Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Theoretical Analysis of Glyoxal Condensation with Ammonia in Aqueous Solution

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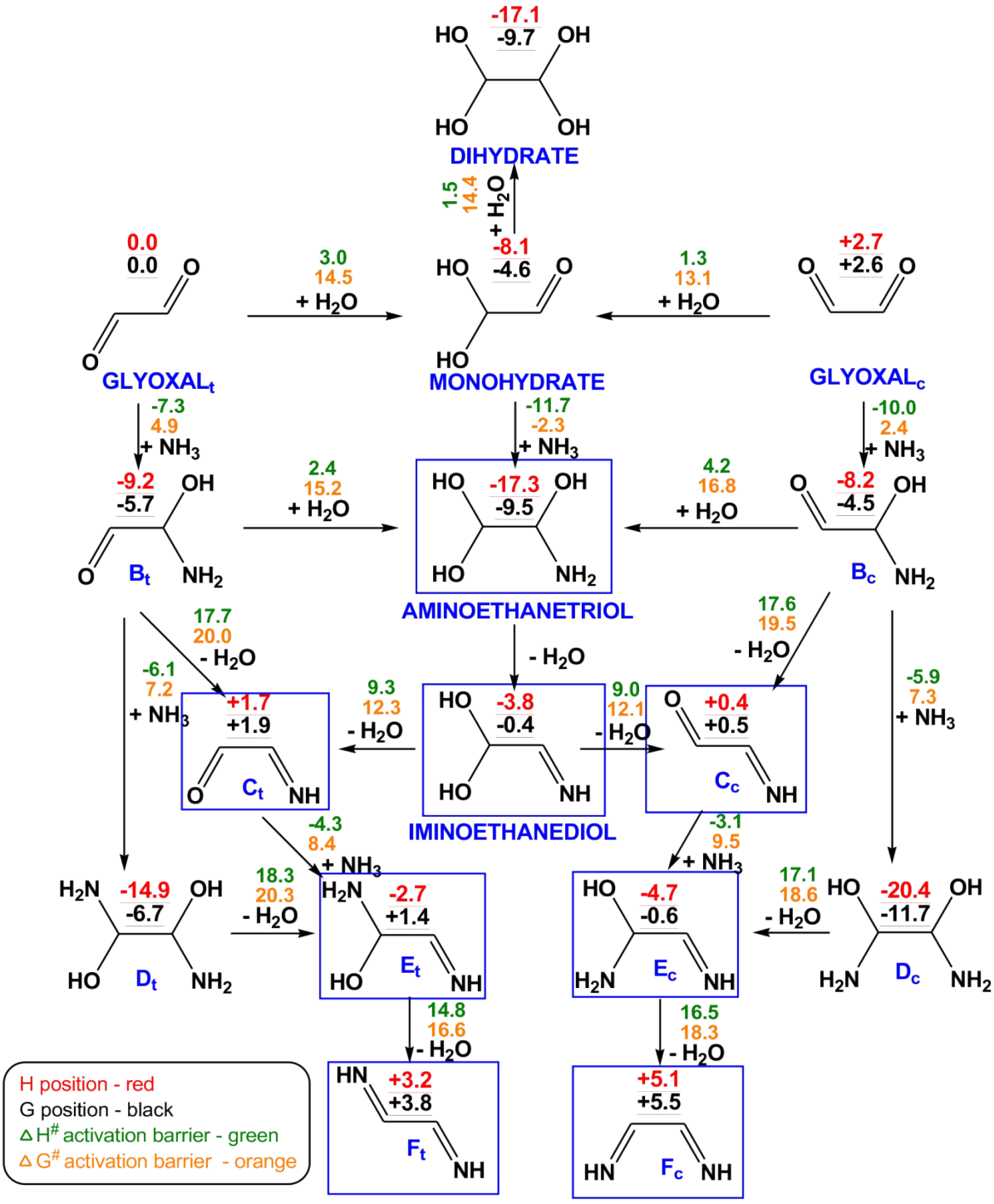


Figure S1. Ethanediimine formation from trans- and cis-glyoxal and ammonia. The G and H values (kcal/mol) of the structure in solution as positions on the PES are marked in black and red, respectively, above the corresponding structure. The Gibbs free energy and enthalpy of activation values ($\Delta G^{\#}$ and $\Delta H^{\#}$) of the stages are marked above the corresponding stage in orange and green, respectively.

