -1.473382
Si 1.162642 0.925057 -1.736251	Si 1.164699 0.924732 -1.737603
H 1.839240 -0.110397 -2.580829	H 1.840608 -0.111204 -2.582141
O 1.349812 -2.935050 -0.622620	O 1.348168 -2.935689 -0.624444
H 0.286130 -3.759689 -2.753482	H 0.284326 -3.759101 -2.755701
O 2.259904 2.180250 -1.649953	O 2.263044 2.178945 -1.650843
Si -0.056520 -3.198145 -1.415345	Si -0.058185 -3.197436 -1.417579

H 6.189416 4.375872 -0.149833	H 6.194093 4.370898 -0.149382
H 7.529230 0.898209 -1.278006	H 7.531139 0.892207 -1.277670
H 7.559720 -2.582849 -0.837645	H 7.558441 -2.588936 -0.837772
H 5.405982 -5.273957 1.057055	H 5.401827 -5.278399 1.055992
H -0.909142 -4.139236 -0.610730	H -0.911850 -4.137884 -0.613318
H -3.369346 -4.345634 0.744977	H -3.372596 -4.342295 0.741708
H -7.646618 -3.695452 -0.492372	H -7.648963 -3.688173 -0.496689
H -7.267493 1.310270 -0.004242	H -7.265553 1.317147 -0.007781
H -4.060024 4.992274 0.065391	H -4.054857 4.996311 0.063202
H -0.262775 6.083037 0.357455	H -0.256725 6.083684 0.356422



Gas phase coordinates	**PCM** coordinates
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N -2.938071 0.756799 2.539575	N -2.919443 0.857531 2.582745
H -3.192734 2.522894 2.298714	H -3.169603 2.517768 2.302489
H -3.261649 0.016024 3.167658	H -3.258234 0.164569 3.255234
O -1.162907 1.305441 1.261495	O -1.150127 1.291416 1.256960
O -3.187358 3.496832 2.049581	O -3.177774 3.506624 2.048743
O -0.484114 4.300989 2.320272	O -0.496461 4.292915 2.320539
H -1.385048 3.969749 2.539946	H -1.407264 3.955766 2.507191

H -0.363872 0.902822 0.792119	H -0.365468 0.854163 0.783839
O 2.485156 -1.431584 1.236684	O 2.480325 -1.429541 1.237253
O 5.225701 -2.800150 2.050159	O 5.193778 -2.807553 2.068825
H 5.966823 -2.191050 1.887968	H 6.059004 -2.364732 2.036330
O 7.243573 0.433622 1.373568	O 7.249797 0.460770 1.373742
H 7.467377 1.226890 1.884646	H 7.590711 1.268158 1.793951
H 3.295807 -1.372703 1.774801	H 3.319482 -1.358193 1.730435
O 0.763444 -3.352590 2.012765	O 0.767154 -3.346019 2.021221
H 0.505322 -4.284116 2.091268	H 0.431457 -4.258295 2.015559
O -4.701093 -2.602544 1.965335	O -4.719177 -2.602348 1.963308
H -5.082741 -1.688156 1.947380	H -5.061457 -1.670967 1.943325
O -5.511686 0.020192 1.486938	O -5.512674 0.015564 1.490092
H -4.711268 0.567659 1.675056	H -4.716004 0.567399 1.674524
O 0.856500 0.371320 -0.135018	O 0.859402 0.379109 -0.132886
H 1.558122 -0.156074 0.321829	H 1.547079 -0.173599 0.319904
O 3.734567 3.989742 -0.292353	O 3.733723 3.987784 -0.297852
H 5.416226 3.419949 -2.170793	H 5.415847 3.416452 -2.175408
Si -0.326719 4.620176 0.699302	Si -0.327883 4.618303 0.692435
H 2.020802 4.729631 -2.026400	H 2.020097 4.725503 -2.032960
Si 2.239651 3.726708 -0.945388	Si 2.238984 3.723739 -0.950882
Si -3.184234 3.808299 0.407255	Si -3.185160 3.805472 0.400713
O -1.653078 4.064806 -0.145761	O -1.653965 4.061763 -0.152293
O 1.041181 3.898684 0.167507	O 1.040276 3.896580 0.161623
O 5.152220 -3.339403 -0.639508	O 5.153117 -3.341387 -0.637243
O 5.811178 -0.743231 -0.430514	O 5.811443 -0.744851 -0.430793
O 3.184292 -4.086809 0.991811	O 3.185070 -4.087572 0.994492
Si 6.181235 -2.180936 -1.180409	Si 6.181963 -2.183239 -1.179148
H 5.996218 -2.061152 -2.655736	H 5.997181 -2.065010 -2.654630
Si 5.241849 3.460135 -0.683446	Si 5.241196 3.458122 -0.688134
Si 4.813453 -3.929672 0.874484	Si 4.814216 -3.930182 0.877293
O 5.507537 1.940375 -0.073208	O 5.507124 1.939050 -0.076292
Si 6.549293 0.685150 -0.133555	Si 6.549178 0.684002 -0.135167
Si -2.391397 -1.255876 -1.357252	Si -2.390849 -1.260327 -1.358462
Si 1.955761 -2.989095 0.915926	Si 1.956301 -2.990218 0.917263
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O -0.857188 -1.755941 -1.641894	O -0.856475 -1.760331 -1.642318
Si -6.642194 -2.675812 -1.051590	Si -6.641375 -2.680923 -1.052099
H -6.736503 -2.503109 -2.532854	H -6.735460 -2.509760 -2.533556
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H -3.270140 -1.692328 -2.474509	H -3.269294 -1.698125 -2.475427
O -5.093033 -3.140485 -0.713221	O -5.092168 -3.144894 -0.712979
O -3.864905 2.544411 -0.382722	O -3.865401 2.540619 -0.388089
Si -4.007303 -3.032681 0.521472	Si -4.006682 -3.035576 0.521796
O -5.145350 0.383697 -1.189137	O -5.145208 0.378786 -1.192516
H -0.077058 1.467968 -2.282937	H -0.076970 1.463098 -2.286527
O -2.439612 0.383828 -1.191207	O -2.439470 0.379536 -1.194106
Si -6.274092 0.190385 -0.004821	Si -6.274116 0.186429 -0.008203
H -3.805953 1.793674 -2.829016	H -3.805842 1.787389 -2.833601
Si -3.789530 1.297555 -1.430082	Si -3.789554 1.292708 -1.434157
Si 1.193240 0.963291 -1.685377	Si 1.193337 0.959325 -1.688224
H 1.873387 -0.059453 -2.542498	H 1.873871 -0.064141 -2.544176
O 1.380850 -2.912036 -0.626000	O 1.381647 -2.914871 -0.624843

H 0.324383 -3.707387 -2.771534	H 0.325744 -3.712663 -2.769748
O 2.289006 2.218163 -1.577990	O 2.288797 2.214557 -1.581929
Si -0.022835 -3.165188 -1.426614	Si -0.021838 -3.169166 -1.425446
H 6.211838 4.395988 -0.035055	H 6.210855 4.394862 -0.040530
H 7.558446 0.935924 -1.208350	H 7.558465 0.933906 -1.210039
H 7.591028 -2.550996 -0.817273	H 7.591776 -2.552604 -0.815383
H 5.434249 -5.270709 1.032593	H 5.435291 -5.270914 1.036886
H -0.876947 -4.118389 -0.637992	H -0.875872 -4.121754 -0.635999
H -3.341009 -4.346290 0.707224	H -3.340120 -4.348841 0.709012
H -7.615180 -3.682649 -0.533688	H -7.614223 -3.687452 -0.533338
H -7.242434 1.316005 0.026471	H -7.242721 1.311859 0.021763
H -4.038802 4.999660 0.157954	H -4.039957 4.996381 0.150040
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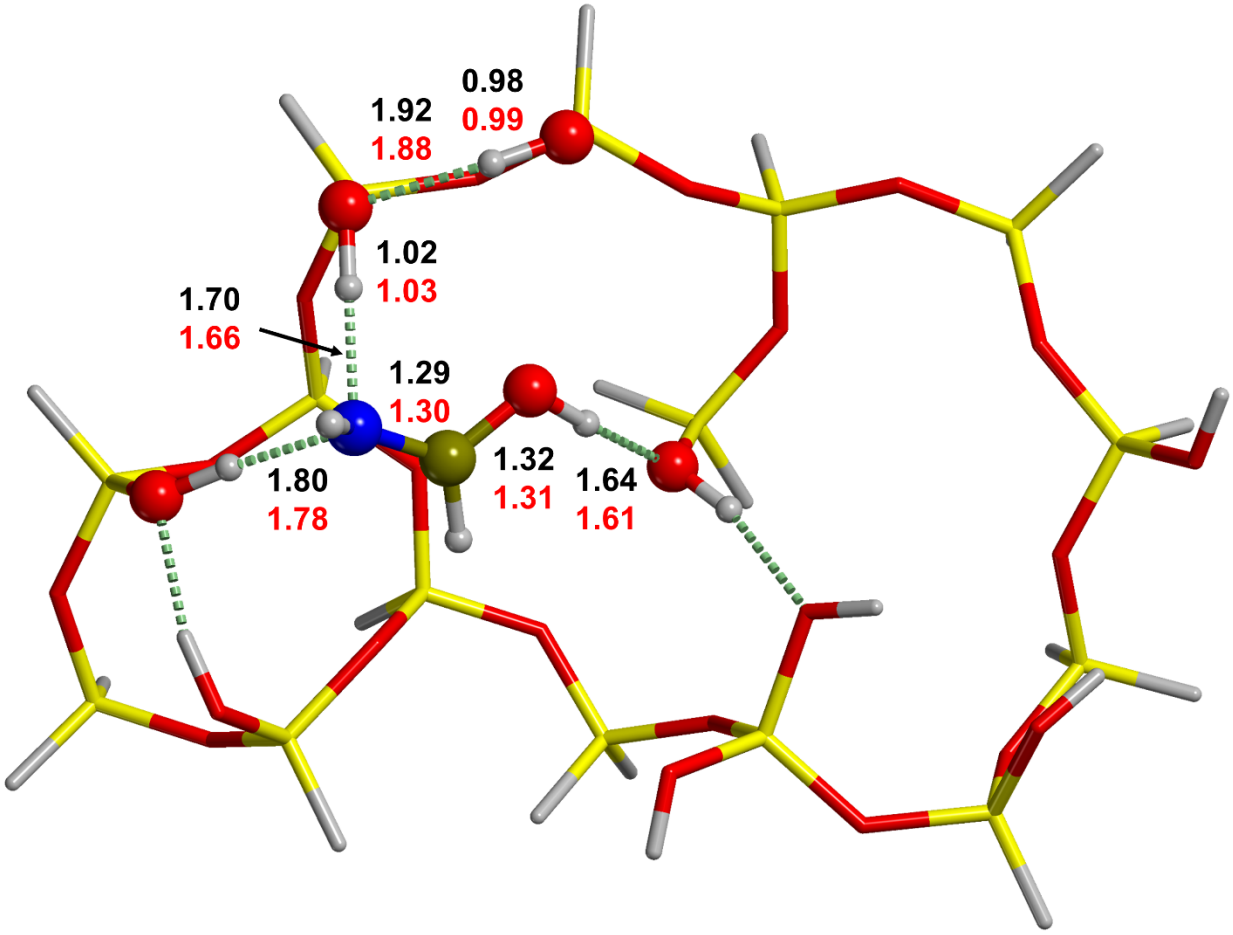

Gas phase coordinates	**PCM** coordinates
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H -3.236049 0.847182 3.419046	H -3.203139 0.864090 3.403358
O -0.933624 1.294278 1.624312	O -0.924295 1.276733 1.604004
O -3.159227 3.510397 2.037098	O -3.147515 3.504971 2.041603

O -0.475249 4.328461 2.312272	O -0.485253 4.320675 2.320332
H -1.372173 3.991859 2.538656	H -1.387462 3.967808 2.516264
H -0.250700 0.907486 0.973391	H -0.236357 0.876312 0.954078
O 2.482421 -1.427349 1.221814	O 2.477184 -1.428270 1.232657
O 5.226977 -2.802558 2.055870	O 5.192925 -2.810614 2.071099
H 5.961683 -2.187461 1.887389	H 6.057914 -2.367533 2.036363
O 7.243078 0.431845 1.369711	O 7.250598 0.455570 1.370153
H 7.469462 1.226052 1.878170	H 7.593663 1.262810 1.788852
H 3.274056 -1.356396 1.785534	H 3.311686 -1.351861 1.732649
O 0.765080 -3.356269 2.018723	O 0.765391 -3.343901 2.026617
H 0.572686 -4.295608 2.163218	H 0.441607 -4.260429 2.034733
O -4.711029 -2.620634 1.968750	O -4.725094 -2.601888 1.968107
H -5.114987 -1.714626 1.961932	H -5.108386 -1.683992 1.935986
O -5.519809 -0.003584 1.481259	O -5.519887 0.001955 1.490275
H -4.607241 0.354440 1.707764	H -4.600216 0.362689 1.714323
O 0.844454 0.379544 -0.129564	O 0.850757 0.388982 -0.122757
H 1.544857 -0.163953 0.312945	H 1.539777 -0.175509 0.315803
O 3.735626 3.985305 -0.304140	O 3.736859 3.983779 -0.304030
H 5.416634 3.410205 -2.181545	H 5.417362 3.408436 -2.181812
Si -0.325147 4.619965 0.686828	Si -0.323573 4.619290 0.687793
H 2.021829 4.721762 -2.039614	H 2.022884 4.720755 -2.039109
Si 2.240453 3.721361 -0.956220	Si 2.241496 3.720224 -0.955832
Si -3.183121 3.808670 0.397350	Si -3.181789 3.808667 0.398823
O -1.651959 4.063146 -0.156602	O -1.650679 4.062835 -0.155414
O 1.042299 3.896569 0.156518	O 1.043603 3.895622 0.157157
O 5.149912 -3.345299 -0.633836	O 5.149411 -3.347122 -0.634550
O 5.810081 -0.748925 -0.431270	O 5.810211 -0.750913 -0.431923
O 3.181993 -4.087864 0.999702	O 3.181648 -4.089360 0.999325
Si 6.179333 -2.188607 -1.177757	Si 6.178987 -2.190624 -1.178590
H 5.994058 -2.072316 -2.653331	H 5.993445 -2.074181 -2.654118
Si 5.242588 3.454072 -0.694266	Si 5.243622 3.452233 -0.694495
Si 4.811199 -3.931746 0.881653	Si 4.810866 -3.933604 0.880963
O 5.507720 1.935676 -0.080404	O 5.508531 1.933731 -0.080798
Si 6.548900 0.679840 -0.137926	Si 6.549414 0.677662 -0.138620
Si -2.392920 -1.260119 -1.355042	Si -2.393089 -1.260172 -1.354101
Si 1.953938 -2.989783 0.921415	Si 1.953828 -2.990994 0.921363
O -7.013376 -1.237618 -0.298593	O -7.013330 -1.236698 -0.296731
O -0.858997 -1.761565 -1.638793	O -0.859337 -1.761946 -1.638194
Si -6.644290 -2.677399 -1.045048	Si -6.644720 -2.676508 -1.043366
H -6.738836 -2.508242 -2.526706	H -6.739522 -2.507220 -2.524993
O -2.917398 -1.872503 0.094356	O -2.917418 -1.872544 0.095356
H -3.272093 -1.698884 -2.471054	H -3.272584 -1.698655 -2.469971
O -5.095265 -3.141947 -0.705881	O -5.095733 -3.141434 -0.704542
O -3.864506 2.543183 -0.389424	O -3.863618 2.543393 -0.387909
Si -4.009226 -3.031643 0.528320	Si -4.009424 -3.031468 0.529451
O -5.146098 0.381094 -1.190321	O -5.145861 0.381655 -1.188711
H -0.077554 1.460427 -2.287811	H -0.077290 1.459916 -2.287129
O -2.440362 0.380002 -1.192959	O -2.440126 0.379947 -1.191887
Si -6.274679 0.191157 -0.005303	Si -6.274250 0.191887 -0.003482
H -3.806416 1.786491 -2.833891	H -3.806186 1.786869 -2.832443
Si -3.789917 1.293749 -1.433757	Si -3.789521 1.294019 -1.432349
Si 1.192647 0.956637 -1.689294	Si 1.192915 0.955793 -1.688902

H 1.872152 -0.068493 -2.544080	H 1.872017 -0.069429 -2.543899
O 1.378737 -2.916203 -0.620572	O 1.378337 -2.917169 -0.620504
H 0.321460 -3.716273 -2.763951	H 0.320451 -3.716839 -2.763732
O 2.289000 2.211264 -1.585176	O 2.289574 2.210162 -1.584909
Si -0.025232 -3.170661 -1.420275	Si -0.025849 -3.171248 -1.419946
H 6.213135 4.391057 -0.048346	H 6.214511 4.388949 -0.048699
H 7.557937 0.927554 -1.213537	H 7.558293 0.925226 -1.214414
H 7.589036 -2.558422 -0.814024	H 7.588678 -2.560786 -0.815165
H 5.431425 -5.272676 1.042879	H 5.430819 -5.274687 1.041967
H -0.879604 -4.121563 -0.629168	H -0.880280 -4.122014 -0.628740
H -3.343484 -4.345097 0.717114	H -3.343943 -4.345087 0.718016
H -7.617620 -3.682540 -0.524506	H -7.618175 -3.681466 -0.522705
H -7.242508 1.317288 0.023465	H -7.241817 1.318236 0.025561
H -4.037185 4.999816 0.145367	H -4.035632 5.000025 0.147098
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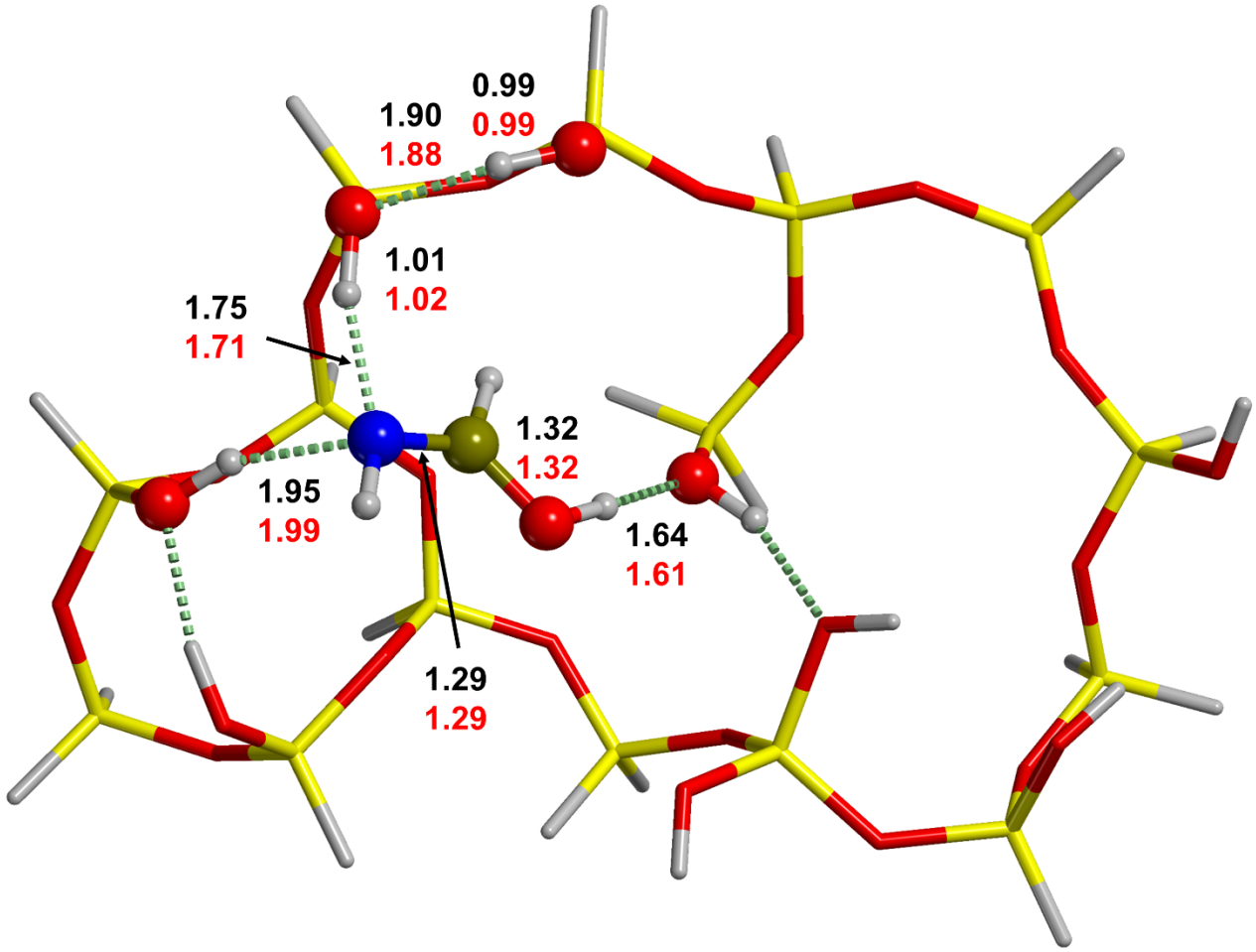

Gas phase coordinates	**PCM** coordinates
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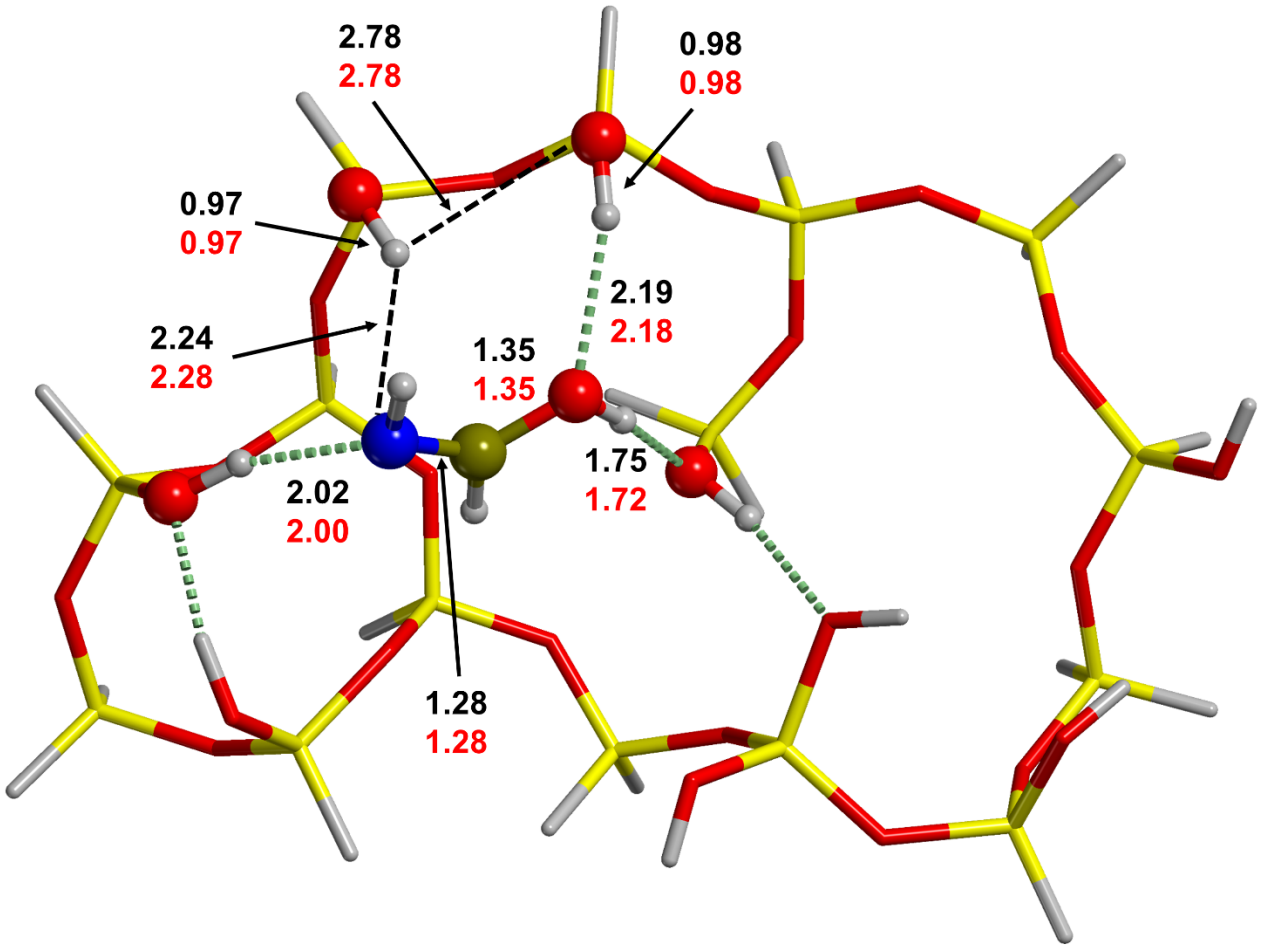
N -2.875118 0.818206 2.364756	N -2.841810 0.855735 2.375842
H -3.224572 2.533158 2.323824	H -3.198000 2.526340 2.314802