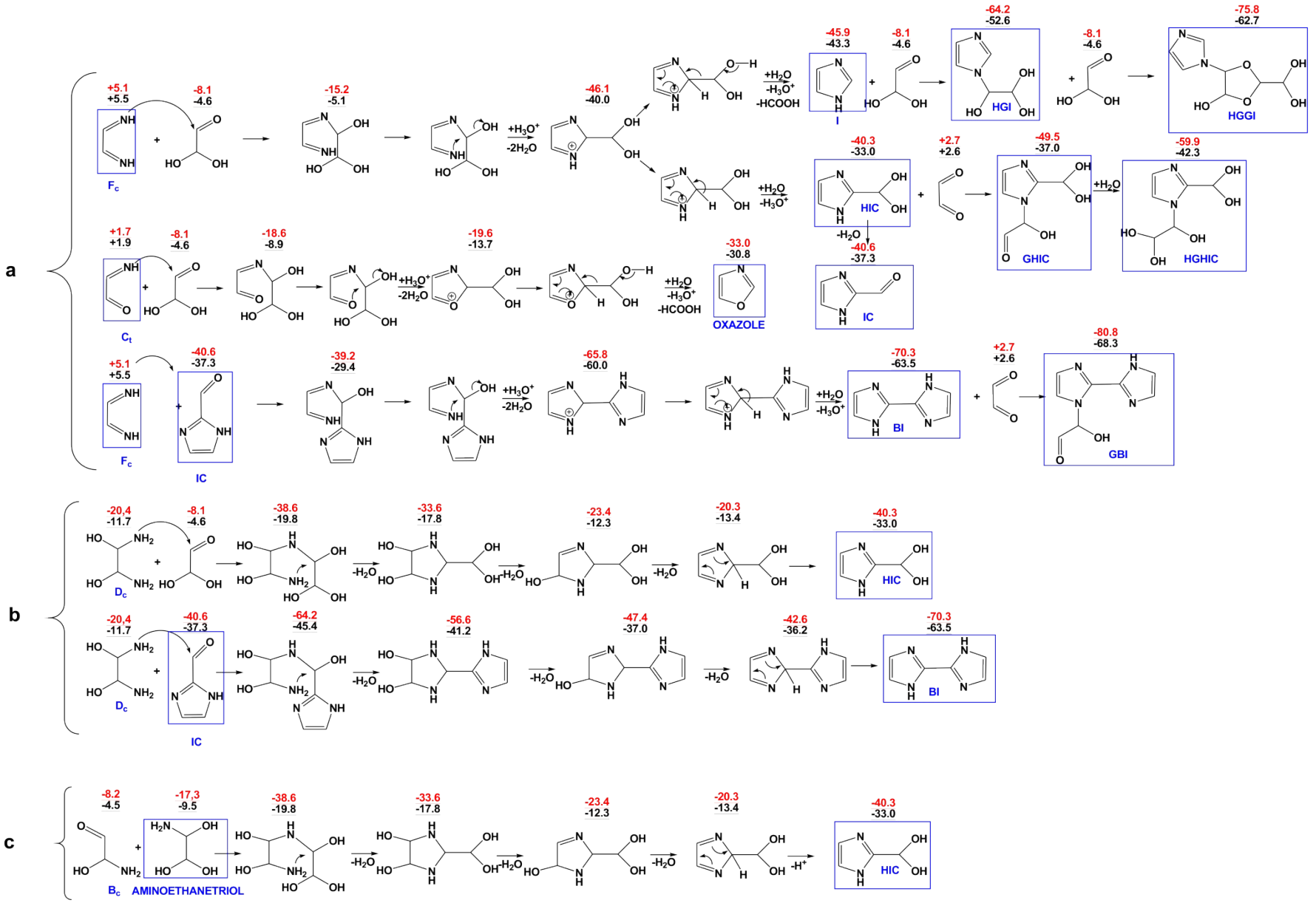


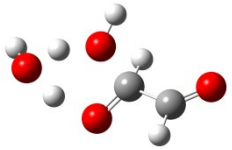
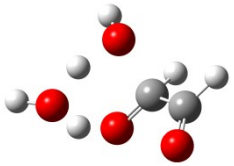
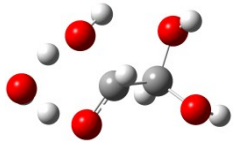
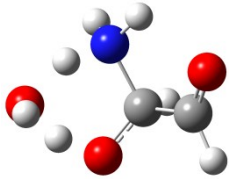
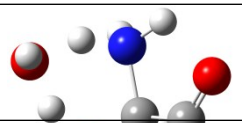
Figure S2. The formation of experimentally identified products of the interaction of glyoxal with ammonia. The G and H values of the structure in solution as a position on the PES are marked in black and red (kcal/mol), respectively, above the corresponding structure.