H -2.944929 0.030334 3.021618	H -2.889543 0.111835 3.083128
O -0.871289 -0.181149 1.743719	O -0.837934 -0.146287 1.747451
O -3.171720 3.511192 2.074311	O -3.168990 3.514759 2.076743
O -0.482710 4.251724 2.334646	O -0.483785 4.242747 2.337257
H -1.410319 4.027202 2.580555	H -1.418014 4.009972 2.560107
H -0.181333 0.017813 1.035980	H -0.158764 0.037384 1.015573
O 2.504273 -1.421184 1.192077	O 2.493474 -1.428319 1.230612
O 5.227624 -2.805826 2.032399	O 5.179318 -2.804569 2.043862
H 5.951190 -2.179263 1.858404	H 6.047489 -2.367109 2.016276
O 7.237118 0.440237 1.364991	O 7.242930 0.459997 1.364469
H 7.460626 1.230626 1.880542	H 7.586740 1.264480 1.787911
H 3.266522 -1.363390 1.796092	H 3.344384 -1.383542 1.708082
O 0.768854 -3.371139 1.996264	O 0.759187 -3.338736 2.007356
H 0.706286 -4.307177 2.240666	H 0.422749 -4.250675 1.995965
O -4.725930 -2.594079 1.956911	O -4.733307 -2.583978 1.961377
H -5.097139 -1.676507 1.955427	H -5.077038 -1.652692 1.946677
O -5.510413 0.050747 1.494712	O -5.509584 0.043652 1.500937
H -4.674453 0.553357 1.671823	H -4.674826 0.548979 1.672909
O 0.918936 0.371644 -0.128005	O 0.930454 0.367462 -0.122985
H 1.674293 -0.146169 0.255488	H 1.684730 -0.162410 0.249655
O 3.729096 4.007177 -0.275563	O 3.730371 4.002973 -0.279929
H 5.406597 3.445260 -2.160083	H 5.407334 3.438848 -2.164268
Si -0.329568 4.637275 0.726903	Si -0.327840 4.635830 0.722631
H 2.013073 4.758341 -2.002514	H 2.014489 4.753740 -2.007192
Si 2.232645 3.749429 -0.927240	Si 2.233703 3.745500 -0.931215
Si -3.188532 3.830693 0.435808	Si -3.187247 3.830467 0.432512
O -1.658214 4.088218 -0.118709	O -1.656876 4.086823 -0.122401
O 1.036476 3.917032 0.188805	O 1.037770 3.914513 0.184871
O 5.137009 -3.321769 -0.664083	O 5.134565 -3.326957 -0.663314
O 5.799572 -0.727551 -0.442583	O 5.798456 -0.732910 -0.443790
O 3.171151 -4.075371 0.966880	O 3.168553 -4.078390 0.968463
Si 6.166469 -2.161726 -1.200741	Si 6.164532 -2.167819 -1.200955
H 5.978894 -2.033909 -2.675072	H 5.976820 -2.040980 -2.675353
Si 5.235000 3.477792 -0.672224	Si 5.235956 3.472547 -0.676410
Si 4.800288 -3.919622 0.847388	Si 4.797752 -3.923543 0.848637
O 5.499918 1.954497 -0.070529	O 5.500194 1.949557 -0.073644
Si 6.540008 0.698327 -0.139411	Si 6.539646 0.692817 -0.141755
Si -2.405319 -1.225184 -1.356909	Si -2.406808 -1.227103 -1.356637
Si 1.943846 -2.975758 0.899064	Si 1.941789 -2.978213 0.900015
O -7.024068 -1.207180 -0.292866	O -7.025402 -1.206015 -0.291979
O -0.872257 -1.725625 -1.647016	O -0.874036 -1.728521 -1.646589
Si -6.657298 -2.641491 -1.050911	Si -6.659453 -2.641060 -1.049032
H -6.754120 -2.460826 -2.531089	H -6.756386 -2.461422 -2.529327
O -2.927934 -1.848314 0.088580	O -2.929537 -1.848921 0.089375
H -3.286652 -1.654635 -2.474839	H -3.288508 -1.656925 -2.474135
O -5.108109 -3.109844 -0.717879	O -5.110453 -3.109946 -0.715870
O -3.872281 2.571603 -0.359453	O -3.871734 2.571141 -0.361741
Si -4.019977 -3.009913 0.515354	Si -4.022103 -3.009663 0.517142
O -5.156866 0.416804 -1.175014	O -5.157508 0.416393 -1.175561
H -0.089291 1.500741 -2.272396	H -0.089541 1.496997 -2.274420
O -2.451194 0.413677 -1.182106	O -2.451839 0.411908 -1.183019
Si -6.283792 0.218632 0.010325	Si -6.284371 0.219646 0.010075

H -3.818786 1.833850 -2.809918	H -3.818943 1.831581 -2.811677
Si -3.800459 1.330396 -1.413730	Si -3.800677 1.329133 -1.415126
Si 1.181396 0.991083 -1.679980	Si 1.180971 0.987134 -1.681807
H 1.858848 -0.027713 -2.543652	H 1.857796 -0.032628 -2.544831
O 1.366204 -2.889834 -0.641372	O 1.363980 -2.893119 -0.640404
H 0.304817 -3.672521 -2.789133	H 0.301909 -3.676835 -2.787451
O 2.278943 2.244237 -1.567856	O 2.279160 2.239820 -1.570743
Si -0.039261 -3.137018 -1.440728	Si -0.041718 -3.140181 -1.439389
H 6.207337 4.409005 -0.020681	H 6.208848 4.403746 -0.025676
H 7.547489 0.953540 -1.214740	H 7.547108 0.946745 -1.217406
H 7.576465 -2.535437 -0.842165	H 7.574390 -2.541975 -0.842300
H 5.419707 -5.262240 0.997259	H 5.416519 -5.266361 0.999399
H -0.893107 -4.093325 -0.655587	H -0.895935 -4.095490 -0.653437
H -3.354979 -4.325305 0.692942	H -3.357738 -4.325258 0.695595
H -7.630591 -3.649844 -0.536575	H -7.633180 -3.648552 -0.533830
H -7.250590 1.345334 0.049310	H -7.250600 1.346860 0.048373
H -4.042230 5.024229 0.194366	H -4.040381 5.024254 0.190318
H -0.244971 6.107967 0.512086	H -0.242537 6.106323 0.506734



Gas phase coordinates	**PCM** coordinates
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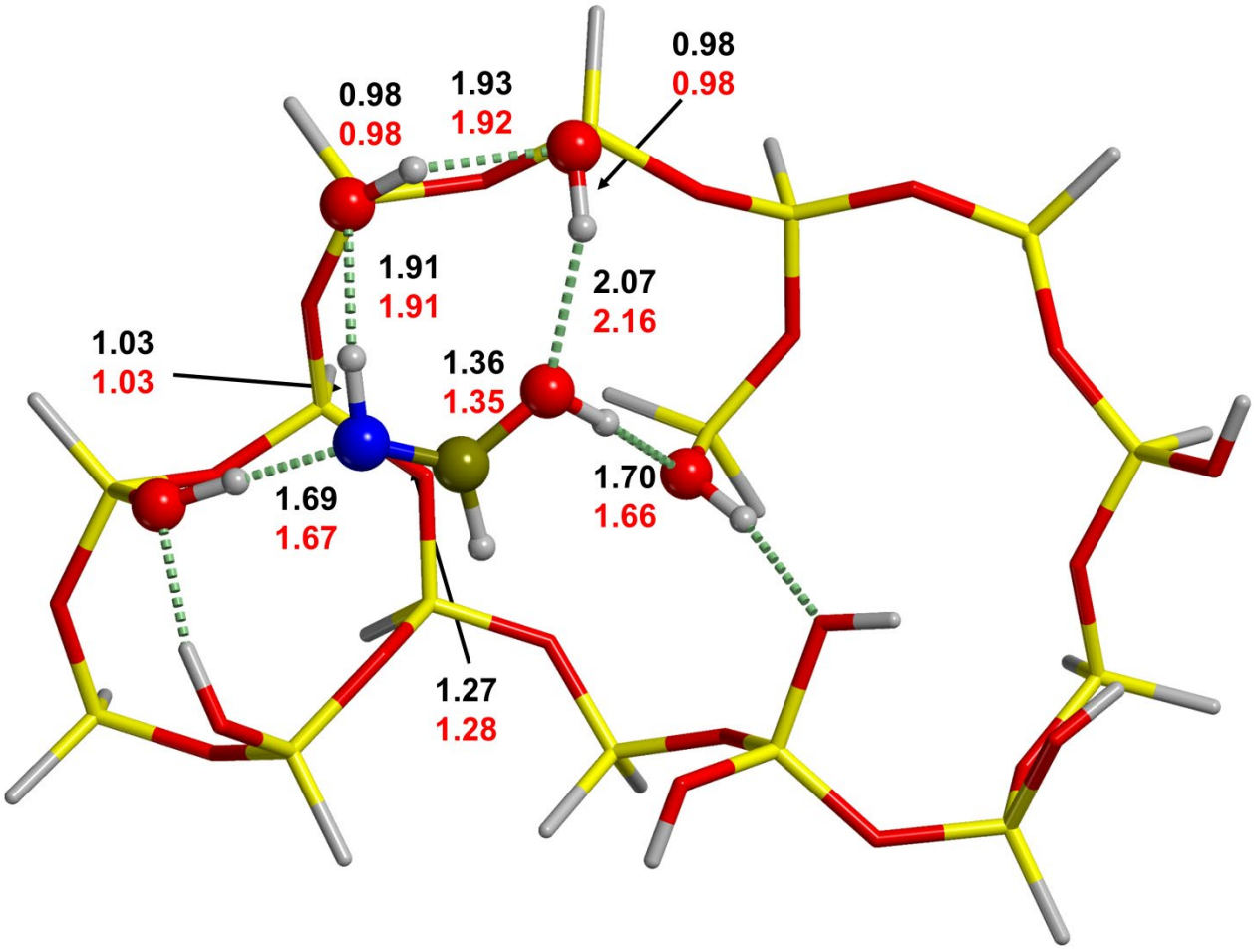
C -1.835824 0.576039 1.875590	C -1.807529 0.558776 1.845073
H -1.874117 -0.113437 1.034227	H -1.815924 -0.141585 1.012619

N -2.866762 0.679414 2.624810	N -2.848293 0.638078 2.588777
H -2.831937 2.907203 2.423659	H -2.830480 2.911303 2.436728
H -2.713256 1.276012 3.451112	H -2.715491 1.247983 3.408852
O -0.674184 1.260611 1.999113	O -0.672548 1.277364 1.966429
O -3.325453 3.637815 2.021670	O -3.328210 3.638907 2.031329
O -0.431006 4.310826 2.293929	O -0.436250 4.317416 2.303473
H -0.344057 3.362237 2.509043	H -0.371430 3.366769 2.523722
H -0.076551 1.000555 1.231500	H -0.060855 1.021819 1.202058
O 2.478449 -1.430859 1.211366	O 2.467809 -1.432101 1.228217
O 5.214499 -2.801930 2.048373	O 5.179360 -2.811701 2.063618
H 5.958110 -2.197169 1.882300	H 6.045746 -2.371369 2.028668
O 7.233306 0.427846 1.353530	O 7.240212 0.449869 1.353815
H 7.473730 1.222707 1.854379	H 7.584976 1.257656 1.770047
H 3.278839 -1.365947 1.763425	H 3.308563 -1.360974 1.718630
O 0.755919 -3.342994 2.021157	O 0.750730 -3.342704 2.022102
H 0.494832 -4.271747 2.117797	H 0.418583 -4.256250 2.024368
O -4.731208 -2.628610 1.965375	O -4.741808 -2.604203 1.967523
H -5.100500 -1.709926 1.981595	H -5.111592 -1.682167 1.944396
O -5.530160 -0.002850 1.475455	O -5.528517 0.006253 1.488209
H -4.682867 0.417853 1.772926	H -4.646453 0.391551 1.741951
O 0.846983 0.405518 -0.128334	O 0.846496 0.411970 -0.124444
H 1.536243 -0.173364 0.285239	H 1.530012 -0.173602 0.291550
O 3.727907 3.978971 -0.328197	O 3.729172 3.977509 -0.327119
H 5.407514 3.397202 -2.204799	H 5.407993 3.395810 -2.204446
Si -0.331798 4.619858 0.662933	Si -0.330008 4.619400 0.665510
H 2.013980 4.712254 -2.064888	H 2.014935 4.711929 -2.063024
Si 2.232185 3.714611 -0.978872	Si 2.233157 3.713855 -0.977407
Si -3.190538 3.810645 0.377004	Si -3.189104 3.811219 0.380220
O -1.659627 4.062457 -0.178481	O -1.658287 4.062713 -0.175667
O 1.034734 3.893992 0.133966	O 1.036118 3.893261 0.135870
O 5.135321 -3.353799 -0.638504	O 5.134082 -3.355619 -0.640297
O 5.797963 -0.757486 -0.443348	O 5.797637 -0.759588 -0.444493
O 3.167480 -4.090092 0.997964	O 3.166518 -4.091808 0.996551
Si 6.165551 -2.199545 -1.186058	Si 6.164517 -2.201522 -1.187796
H 5.979699 -2.087115 -2.661860	H 5.978234 -2.088543 -2.663502
Si 5.234200 3.445295 -0.717561	Si 5.235166 3.443468 -0.717137
Si 4.796775 -3.935789 0.878739	Si 4.795826 -3.938000 0.876861
O 5.498224 1.928337 -0.099679	O 5.498888 1.926219 -0.099841
Si 6.538231 0.671395 -0.154230	Si 6.538466 0.668954 -0.155137
Si -2.405928 -1.263685 -1.361932	Si -2.406710 -1.262793 -1.360643
Si 1.940396 -2.991104 0.917243	Si 1.939769 -2.992391 0.916583
O -7.025923 -1.233978 -0.303667	O -7.026360 -1.231920 -0.300903
O -0.872597 -1.767307 -1.645018	O -0.873634 -1.766824 -1.644381
Si -6.658417 -2.676258 -1.046004	Si -6.659562 -2.674075 -1.043834
H -6.753528 -2.511015 -2.528177	H -6.755089 -2.508311 -2.525922
O -2.930297 -1.871618 0.089378	O -2.930819 -1.871034 0.090632
H -3.286023 -1.704686 -2.476334	H -3.287303 -1.703136 -2.474911
O -5.109693 -3.141230 -0.706388	O -5.110883 -3.139667 -0.704862
O -3.873567 2.543503 -0.405906	O -3.872797 2.544560 -0.402893
Si -4.022985 -3.028573 0.527004	Si -4.023747 -3.027775 0.528222
O -5.157404 0.380289 -1.200345	O -5.157595 0.382030 -1.197640
H -0.088490 1.452259 -2.303163	H -0.088680 1.452702 -2.301710

O -2.451795 0.376920 -1.204311 Si -6.285786 0.194916 -0.014256 H -3.817319 1.780170 -2.848454 Si -3.800719 1.291383 -1.447089 Si 1.181444 0.948667 -1.703978 H 1.859762 -0.079175 -2.556178 O 1.364548 -2.921209 -0.624675 H 0.305547 -3.726165 -2.765371 O 2.279019 2.202800 -1.603687 Si -0.040022 -3.176566 -1.423034 H 6.205902 4.383150 -0.074656 H 7.546989 0.915243 -1.231000 H 7.575083 -2.569655 -0.821963 H 5.415846 -5.276841 1.043344 H -0.894900 -4.124518 -0.628935 H -3.358364 -4.342111 0.719094 H -7.632461 -3.679029 -0.522369 H -7.252527 1.321921 0.011765 H -4.043821 5.001785 0.122055 H -0.246810 6.088341 0.432861	O -2.451989 0.377775 -1.202465 Si -6.285662 0.196635 -0.011254 H -3.817574 1.782017 -2.845711 Si -3.800690 1.292761 -1.444513 Si 1.181279 0.948496 -1.703095 H 1.858989 -0.079287 -2.555849 O 1.363455 -2.921797 -0.625129 H 0.303512 -3.725697 -2.765756 O 2.279297 2.202235 -1.602737 Si -0.041451 -3.176429 -1.423127 H 6.207380 4.380791 -0.074230 H 7.546962 0.912827 -1.232146 H 7.574042 -2.572215 -0.824270 H 5.414509 -5.279309 1.040826 H -0.896389 -4.124363 -0.629071 H -3.359497 -4.341594 0.719667 H -7.633769 -3.676700 -0.520221 H -7.252025 1.323948 0.015446 H -4.042077 5.002723 0.125935 H -0.244611 6.087931 0.435897



Gas phase coordinates	**PCM** coordinates
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N -3.029174 0.743657 2.223622	N -3.028725 0.717914 2.221597
H -2.405264 3.956378 2.486625	H -2.388281 3.908829 2.488354
H -3.123561 1.729393 2.514719	H -3.110317 1.712424 2.489379
O -0.829279 1.373206 1.734046	O -0.851932 1.350045 1.676897
O -3.206817 3.580019 2.060483	O -3.210583 3.568608 2.066732
O -0.504763 4.244324 2.312564	O -0.506189 4.248864 2.322094
H -0.403960 3.273401 2.438923	H -0.345339 3.292778 2.476259
H -0.135133 1.010403 1.104141	H -0.145156 0.982765 1.052848
O 2.495455 -1.436640 1.228169	O 2.481384 -1.434569 1.240136
O 5.220825 -2.798775 2.052232	O 5.188612 -2.809938 2.067572
H 5.978453 -2.208828 1.897319	H 6.055475 -2.370411 2.033963
O 7.239694 0.431340 1.359424	O 7.246903 0.453569 1.361464
H 7.489903 1.225308 1.856824	H 7.589164 1.261503 1.779477
H 3.311769 -1.382252 1.758172	H 3.328432 -1.368093 1.720628
O 0.763127 -3.333099 2.032375	O 0.761132 -3.341968 2.031642
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H -5.124615 -1.728115 1.986770	H -5.130844 -1.694845 1.943337
O -5.526676 -0.002919 1.487208	O -5.523509 0.004353 1.498806
H -4.574807 0.283378 1.717900	H -4.553961 0.279888 1.705655
O 0.873226 0.390026 -0.119974	O 0.868278 0.389854 -0.118969
H 1.568566 -0.179720 0.296005	H 1.560638 -0.181430 0.302887
O 3.728393 3.980391 -0.313501	O 3.730884 3.980348 -0.310123
H 5.406168 3.402265 -2.192866	H 5.408201 3.403116 -2.190170
Si -0.330638 4.616516 0.683439	Si -0.327795 4.617046 0.687884
H 2.011639 4.714122 -2.047207	H 2.014127 4.715981 -2.043019
Si 2.232094 3.715436 -0.962605	Si 2.234406 3.716387 -0.959218
Si -3.189010 3.805074 0.400162	Si -3.186475 3.806767 0.404390
O -1.659021 4.058889 -0.156949	O -1.656482 4.060505 -0.152744
O 1.035878 3.892476 0.151934	O 1.038406 3.892965 0.155628
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O 5.802531 -0.754079 -0.436651	O 5.803440 -0.754710 -0.437213
O 3.176830 -4.090678 1.004143	O 3.176842 -4.091550 1.001386
Si 6.170476 -2.194961 -1.181467	Si 6.170804 -2.195139 -1.183190
H 5.982676 -2.081013 -2.656906	H 5.982831 -2.079993 -2.658514
Si 5.234673 3.448506 -0.705358	Si 5.236933 3.448268 -0.702603
Si 4.805836 -3.934783 0.883056	Si 4.805882 -3.936099 0.880187
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Si 6.541884 0.675132 -0.146828	Si 6.543307 0.674033 -0.146394
Si -2.402049 -1.266564 -1.345549	Si -2.401437 -1.263786 -1.345337
Si 1.948666 -2.992696 0.926213	Si 1.949030 -2.993103 0.924475
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O -0.868625 -1.768492 -1.631128	O -0.868219 -1.766000 -1.631520
Si -6.652876 -2.683299 -1.025915	Si -6.652687 -2.679362 -1.026189
H -6.749990 -2.516449 -2.507778	H -6.749956 -2.511340 -2.507909
O -2.924057 -1.876622 0.105721	O -2.923441 -1.874788 0.105536
H -3.283144 -1.707080 -2.459352	H -3.282836 -1.703154 -2.459354
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Si -4.015163 -3.035052 0.543392	Si -4.014868 -3.033195 0.542471

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O -2.449183 0.373818 -1.185997	O -2.448007 0.376488 -1.184516
Si -6.281517 0.187028 0.008645	Si -6.280233 0.190044 0.010527
H -3.818016 1.777722 -2.826826	H -3.816609 1.782107 -2.824069
Si -3.799226 1.287351 -1.426042	Si -3.797782 1.290652 -1.423666
Si 1.182916 0.949383 -1.689555	Si 1.184210 0.951242 -1.688147
H 1.861084 -0.076879 -2.543776	H 1.861917 -0.074587 -2.543256
O 1.370825 -2.921557 -0.614903	O 1.370994 -2.920586 -0.616503
H 0.309864 -3.725016 -2.755190	H 0.309463 -3.722047 -2.757257
O 2.279496 2.204381 -1.589205	O 2.281218 2.205801 -1.586988
Si -0.034515 -3.177258 -1.411795	Si -0.034544 -3.175210 -1.413391
H 6.206342 4.386495 -0.062598	H 6.209003 4.385441 -0.059260
H 7.549075 0.921111 -1.224579	H 7.550426 0.920509 -1.224099
H 7.580792 -2.564225 -0.819559	H 7.581050 -2.565148 -0.821767
H 5.426310 -5.275468 1.045355	H 5.425937 -5.277113 1.041365
H -0.887551 -4.126880 -0.617711	H -0.887781 -4.125161 -0.619917
H -3.349130 -4.348213 0.733150	H -3.349241 -4.346722 0.731123
H -7.625368 -3.687537 -0.502207	H -7.625436 -3.683682 -0.503117
H -7.249230 1.313138 0.037163	H -7.247570 1.316451 0.040049
H -4.043675 4.995741 0.147642	H -4.040783 4.997910 0.152907
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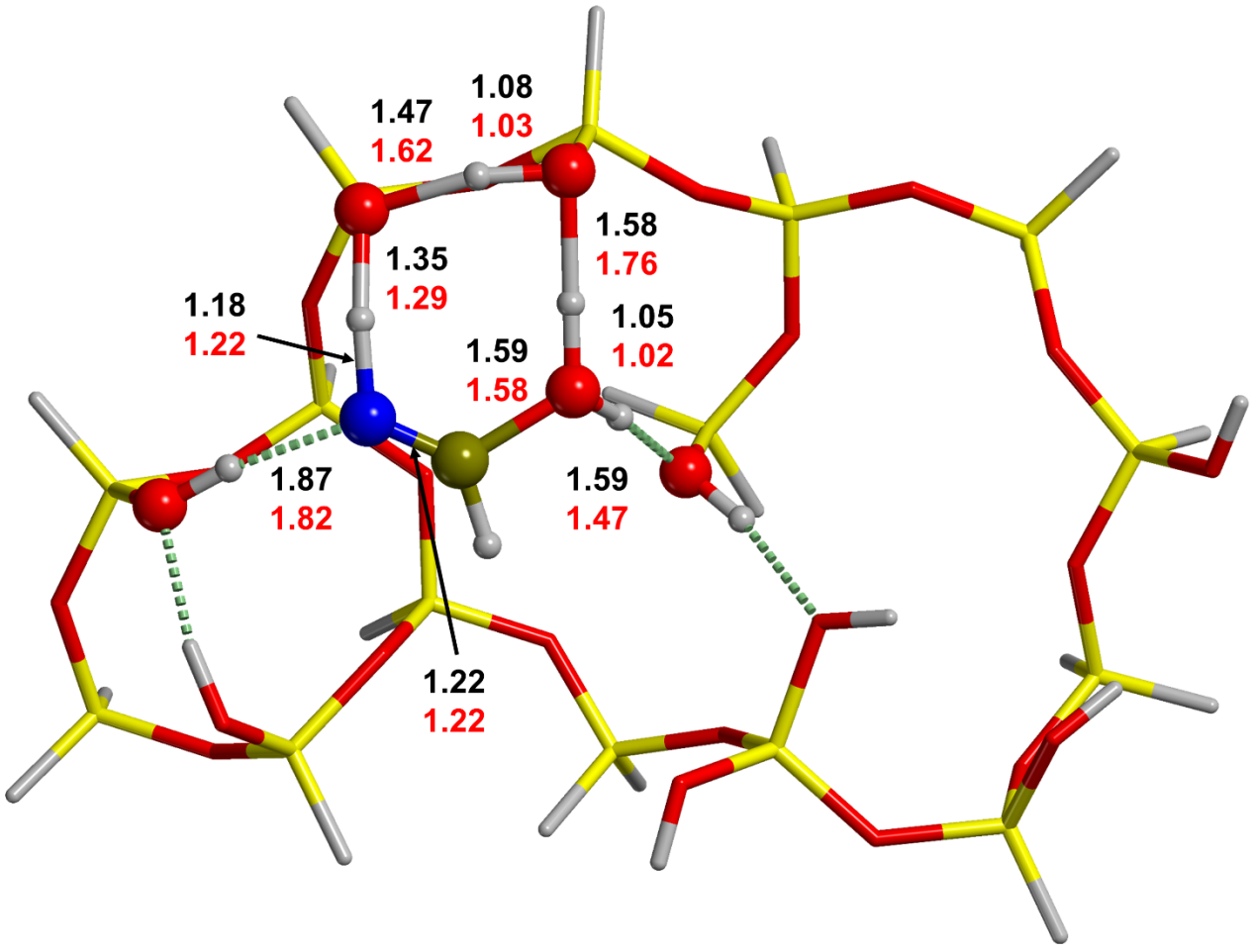

Gas phase coordinates	**PCM** coordinates

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N -2.964953 1.028143 2.209316	N -2.981723 1.012933 2.186493
H -1.656978 3.901630 2.335991	H -1.575370 3.925212 2.401524
H -3.049370 2.199892 2.253449	H -3.050867 2.229304 2.216955
O -0.527971 1.363559 1.888292	O -0.540490 1.248146 1.835232
O -3.048761 3.526814 2.029723	O -3.099561 3.503459 2.041628
O -0.585526 3.972199 2.231448	O -0.557119 3.995746 2.257379
H -0.551043 2.408804 2.025795	H -0.555099 2.254259 1.988665
H 0.032001 1.072683 1.072985	H 0.031373 0.961360 0.985755
O 2.473411 -1.430994 1.205416	O 2.445023 -1.402890 1.163783
O 5.208383 -2.807036 2.040022	O 5.433272 -2.911549 2.029259
H 5.964349 -2.214253 1.887383	H 5.454265 -1.964254 1.799902
O 7.230522 0.423697 1.350533	O 7.227134 0.455542 1.356056
H 7.476847 1.216043 1.852513	H 7.548245 1.263591 1.790292
H 3.273724 -1.359401 1.756994	H 2.650075 -1.152530 2.081484
O 0.754095 -3.338957 2.023020	O 0.779118 -3.352270 2.038747
H 0.495495 -4.267165 2.132074	H 0.743736 -4.277194 2.334965
O -4.721021 -2.623843 1.983003	O -4.733413 -2.605046 1.978910
H -5.103495 -1.708271 1.986659	H -5.100498 -1.680401 1.950304
O -5.529810 -0.008206 1.498741	O -5.528989 0.000572 1.510693
H -4.670204 0.437657 1.734538	H -4.640646 0.423419 1.711888
O 0.861118 0.408677 -0.105814	O 0.846563 0.405927 -0.106532
H 1.548049 -0.178754 0.307507	H 1.503106 -0.230376 0.299828
O 3.720432 3.979451 -0.310858	O 3.715553 3.987590 -0.304159
H 5.395689 3.404467 -2.193431	H 5.391074 3.417456 -2.187971
Si -0.337078 4.615660 0.692202	Si -0.342482 4.617509 0.700746
H 2.002061 4.717882 -2.040964	H 1.995945 4.726661 -2.032761
Si 2.223228 3.716729 -0.958784	Si 2.218517 3.724109 -0.952166
Si -3.196229 3.806413 0.410513	Si -3.200744 3.805349 0.418430
O -1.666751 4.060588 -0.147836	O -1.671686 4.062170 -0.139857
O 1.028414 3.892017 0.157534	O 1.023741 3.896286 0.164676
O 5.129556 -3.351768 -0.648816	O 5.133183 -3.341447 -0.653665
O 5.791795 -0.755887 -0.446678	O 5.792427 -0.745106 -0.447688
O 3.165927 -4.094145 0.989962	O 3.170779 -4.088635 0.984393
Si 6.158070 -2.195356 -1.195040	Si 6.160225 -2.182996 -1.198335
H 5.968610 -2.078111 -2.670008	H 5.970309 -2.063710 -2.673081
Si 5.225957 3.447583 -0.705627	Si 5.221614 3.458091 -0.700067
Si 4.794877 -3.938888 0.867308	Si 4.799520 -3.931284 0.861628
O 5.491986 1.928682 -0.093405	O 5.489553 1.938565 -0.090232
Si 6.532280 0.672285 -0.154628	Si 6.531303 0.683482 -0.153606
Si -2.414124 -1.261869 -1.347087	Si -2.413089 -1.259313 -1.347111
Si 1.938283 -2.995318 0.915845	Si 1.941834 -2.991134 0.912225
O -7.031554 -1.237251 -0.277558	O -7.030313 -1.241741 -0.276555
O -0.881314 -1.764025 -1.635545	O -0.879754 -1.759231 -1.636668
Si -6.665361 -2.676943 -1.025549	Si -6.662597 -2.679854 -1.026832
H -6.764113 -2.506832 -2.506932	H -6.761868 -2.507587 -2.507931
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H -3.296764 -1.699486 -2.460810	H -3.295457 -1.696254 -2.461314
O -5.115664 -3.142502 -0.691219	O -5.112284 -3.144111 -0.693549