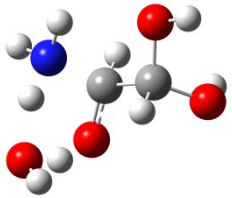
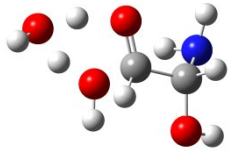
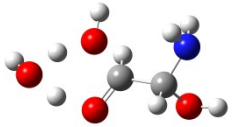
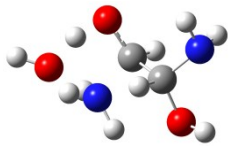
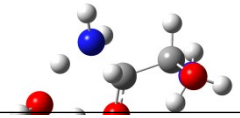
Table S1. The Gibbs free energies and enthalpies of the structures in solution and the PES positions of all structures of the proposed mechanisms of interaction between glyoxal and ammonia

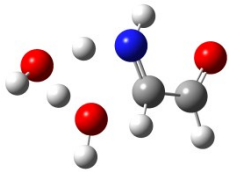
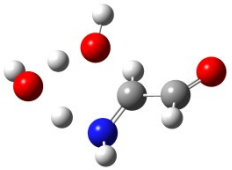
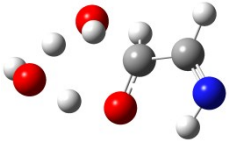
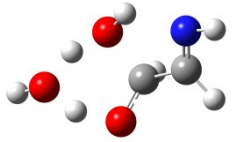
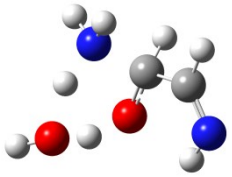
Structure	**Abbreviation**	G, a.u.	G, kcal/mol	Gposition	H, a.u.	H, kcal/mol	Hposition
trans-Glyoxal (trans-GO)	HOC-COH_t	-227.879412	-142996.5	0.0	-227.851613	-142979.1	0.0
Water	H_2O	-76.448667	-47972.3	0.0	-76.4296	-47960.3	0.0
Ammonia	NH_3	-56.563306	-35494.0	0.0	-56.543448	-35481.6	0.0
Hydronium	H_3O^+	-76.830949	-48212.2	0.0	-76.812793	-48200.8	0.0
Formic acid	HCOOH	-189.814648	-119110.5	0.0	-189.789481	-119094.7	0.0
cis-Glyoxal (cis-GO)	HOC-COH_c	-227.875282	-142993.9	2.6	-227.847284	-142976.3	2.7
B from trans-GO	B_t_OHC-$CHOHNH_2$	-284.442632	-178490.5	-5.7	-284.40967	-178469.8	-9.2
B from cis-GO	B_c_OHC-$CHOHNH_2$	-284.440698	-178489.2	-4.5	-284.408123	-178468.8	-8.2
Iminoacetaldehyde from cis-GO	C_c_OHC-CHNH	-207.993268	-130517.8	0.5	-207.964896	-130499.9	0.4
Iminoacetaldehyde from trans-GO	C_t_OHC-CHNH	-207.991031	-130516.3	1.9	-207.962707	-130498.6	1.7
Imino-aminoethanol from cis-GO	E_c_NH_2HOHC-CHNH	-264.549056	-166007.0	-0.6	-264.516326	-165986.5	-4.7
Imino-aminoethanol from trans-GO	E_t_NH_2HOHC-CHNH	-264.545815	-166005.0	1.4	-264.513167	-165984.5	-2.7
Diiminoethane from cis-GO	F_c_HNHC-CHNH	-188.099923	-118034.5	5.5	-188.071189	-118016.5	5.1
Diiminoethane from trans-GO	F_t_HNHC-CHNH	-188.102608	-118036.2	3.8	-188.074205	-118018.4	3.2
Diaminoethanediol from cis-GO	D_c_NH_2HOHC-$CHOHNH_2$	-341.006158	-213984.6	-11.7	-340.97102	-213962.6	-20.4
Diaminoethanediol from trans-GO	D_t_NH_2HOHC-$CHOHNH_2$	-340.998213	-213979.6	-6.7	-340.962186	-213957.0	-14.9
Glyoxal monohydrate	Monohydrate	-304.326221	-190967.6	-4.6	-304.294176	-190947.5	-8.1
Glyoxal dihydrate	Dihydrate	-380.773717	-238939.1	-9.7	-380.73804	-238916.7	-17.1
Aminoethanetriol	HOHOHC-$CHOHNH_2$	-360.887994	-226460.6	-9.5	-360.852274	-226438.2	-17.3
Iminoethanediol	HOHOHC-CHNH	-284.434161	-178485.1	-0.4	-284.401101	-178464.4	-3.8
HNHC-CHN-HOHC-CHOHOH	1a	-492.426490	-309002.3	-5.1	-492.384765	-308976.1	-15.2
HNHC-CHN-HOHC-$CHOHOH^+$	2a	-416.424828	-261310.5	-40.0	-416.387517	-261287.1	-46.1
Imidazole	I	-226.242461	-141969.3	-43.3	-226.214587	-141951.8	-45.9
Hydrated N-glyoxal substituted imidazole	HGI	-530.566856	-332935.7	-52.6	-530.525027	-332909.5	-64.2
Hydrated imidazole-2-carboxaldehyde	HIC	-416.031375	-261063.6	-33.0	-415.995213	-261040.9	-40.3
1H-imidazole-2-carboxaldehyde	IC	-339.598852	-213101.5	-37.3	-339.566079	-213080.9	-40.6