O -3.880725 2.541632 -0.374928	O -3.883930 2.540973 -0.368804
Si -4.026012 -3.033549 0.539908	Si -4.022494 -3.035771 0.537510
O -5.165753 0.380614 -1.173410	O -5.166600 0.379680 -1.170324
H -0.099883 1.457970 -2.284933	H -0.102235 1.464669 -2.281280
O -2.460161 0.378190 -1.183931	O -2.461010 0.380439 -1.181429
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H -3.830130 1.786399 -2.820116	H -3.832980 1.789551 -2.815158
Si -3.809976 1.292986 -1.420420	Si -3.811946 1.294016 -1.416225
Si 1.171666 0.952836 -1.690490	Si 1.170033 0.960113 -1.687885
H 1.848266 -0.071949 -2.547722	H 1.847646 -0.062563 -2.546834
O 1.358682 -2.920524 -0.624437	O 1.361812 -2.914656 -0.627816
H 0.294775 -3.718762 -2.765215	H 0.298377 -3.710855 -2.769587
O 2.269059 2.207008 -1.588707	O 2.265979 2.215411 -1.584414
Si -0.047730 -3.173723 -1.420236	Si -0.044474 -3.168281 -1.423700
H 6.198897 4.383642 -0.061975	H 6.193597 4.394300 -0.055188
H 7.538348 0.920039 -1.233021	H 7.536847 0.934068 -1.231833
H 7.568603 -2.566182 -0.835582	H 7.571269 -2.552721 -0.839749
H 5.414796 -5.280264 1.025980	H 5.421042 -5.272175 1.018109
H -0.900365 -4.124590 -0.627212	H -0.895824 -4.121360 -0.631953
H -3.360487 -4.347486 0.726045	H -3.355391 -4.349212 0.721488
H -7.637798 -3.681774 -0.502878	H -7.633744 -3.686623 -0.505494
H -7.258253 1.317513 0.046871	H -7.259931 1.312255 0.051842
H -4.050527 4.998096 0.161570	H -4.056490 4.996411 0.171499
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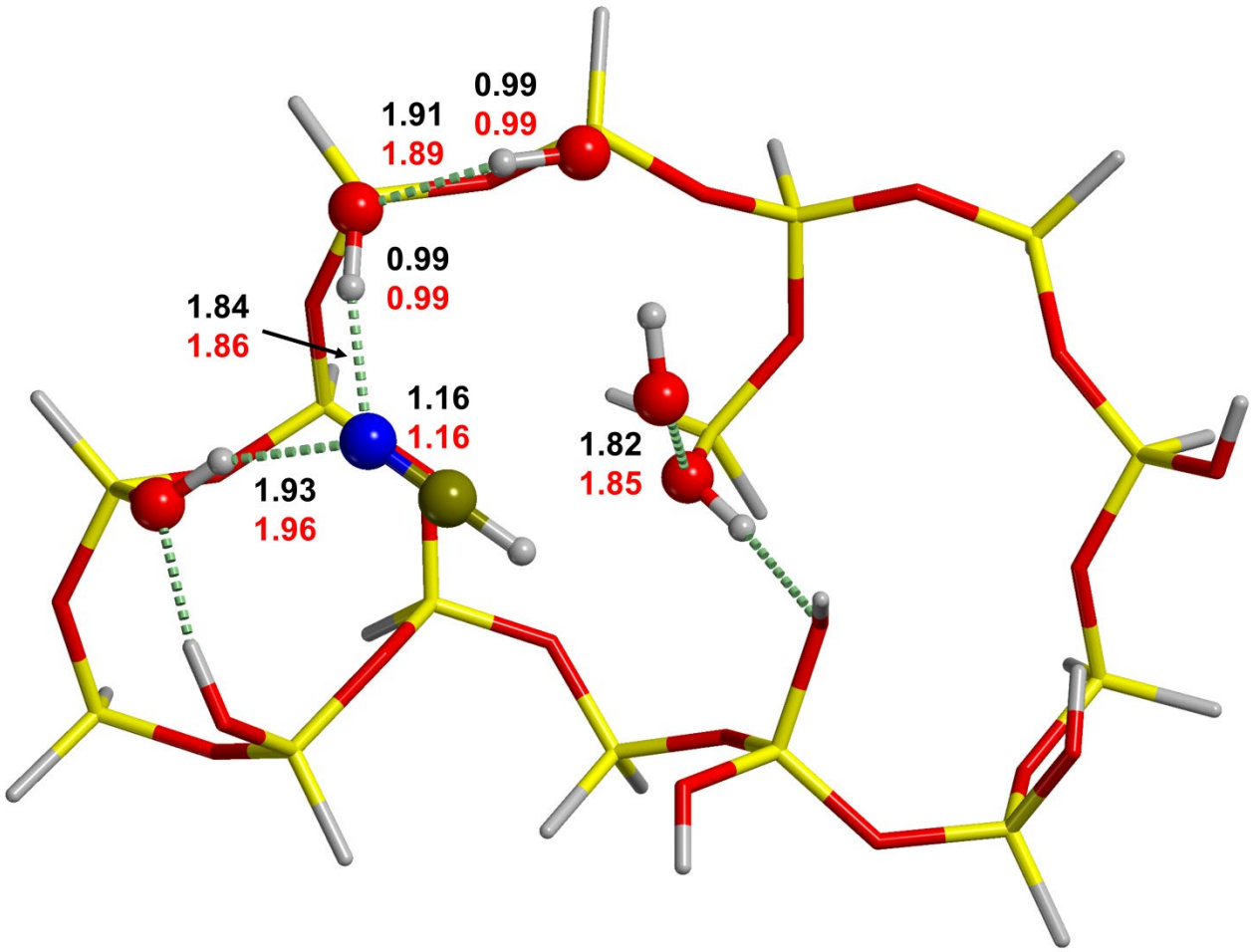

Gas phase coordinates	**PCM** coordinates
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H -1.178281 -0.529209 2.427263	H -1.054160 -0.439775 2.221462
N -2.993929 0.773538 2.392678	N -2.942000 0.752236 2.349483
H -1.396342 4.056053 2.538230	H -1.407405 4.049345 2.527537
H -3.207346 2.599027 2.289696	H -3.185548 2.593967 2.284599
O 0.467829 1.282677 2.398442	O 0.585706 1.475384 2.410345
O -3.165728 3.552922 2.035881	O -3.166729 3.550681 2.039971
O -0.457923 4.200595 2.272784	O -0.464691 4.204930 2.274988
H 0.356222 2.243193 2.546430	H 0.294888 2.411835 2.451250
H 0.555724 1.194886 1.421097	H 0.647212 1.282872 1.446326
O 2.416974 -1.419132 1.188848	O 2.431821 -1.423501 1.160214
O 5.380845 -2.929585 2.010064	O 5.404034 -2.936860 2.010027
H 5.479273 -1.992315 1.763590	H 5.382527 -1.985911 1.796250
O 7.214404 0.432067 1.319959	O 7.209531 0.424554 1.317456
H 7.408321 1.237619 1.823551	H 7.532223 1.234878 1.746224
H 2.369840 -1.108487 2.109487	H 2.550870 -1.154889 2.087675
O 0.731709 -3.355597 2.012861	O 0.733336 -3.347810 2.025046
H 0.727398 -4.262052 2.357679	H 0.687564 -4.272230 2.321061
O -4.746728 -2.592702 1.969441	O -4.767174 -2.579904 1.980361
H -5.135876 -1.683573 1.975734	H -5.126889 -1.655073 1.962408
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H -4.797817 0.543734 1.756345	H -4.796897 0.542412 1.754082
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H 1.497888 -0.264231 0.184521	H 1.471835 -0.265849 0.205737
O 3.717713 3.972048 -0.345386	O 3.713236 3.965454 -0.353820
H 5.389023 3.387437 -2.228503	H 5.382350 3.376628 -2.237571
Si -0.336311 4.626585 0.660054	Si -0.339496 4.623330 0.654643
H 2.001009 4.715165 -2.075140	H 1.994956 4.705817 -2.083190
Si 2.218898 3.714634 -0.991722	Si 2.213649 3.707307 -0.998071
Si -3.198885 3.828984 0.381822	Si -3.202636 3.826179 0.380983
O -1.668935 4.075705 -0.178105	O -1.673196 4.071290 -0.181039
O 1.025740 3.896475 0.125315	O 1.021737 3.891718 0.119875
O 5.096077 -3.365439 -0.674078	O 5.088739 -3.373129 -0.669783
O 5.769265 -0.772049 -0.476166	O 5.763024 -0.779593 -0.477599
O 3.130723 -4.097321 0.967358	O 3.124874 -4.101160 0.975144
Si 6.128939 -2.214086 -1.222779	Si 6.121413 -2.223195 -1.221802
H 5.938761 -2.098145 -2.697758	H 5.929713 -2.110040 -2.696801
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Si 4.760203 -3.949012 0.843151	Si 4.754272 -3.953652 0.848926
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Si 6.515918 0.653445 -0.186747	Si 6.510471 0.646200 -0.191727
Si -2.439420 -1.245186 -1.369178	Si -2.446764 -1.251628 -1.361005
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O -2.961428 -1.853868 0.082668	O -2.967442 -1.857323 0.092567
H -3.324785 -1.680707 -2.481561	H -3.333456 -1.688994 -2.471606

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O -3.889379 2.565643 -0.401074	O -3.894392 2.561564 -0.398737
Si -4.057112 -3.007478 0.521642	Si -4.063056 -3.009704 0.534930
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O -2.478508 0.395280 -1.208315	O -2.485120 0.389159 -1.203273
Si -6.309440 0.225586 -0.006225	Si -6.314834 0.223109 0.003197
H -3.843953 1.806853 -2.845383	H -3.851814 1.798035 -2.841621
Si -3.824731 1.315407 -1.445081	Si -3.831278 1.309290 -1.440393
Si 1.155259 0.954104 -1.718645	Si 1.148296 0.945744 -1.718528
H 1.826893 -0.074699 -2.574969	H 1.818670 -0.084944 -2.573572
O 1.327045 -2.918480 -0.647241	O 1.319890 -2.924821 -0.639821
H 0.258079 -3.715326 -2.786019	H 0.248387 -3.725432 -2.775922
O 2.257941 2.203845 -1.619534	O 2.251510 2.195294 -1.623001
Si -0.081054 -3.166964 -1.441538	Si -0.089134 -3.174355 -1.432145
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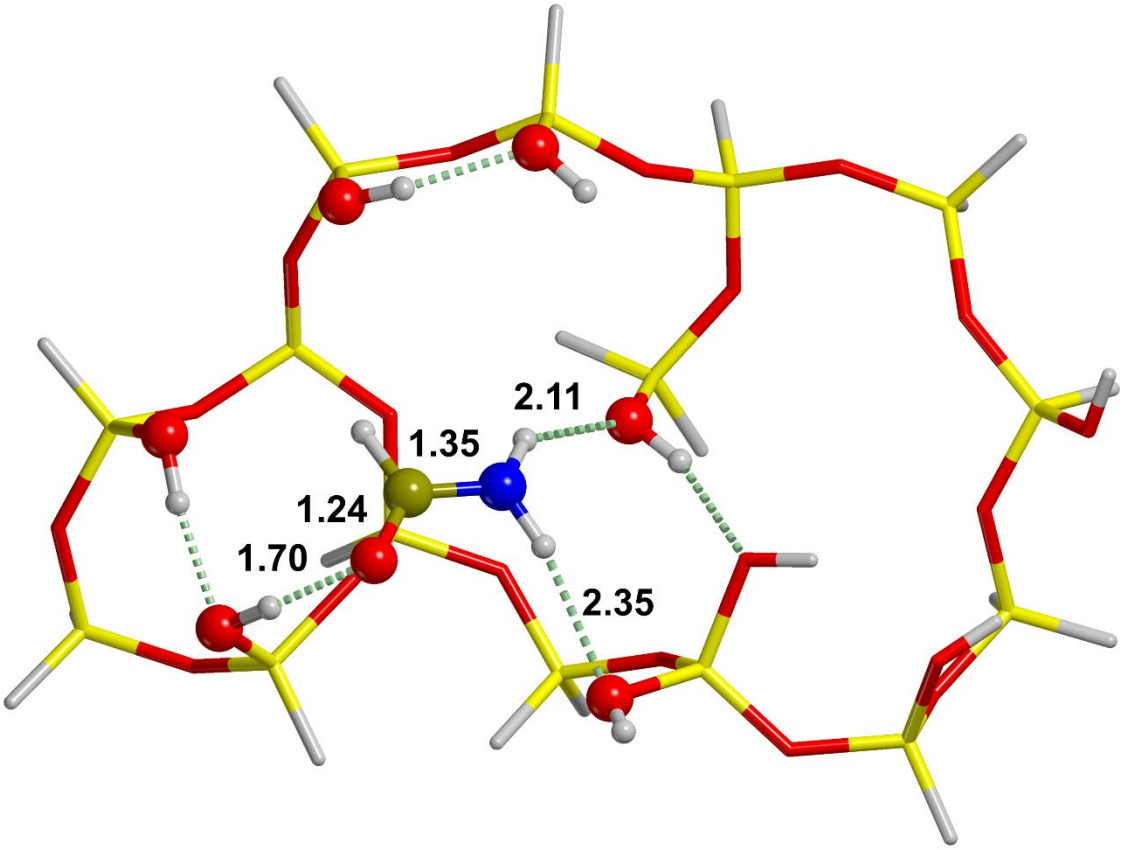
H 7.522123 0.895485 -1.266307	H 7.515615 0.885806 -1.272817
H 7.538214 -2.590264 -0.863943	H 7.530938 -2.599164 -0.863731
H 5.374671 -5.292728 1.003223	H 5.368449 -5.297268 1.010945
H -0.936985 -4.113153 -0.646471	H -0.944546 -4.118710 -0.634345
H -3.396903 -4.323902 0.709105	H -3.403099 -4.325991 0.724239
H -7.672414 -3.642154 -0.517285	H -7.679673 -3.645142 -0.498941
H -7.271619 1.356307 0.025064	H -7.276592 1.354220 0.033318
H -4.048624 5.023607 0.131900	H -4.052231 5.020609 0.129652
H -0.246434 6.095125 0.432508	H -0.249358 6.091396 0.424163

Figure S9: PBE-D2/TZVP optimized geometries for the formamide dehydration reaction catalysed by hydrophilic silica. In the figures the most representative bond lengths (in Å) in gas phase (black) and in PCM (F) (red) are reported. In the left and the right columns the cartesian coordinates of the optimized structures in gas phase and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue, silicons in yellow.

Formamide + Silica 4.5 decarbonylation reaction



Gas phase coordinates	**PCM (F)** coordinates
74 SiH_R_G C -2.1782691305 -0.5279780878 2.4298038227 H -2.8028971305 0.3192259122 2.0800648227 N -0.8771701305 -0.4408710878 2.0909488227 H -0.3033561305 -1.2711490878 2.2464358227 H -0.5617991305 0.2054679122 1.3636178227 O -2.6512601305 -1.4665280878 3.0929918227 O -3.1019031305 3.5194139122 2.1054548227 O -0.4156461305 4.2643239122 2.4384388227 H -2.2548491305 3.6980369122 2.5614168227 H 0.2686198695 3.6619239122 2.7731528227 O 2.4992818695 -1.4553660878 1.2016058227 O 5.1547828695 -2.8666130878 1.9337558227 H 5.9594028695 -2.3284440878 1.8380228227 O 7.2495318695 0.3351399122 1.3690508227 H 7.5318088695 1.1052149122 1.8865208227 H 3.4025748695 -1.4623040878 1.5723938227 O 0.6168668695 -3.3794150878 1.7654958227 H 0.8054758695 -3.8400340878 2.5975868227 O -4.7951571305 -2.4081580878 1.8078458227 H -4.1002161305 -2.1224250878 2.4772578227	

O -5.5535701305 0.2742719122 1.4557918227 H -5.3728541305 -0.6638620878 1.7050038227 O 0.8821698695 0.4737879122 -0.1497911773 H 1.5856118695 -0.0850730878 0.2529458227 O 3.8110168695 4.0086909122 -0.1873121773 H 5.4863478695 3.4683829122 -2.0800631773 Si -0.2401891305 4.6829819122 0.8166468227 H 2.1156988695 4.8363089122 -1.8997051773 Si 2.3130558695 3.7950439122 -0.8513001773 Si -3.1116781305 3.9348229122 0.4931588227 O -1.5746231305 4.1802399122 -0.0484141773 O 1.1152678695 3.9534649122 0.2643388227 O 5.0920178695 -3.3307620878 -0.7687661773 O 5.7989618695 -0.7555470878 -0.4746571773 O 3.1064128695 -4.0933670878 0.8338428227 Si 6.1438818695 -2.1749700878 -1.2699821773 H 5.9647868695 -2.0041190878 -2.7410061773 Si 5.3090768695 3.4637569122 -0.5925231773 Si 4.7385158695 -3.9631740878 0.7247008227 O 5.5447498695 1.9203469122 -0.0312801773 Si 6.5629608695 0.6483659122 -0.1302651773 Si -2.4094611305 -1.0836970878 -1.4327881773 Si 1.8988448695 -2.9708730878 0.7912228227 O -7.0315971305 -1.0130920878 -0.3858571773 O -0.8841861305 -1.6030540878 -1.7306011773 Si -6.6868451305 -2.4326120878 -1.1811551773 H -6.7742431305 -2.2103940878 -2.6562301773 O -2.9489891305 -1.7363180878 -0.0066621773 H -3.2934581305 -1.4672240878 -2.5652201773 O -5.1474981305 -2.9370150878 -0.8551101773 O -3.8139421305 2.7101429122 -0.3385661773 Si -4.0629951305 -2.8895930878 0.3844478227 O -5.1326311305 0.6010639122 -1.2168531773 H -0.0422361305 1.6246509122 -2.2655471773 O -2.4273681305 0.5504009122 -1.2138711773 Si -6.2677191305 0.3908359122 -0.0415171773 H -3.7630161305 2.0378679122 -2.8077521773 Si -3.7593451305 1.4965839122 -1.4255751773 Si 1.2169068695 1.0771379122 -1.6822611773 H 1.8798998695 0.0700189122 -2.5707521773 O 1.3292908695 -2.8332370878 -0.7484721773 H 0.2634208695 -3.5388460878 -2.9205811773 O 2.3357128695 2.3070659122 -1.5322861773 Si -0.0769071305 -3.0339560878 -1.5594721773 H 6.2948178695 4.3597699122 0.0876148227 H 7.5792858695 0.9147259122 -1.1944981773 H 7.5455948695 -2.5830070878 -0.9163851773 H 5.3336948695 -5.3200510878 0.8404958227 H -0.9506661305 -3.9959180878 -0.8036981773 H -3.4218801305 -4.2208100878 0.5288448227 H -7.6797941305 -3.4371920878 -0.6979151773 H -7.2148871305 1.5328619122 0.0243708227	

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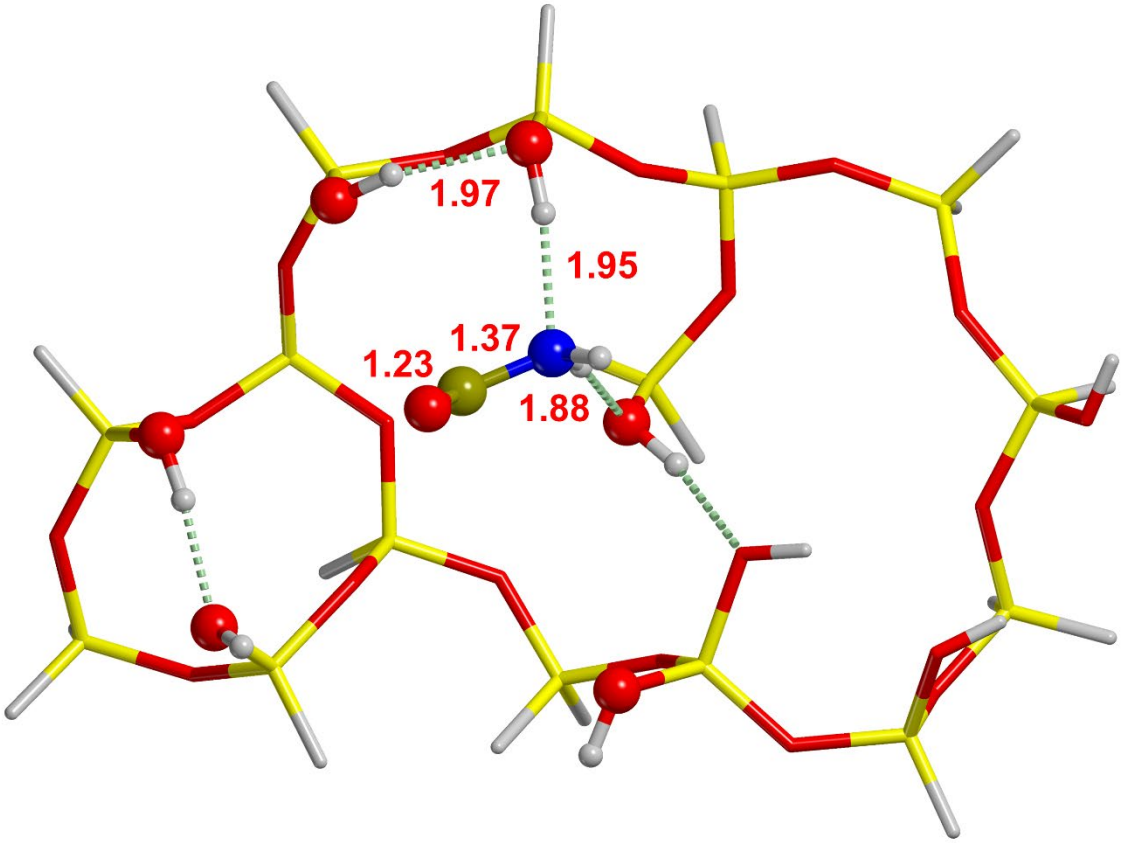

Gas phase coordinates	**PCM (F)** coordinates
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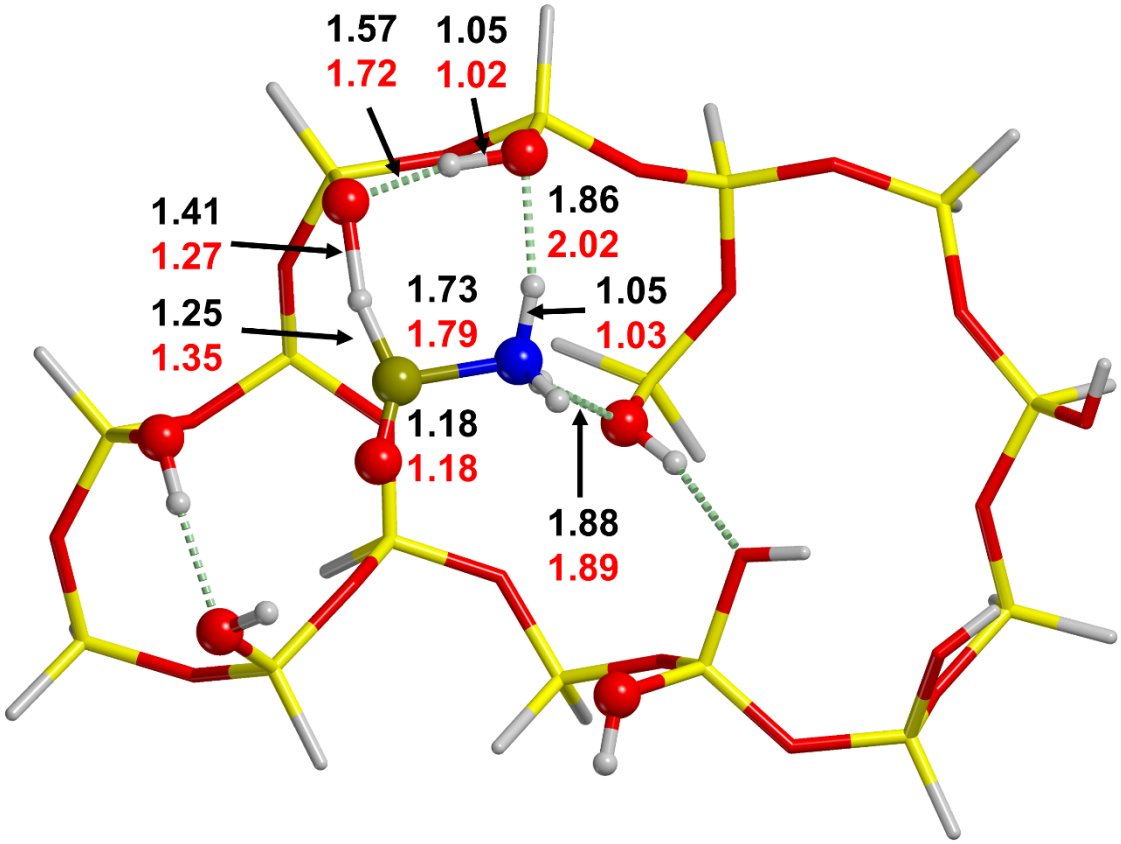
	O -4.8651767753 -2.4689957714 1.8798646185 H -4.4869287753 -2.7348847714 2.7354326185 O -5.6035307753 0.1996872286 1.4728256185 H -5.2944887753 -0.6953237714 1.7536516185 O 0.8504562247 0.3849082286 -0.1874903815 H 1.5358522247 -0.2031587714 0.2147076185 O 3.7226782247 3.9601882286 -0.3852743815 H 5.3967992247 3.3648612286 -2.2625273815 Si -0.3327067753 4.6220922286 0.6100236185 H 2.0091732247 4.6949722286 -2.1217473815 Si 2.2248102247 3.7000822286 -1.0327043815 Si -3.1954297753 3.8240212286 0.3312406185 O -1.6641027753 4.0670552286 -0.2272933815 O 1.0298742247 3.8883382286 0.0813566185 O 5.0980662247 -3.3795777714 -0.6729783815 O 5.7721702247 -0.7854997714 -0.4876383815 O 3.1296692247 -4.1018657714 0.9690526185 Si 6.1323802247 -2.2316237714 -1.2260493815 H 5.9446782247 -2.1233777714 -2.7019303815 Si 5.2260442247 3.4187192286 -0.7751943815 Si 4.7594212247 -3.9549827714 0.8467526185 O 5.4845262247 1.9027362286 -0.1525913815 Si 6.5190262247 0.6411502286 -0.2045393815 Si -2.4352647753 -1.2594787714 -1.3916493815 Si 1.9071962247 -2.9978847714 0.8865366185 O -7.0533577753 -1.2063927714 -0.3259963815 O -0.9045607753 -1.7706497714 -1.6754363815 Si -6.6933157753 -2.6526117714 -1.0643853815 H -6.7900247753 -2.4920187714 -2.5468553815 O -2.9599437753 -1.8602507714 0.0625256185 H -3.3190077753 -1.7004497714 -2.5031753815 O -5.1460377753 -3.1231677714 -0.7255173815 O -3.8850057753 2.5572082286 -0.4462323815 Si -4.0569027753 -3.0109987714 0.5057836185 O -5.1795117753 0.3970752286 -1.2314003815 H -0.1076777753 1.4431882286 -2.3457393815 O -2.4738267753 0.3818282286 -1.2395103815 Si -6.3066237753 0.2202622286 -0.0429703815 H -3.8359067753 1.7853852286 -2.8862463815 Si -3.8191157753 1.3011682286 -1.4832163815 Si 1.1610862247 0.9364542286 -1.7467133815 H 1.8335032247 -0.0974277714 -2.5965923815 O 1.3292142247 -2.9307187714 -0.6547033815 H 0.2633772247 -3.7383347714 -2.7910013815 O 2.2642062247 2.1859262286 -1.6524903815 Si -0.0777037753 -3.1827217714 -1.4499893815 H 6.2027862247 4.3545482286 -0.1369863815 H 7.5271262247 0.8770202286 -1.2836853815 H 7.5408832247 -2.6065677714 -0.8629173815 H 5.3729822247 -5.2981227714 1.0149236185 H -0.9353907753 -4.1242997714 -0.6513513815 H -3.3976257753 -4.3267347714 0.7012606185

	H -7.6707957753 -3.6494617714 -0.5357303815 H -7.2685107753 1.3515952286 -0.0191213815 H -4.0438117753 5.0179972286 0.0737396185 H -0.2417057753 6.0892032286 0.3748946185



Gas phase coordinates	**PCM (F)** coordinates
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C -2.3050944319 0.9717098544 2.4402496427	C -2.2069128592 1.0748314422 2.5298791773
H -2.8202494319 2.0922338544 2.2359416427	H -2.7240428592 2.2876284422 2.2357641773
N -0.6242914319 1.2554598544 2.1629046427	N -0.4365908592 1.2308774422 2.2909211773
H -0.0813984319 0.7031008544 2.8364166427	H 0.0517191408 0.6419084422 2.9745521773
H -0.3178904319 0.9609058544 1.2058436427	H -0.1403488592 0.9391044422 1.3332781773
O -2.5640234319 -0.1372991456 2.7555066427	O -2.5258938592 -0.0023155578 2.8854411773
O -3.0160134319 3.4618648544 1.9806066427	O -3.0687358592 3.4796694422 1.9780481773
O -0.5438934319 4.1365988544 2.2612996427	O -0.5102258592 4.2128114422 2.2664381773
H -1.5768094319 3.9727758544 2.3432066427	H -1.4987558592 4.0356604422 2.3984051773
H -0.4236834319 2.2812208544 2.2733306427	H -0.1820908592 2.2256104422 2.4248621773
O 2.4723455681 -1.4409041456 1.2348976427	O 2.4735291408 -1.4438035578 1.2226271773
O 5.2004525681 -2.8105221456 2.0180376427	O 5.1697271408 -2.8253505578 2.0397661773
H 5.9620175681 -2.2233381456 1.8700196427	H 6.0387761408 -2.3898825578 2.0090141773
O 7.2396795681 0.4053698544 1.3509556427	O 7.2437321408 0.4288854422 1.3425391773
H 7.4928755681 1.1958258544 1.8526206427	H 7.5906861408 1.2345594422 1.7610591773
H 3.3242525681 -1.4081221456 1.7093406427	H 3.3292621408 -1.3934955578 1.6899371773

O 0.7452535681 -3.3823121456 1.9734366427	O 0.7375791408 -3.3451825578 1.9892231773
H 0.5784515681 -4.3292421456 2.0994056427	H 0.3840851408 -4.2504225578 1.9680701773
O -4.7588494319 -2.5021181456 1.9157386427	O -4.8427408592 -2.4788075578 1.8691441773
H -4.1157504319 -2.2421461456 2.6013106427	H -4.3980618592 -2.6598965578 2.7153801773
O -5.5793074319 0.1880408544 1.4740736427	O -5.5959578592 0.2036234422 1.4796171773
H -5.3361184319 -0.7193191456 1.7552546427	H -5.2425158592 -0.6784495578 1.7457951773
O 0.8443775681 0.3909818544 -0.1636143573	O 0.8543571408 0.3865684422 -0.1723388227
H 1.5443405681 -0.1585261456 0.2616736427	H 1.5485101408 -0.1781075578 0.2474091773
O 3.7483805681 3.9823218544 -0.3113753573	O 3.7471501408 3.9727664422 -0.3341238227
H 5.4284175681 3.4080668544 -2.1899073573	H 5.4266121408 3.3902254422 -2.2106178227
Si -0.3105424319 4.6292998544 0.6792966427	Si -0.3112468592 4.6261634422 0.6544891773
H 2.0388115681 4.7326858544 -2.0450623573	H 2.0378781408 4.7175824422 -2.0704948227
Si 2.2526315681 3.7270388544 -0.9655753573	Si 2.2511651408 3.7159434422 -0.9871818227
Si -3.1715144319 3.8306868544 0.3845156427	Si -3.1727658592 3.8282764422 0.3630751773
O -1.6389474319 4.0812428544 -0.1673263573	O -1.6400978592 4.0757234422 -0.1898858227
O 1.0543825681 3.9025618544 0.1470036427	O 1.0531501408 3.8965064422 0.1248421773
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O 3.1613495681 -4.0937651456 0.9593646427	O 3.1550361408 -4.0980075578 0.9676361773
Si 6.1678755681 -2.1977861456 -1.2082643573	Si 6.1625521408 -2.2122995578 -1.2075648227
H 5.9841355681 -2.0747771456 -2.6834873573	H 5.9787321408 -2.0948285578 -2.6832298227
Si 5.2534745681 3.4466138544 -0.7025843573	Si 5.2518551408 3.4345884422 -0.7234358227
Si 4.7912555681 -3.9437271456 0.8431006427	Si 4.7850261408 -3.9494705578 0.8506251773
O 5.5120585681 1.9246908544 -0.0946893573	O 5.5095211408 1.9148404422 -0.1097368227
Si 6.5482205681 0.6649178544 -0.1565653573	Si 6.5448621408 0.6541694422 -0.1668908227
Si -2.4004454319 -1.2341071456 -1.3878413573	Si -2.4051628592 -1.2437745578 -1.3899288227
Si 1.9377775681 -2.9904441456 0.8846596427	Si 1.9321701408 -2.9941905578 0.8888301773
O -7.0215354319 -1.1972891456 -0.3345753573	O -7.0261138592 -1.1999285578 -0.3363228227
O -0.8683444319 -1.7405651456 -1.6725403573	O -0.8734208592 -1.7523105578 -1.6728458227
Si -6.6577014319 -2.6355111456 -1.0865953573	Si -6.6632918592 -2.6412585578 -1.0828608227
H -6.7504944319 -2.4599811456 -2.5676233573	H -6.7561318592 -2.4713485578 -2.5645418227
O -2.9284274319 -1.8502361456 0.0586926427	O -2.9333868592 -1.8540105578 0.0590121773
H -3.2805694319 -1.6648071456 -2.5062443573	H -3.2856868592 -1.6781895578 -2.5065788227
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O -3.8574314319 2.5711438544 -0.4078563573	O -3.8595828592 2.5661484422 -0.4243888227
Si -4.0252224319 -3.0067191456 0.4871866427	Si -4.0308828592 -3.0081325578 0.4920541773
O -5.1471214319 0.4174908544 -1.2184223573	O -5.1507528592 0.4102374422 -1.2265538227
H -0.0734844319 1.4808598544 -2.3079483573	H -0.0765478592 1.4661394422 -2.3206858227
O -2.4414094319 0.4055238544 -1.2191523573	O -2.4450488592 0.3965174422 -1.2275238227
Si -6.2773114319 0.2273038544 -0.0349793573	Si -6.2809368592 0.2253204422 -0.0422708227
H -3.8006114319 1.8241278544 -2.8553383573	H -3.8035108592 1.8097164422 -2.8689938227
Si -3.7871094319 1.3256668544 -1.4572073573	Si -3.7901798592 1.3166114422 -1.4689638227
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H 1.8702425681 -0.0548471456 -2.5690293573	H 1.8661581408 -0.0718145578 -2.5760828227
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H 0.3050555681 -3.6954391456 -2.8047713573	H 0.2985931408 -3.7122705578 -2.7976968227
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H 6.2273145681 4.3770628544 -0.0521903573	H 6.2263661408 4.3668944422 -0.0767168227
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H -0.8991724319 -4.1045301456 -0.6724963573	H -0.9056688592 -4.1124035578 -0.6637418227
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H -4.0206204319 5.0262628544 0.1367306427	H -4.0211258592 5.0234424422 0.1107981773
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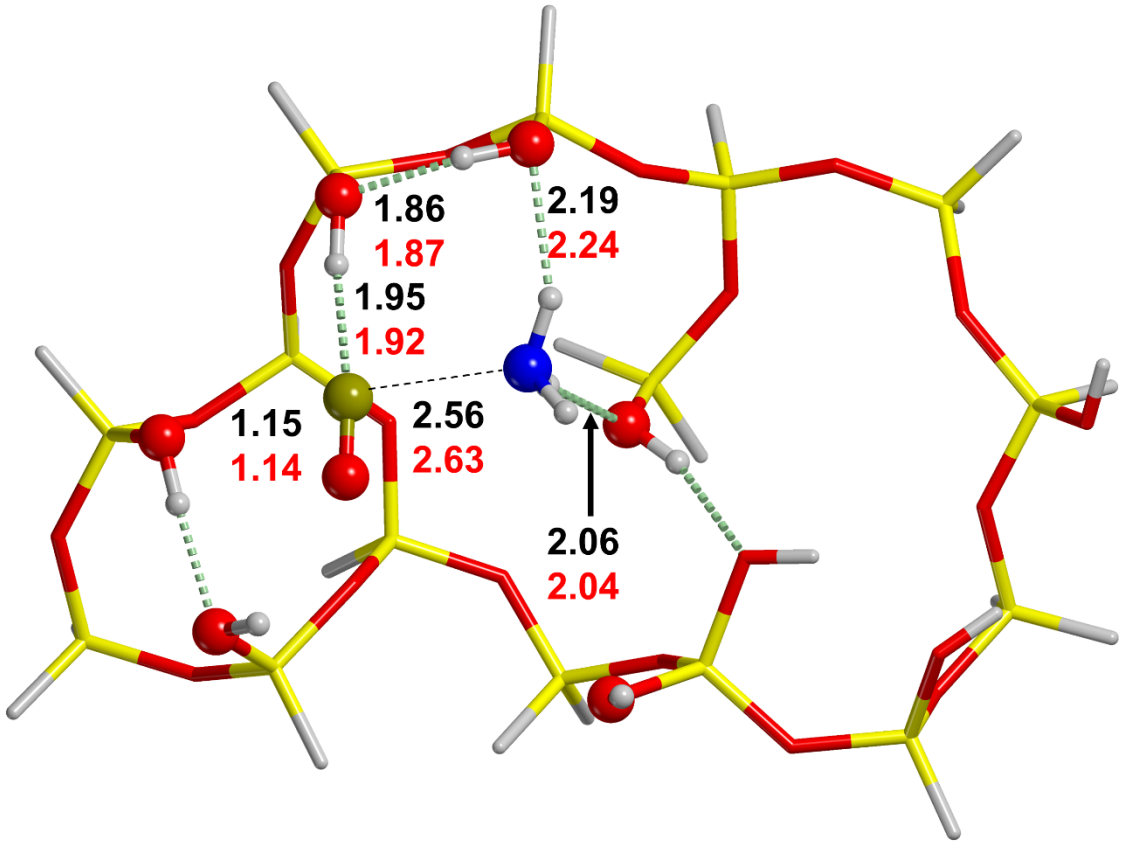

Gas phase coordinates	**PCM (F)** coordinates
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H -3.1443514710 2.5961816642 2.2736848689	H -3.1383873435 2.6081727077 2.2796898273
N -0.4953074710 1.1617466642 2.4174828689	N -0.5779073435 1.1071227077 2.3826798273
H 0.0340525290 0.5492376642 3.0421898689	H -0.1414023435 0.4801177077 3.0627618273
H -0.2189114710 0.9184936642 1.4571828689	H -0.2120953435 0.8536237077 1.4556798273
O -3.0170944710 -0.3486403358 3.2143198689	O -3.1504453435 -0.2172802923 3.4714428273
O -3.1143024710 3.5472286642 1.9890228689	O -3.1254513435 3.5545017077 1.9740098273
O -0.4549644710 4.2739506642 2.2708058689	O -0.4540833435 4.2690307077 2.2609848273
H -1.3992524710 4.0818706642 2.4916448689	H -1.3985563435 4.0718587077 2.4770468273
H -0.1822474710 2.1243896642 2.5821418689	H -0.2499153435 2.0572227077 2.5805918273
O 2.5187175290 -1.4645053358 1.2950828689	O 2.4959726565 -1.4433032923 1.2287088273
O 5.2019765290 -2.8039993358 2.0256878689	O 5.1789706565 -2.8212622923 2.0583198273
H 5.9904935290 -2.2481133358 1.9006148689	H 6.0486566565 -2.3864982923 2.0368778273
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H 7.4760525290 1.1984956642 1.8815038689	H 7.6030106565 1.2389757077 1.8057048273
H 3.4460405290 -1.4529033358 1.6021248689	H 3.3514676565 -1.4041762923 1.6978428273

O 0.6589805290 -3.4366353358 1.8296318689	O 0.7457116565 -3.3436332923 1.9667338273
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H -0.1958244710 6.1059576642 0.4304618689	H -0.1968083435 6.1018927077 0.4140038273

Figure S10: PBE-D2/TZVP optimized geometries for the formamide decarbonylation reaction catalysed by hydrophilic silica. In the figures the most representative bond lengths (in Å) in gas phase (black) and in PCM (F) (red) are reported. In the left and the right columns the cartesian coordinates of the optimized structures in gas phase and in PCM (F), respectively, are reported. Hydrogens in white, oxygens in red, carbons in ochre, nitrogens in blue, silicons in yellow.

Table S1: CCSD(T) energies with thermodynamic corrections computed at PBE level for the formamide dehydration in gas phase.

	NC		$1H_2O$				$2H_2O$				SiL				SiH			
	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0
M1	0.0	0.0	-33.8	22.9	0.0	0.0	-90.4	27.7	0.0	0.0	-45.6	44.4	0.0	0.0	-108.8	-7.5	0.0	0.0
TS1	180.1	184.1	38.6	110.6	72.3	87.7	-27.7	107.2	62.7	79.5	13.4	109.8	58.9	65.3	-41.5	69.7	67.3	77.2
M2	43.2	46.2	2.0	64.4	35.8	41.5	-55.5	68.5	34.8	40.7	-5.3	91.1	40.3	46.7	-66.3	39.3	42.5	46.8
TS2	81.4	85.9	122.6	181.0	156.4	158.1	69.9	191.6	160.2	163.9	41.1	130.7	86.6	86.2	-40.5	64.0	68.3	71.5
M3	65.4	67.4	30.5	80.1	64.3	57.1	-28.6	90.6	61.7	62.8	25.8	114.6	71.4	70.2	-82.4	18.9	26.4	26.4
TS3	159.9	160.5	62.2	116.9	96.0	93.9					43.0	133.4	88.6	89.0	34.9	138.8	143.7	146.3
M4	57.7	59.5	46.0	95.4	79.8	72.4	4.1	113.4	94.4	85.7	40.6	129.0	86.1	84.5	-75.7	27.0	33.1	34.5
TS4	304.2	303.8	196.0	262.0	229.7	239.0	134.2	261.2	224.6	233.5	133.9	226.4	179.5	181.9	-49.2	53.9	59.7	61.4
M5	59.2	37.6	35.3	69.9	69.0	47.0	-20.9	76.7	69.4	48.9	20.5	112.2	66.1	67.8	-65.4	36.3	43.4	43.8
TS5											180.5	272.9	226.1	228.5	90.0	200.3	198.8	207.8
M6											31.9	106.8	77.5	62.3	-45.8	46.1	63.0	53.6
Prods	81.3	21.6	81.3	21.6	115.1	-1.3	81.3	21.6	171.7	-6.1	81.3	21.6	126.9	-22.8	81.3	21.6	190.2	29.1

NC stands for the non-catalysed reaction, $1H_2O$ and $2H_2O$ for the $1H_2O$- and $2H_2O$-mediated reaction, respectively, while SiL and SiH for the Silica 1.5- and Silica 4.5-mediated reactions, respectively.

Mn and TSn correspond to the structures shown in the previous Figures.

ΔH and ΔG energies are referred to non-interacting reactants, while for ΔH^0 and ΔG^0 the reference minimum is M1.

Prods are the energies of non-interacting products.

Table S2: CCSD(T) energies with thermodynamic corrections computed at PBE level for the formamide dehydration in PCM (F).

	NC		$1H_2O$				$2H_2O$				SiL				SiH			
	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0
M1	0.0	0.0	-16.6	-39.1	0.0	0.0	-39.2	-76.3	0.0	0.0	-14.9	-35.8	0.0	0.0	-61.3	-76.3	0.0	0.0
TS1	189.9	193.0	61.2	52.7	77.9	91.8	25.3	1.8	64.6	78.1	46.1	30.8	61.0	66.6	4.4	-0.8	65.7	75.4
M2	53.3	55.4	27.9	10.4	44.5	49.5	0.4	-31.9	39.7	44.4	39.4	20.4	54.3	56.2	-13.5	-24.3	47.8	52.0
TS2	84.0	87.7	144.6	120.1	161.2	159.2	125.6	90.1	164.9	166.4	61.6	42.3	76.5	78.1	14.6	2.4	76.0	78.7
M3	61.6	63.0	40.7	20.1	57.3	59.2	24.7	-13.4	63.9	62.9	49.6	29.2	64.6	65.0	-27.0	-39.6	34.4	36.6
TS3	166.5	165.8	78.0	56.9	94.7	96.0					65.9	44.2	80.8	80.0	86.9	77.0	148.3	153.2
M4	60.8	62.1	57.3	34.5	73.9	73.6	42.3	0.8	81.5	77.1	57.0	35.1	71.9	70.9	-20.6	-32.0	40.7	44.3
TS4	306.6	306.4	208.5	195.3	225.1	234.3	180.3	151.0	219.5	227.3	167.9	145.7	182.9	181.5	3.0	-8.1	64.3	68.2
M5	57.2	41.0	49.0	15.0	65.6	54.1	31.7	-19.4	70.9	57.0	50.2	30.0	65.2	65.8	-10.6	-23.8	50.7	52.4
TS5											203.4	183.5	218.3	219.3	133.9	128.6	195.2	204.9
M6											59.8	21.9	74.7	57.7	6.6	-16.5	67.9	59.8
Prods	64.9	71.1	64.9	71.1	81.5	110.1	64.9	71.1	104.1	147.4	64.9	71.1	79.8	106.9	64.9	71.1	126.2	147.3

NC stands for the non-catalysed reaction, $1H_2O$ and $2H_2O$ for the $1H_2O$- and $2H_2O$-mediated reaction, respectively, while SiL and SiH for the Silica 1.5- and Silica 4.5-mediated reactions, respectively.

Mn and TSn correspond to the structures shown in the previous Figures.

ΔH and ΔG energies are referred to non-interacting reactants, while for ΔH^0 and ΔG^0 the reference minimum is M1.

Prods are the energies of non-interacting products.

Table S3: CCSD(T) energies with thermodynamic corrections computed at PBE level for the formamide decarbonylation in gas phase.

	NC		$1H_2O$				$2H_2O$				SiL				SiH			
	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0
M1	0.0	0.0	-36.9	22.3	0.0	0.0	-79.0	44.0	0.0	0.0	-20.6	69.4	0.0	0.0	-78.0	23.3	0.0	0.0
R	0.0	0.0	-17.6	29.2	19.3	7.0	-49.2	61.1	29.9	17.1	-3.3	89.1	17.3	19.7	-61.8	35.8	16.2	12.5
TS	337.9	332.2	212.2	276.0	249.1	253.7	141.2	270.2	220.3	226.1	172.4	260.9	193.0	191.5	111.7	215.8	189.6	192.4
P	27.2	-3.4	13.4	42.2	50.3	20.0	-34.8	52.5	44.3	8.5	5.1	87.6	25.7	18.1	-4.7	81.8	73.3	58.4
Prods	25.8	-33.0	25.8	-33.0	62.7	-55.3	25.8	-33.0	104.8	-77.1	25.8	-33.0	46.3	-102.4	25.8	-33.0	103.7	-56.4

NC stands for the non-catalysed reaction, $1H_2O$ and $2H_2O$ for the $1H_2O$- and $2H_2O$-mediated reaction, respectively, while SiL and SiH for the Silica 1.5- and Silica 4.5-mediated reactions, respectively.
Mn and TSn correspond to the structures shown in the previous Figures.
ΔH and ΔG energies are referred to non-interacting reactants, while for ΔH^0 and ΔG^0 the reference minimum is M1.
Prods are the energies of non-interacting products.

Table S4: CCSD(T) energies with thermodynamic corrections computed at PBE level for the formamide decarbonylation in PCM (F).

	NC		$1H_2O$				$2H_2O$				SiL				SiH			
	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0	ΔH	ΔG	ΔH^0	ΔG^0
M1	0.0	0.0	-10.3	-32.7	0.0	0.0	-27.8	-64.9	0.0	0.0	10.7	-10.2	0.0	0.0	-31.5	-46.4	0.0	0.0
R	0.0	0.0	5.4	-30.9	15.7	1.8	-14.9	-61.3	13.0	3.6	20.0	-9.2	9.3	1.0	-10.8	-38.9	20.7	7.5
TS	354.1	348.3	231.5	213.1	241.7	245.8	198.2	156.6	226.0	221.6	195.7	176.5	185.0	186.6	153.5	139.3	185.0	185.7
P	41.5	29.8	50.0	28.3	60.3	61.0	5.7	-26.4	33.6	38.5	34.2	11.4	23.5	21.6	35.1	20.9	66.6	67.3
Prods	32.3	39.4	32.3	39.4	42.6	72.1	32.3	39.4	60.1	104.3	32.3	39.4	21.6	49.6	32.3	39.4	63.8	85.8

NC stands for the non-catalysed reaction, $1H_2O$ and $2H_2O$ for the $1H_2O$- and $2H_2O$-mediated reaction, respectively, while SiL and SiH for the Silica 1.5- and Silica 4.5-mediated reactions, respectively.
Mn and TSn correspond to the structures shown in the previous Figures.
ΔH and ΔG energies are referred to non-interacting reactants, while for ΔH^0 and ΔG^0 the reference minimum is M1.
Prods are the energies of non-interacting products.

Basis sets

TZVP

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 0.4065901283400E+03 -0.2077271512500E-01
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    D   1 1.
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    S   1 1.
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 0.1030724100000E+00  0.1000000000000E+01
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S   5   1.00
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S   2   1.00
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     13.8681080            0.20091165
S   1   1.00
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S   1   1.00
      1.4659925            1.0000000
S   1   1.00
      0.25271086           1.0000000
S   1   1.00
      0.92491673E-01       1.0000000
P   5   1.00
    483.0235200            0.19161547E-02
    114.2508100            0.15309765E-01
     36.3877860            0.71094358E-01
     13.4117040            0.21243244
      5.2884033            0.38976302
P   1   1.00
      2.1374219            1.0000000
P   1   1.00
      0.86468463           1.0000000
P   1   1.00
      0.25489855           1.0000000
P   1   1.00
      0.79397031E-01       1.0000000
D   1   1.00
      0.3500000            1.0000000
****
```

cc-pVTZ

```
  C     0
  S   8   1.00
     8236.0000000            0.0005310
     1235.0000000            0.0041080
      280.8000000            0.0210870
       79.2700000            0.0818530
       25.5900000            0.2348170
        8.9970000            0.4344010
        3.3190000            0.3461290
        0.3643000           -0.0089830
  S   8   1.00
     8236.0000000           -0.0001130
     1235.0000000           -0.0008780
      280.8000000           -0.0045400
       79.2700000           -0.0181330
```

```
    25.5900000           -0.0557600
     8.9970000           -0.1268950
     3.3190000           -0.1703520
     0.3643000            0.5986840
S   1   1.00
     0.9059000            1.0000000
S   1   1.00
     0.1285000            1.0000000
P   3   1.00
    18.7100000            0.0140310
     4.1330000            0.0868660
     1.2000000            0.2902160
P   1   1.00
     0.3827000            1.0000000
P   1   1.00
     0.1209000            1.0000000
D   1   1.00
     1.0970000            1.0000000
D   1   1.00
     0.3180000            1.0000000
F   1   1.00
     0.7610000            1.0000000
****
N    0
S   8   1.00
  11420.0000000            0.0005230
   1712.0000000            0.0040450
    389.3000000            0.0207750
    110.0000000            0.0807270
     35.5700000            0.2330740
     12.5400000            0.4335010
      4.6440000            0.3474720
      0.5118000           -0.0085080
S   8   1.00
  11420.0000000           -0.0001150
   1712.0000000           -0.0008950
    389.3000000           -0.0046240
    110.0000000           -0.0185280
     35.5700000           -0.0573390
     12.5400000           -0.1320760
      4.6440000           -0.1725100
      0.5118000            0.5999440
S   1   1.00
     1.2930000            1.0000000
S   1   1.00
     0.1787000            1.0000000
P   3   1.00
    26.6300000            0.0146700
     5.9480000            0.0917640
     1.7420000            0.2986830
P   1   1.00
     0.5550000            1.0000000
```

```
P   1   1.00
     0.1725000           1.0000000
D   1   1.00
     1.6540000           1.0000000
D   1   1.00
     0.4690000           1.0000000
F   1   1.00
     1.0930000           1.0000000
****
O    0
S   8   1.00
  15330.0000000           0.0005080
   2299.0000000           0.0039290
    522.4000000           0.0202430
    147.3000000           0.0791810
     47.5500000           0.2306870
     16.7600000           0.4331180
      6.2070000           0.3502600
      0.6882000          -0.0081540
S   8   1.00
  15330.0000000          -0.0001150
   2299.0000000          -0.0008950
    522.4000000          -0.0046360
    147.3000000          -0.0187240
     47.5500000          -0.0584630
     16.7600000          -0.1364630
      6.2070000          -0.1757400
      0.6882000           0.6034180
S   1   1.00
     1.7520000           1.0000000
S   1   1.00
     0.2384000           1.0000000
P   3   1.00
    34.4600000           0.0159280
     7.7490000           0.0997400
     2.2800000           0.3104920
P   1   1.00
     0.7156000           1.0000000
P   1   1.00
     0.2140000           1.0000000
D   1   1.00
     2.3140000           1.0000000
D   1   1.00
     0.6450000           1.0000000
F   1   1.00
     1.4280000           1.0000000
****
H    0
S   3   1.00
    33.8700000           0.0060680
     5.0950000           0.0453080
     1.1590000           0.2028220
```

```
S   1   1.00
     0.3258000           1.0000000
S   1   1.00
     0.1027000           1.0000000
P   1   1.00
     1.4070000           1.0000000
P   1   1.00
     0.3880000           1.0000000
D   1   1.00
     1.0570000           1.0000000
****
```