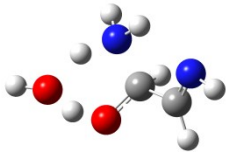
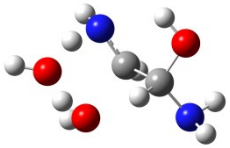
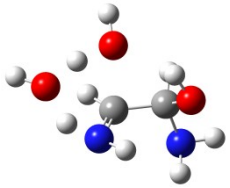
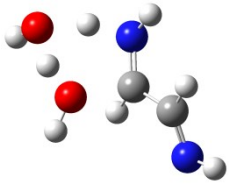
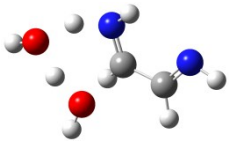
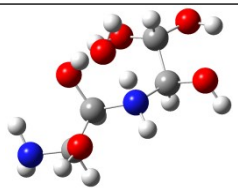
	OHC-CN-HOHC-CHOHOH	-512.317789	-321484.3	-8.9	-512.276251	-321458.2	-18.6
	OHC-CN-HOHC-CHOHOH^{+}	-436.268308	-273762.5	-13.7	-436.231508	-273739.4	-19.6
1.3-oxazole	oxazole	-246.107829	-154435.0	-30.8	-246.080193	-154417.7	-33.0
	HNHC-CHN-CHOH-(CNHCHCHN)	-527.685716	-331127.8	-29.4	-527.643108	-331101.1	-39.2
	HNHC-CHN-CHOH-(CNHCHCHN)$^{+}$	-451.677312	-283431.8	-60.0	-451.639044	-283407.8	-65.8
2.2’-bisimidazole	BI	-451.300663	-283195.5	-63.5	-451.263044	-283171.8	-70.3
N-glyoxal substituted hydrated 1H-imidazole-2-carbaldehyde	GHIC	-643.908021	-404058.4	-37.0	-643.861437	-404029.2	-49.5
Hydrated N-glyoxal substituted hydrated 1H-imidazole-2-carbaldehyde	HGHIC	-720.355833	-452030.1	-42.3	-720.307656	-451999.9	-59.9
N-glyoxal substituted 2.2’-bisimidazole	GBI	-679.178542	-426191.0	-68.3	-679.131449	-426161.4	-80.8
Hydrated glyoxal dimer substituted imidazole	HGGI	-758.443813	-475930.7	-62.7	-758.395022	-475900.1	-75.8
2-(2-amino-1.2-dihydroxyethylamino)ethane-1.1.2-triol	1b	-645.328713	-404949.9	-19.8	-645.281251	-404920.1	-38.6
2-(dihydroxymethyl) imidazolidine-4.5-diol	2b	-568.886083	-356981.4	-17.8	-568.843681	-356954.8	-33.6
2-(dihydroxymethyl)5-hydroxy-2.5-dihydro-1H-imidazol	3b	-492.43784	-309009.4	-12.3	-492.397872	-308984.3	-23.4
(2H-imidazol-2-yl) methanediol	4b	-416.000138	-261044.0	-13.4	-415.963334	-261020.9	-20.3
1-amino-2-(hydroxy(1H-imidazol-2-yl) methylamino) ethane-1.2-diol		-680.590081	-427076.7	-45.4	-680.542108	-427046.6	-64.2
2-(1H-imidazol-2-yl) imidazolidine-4.5-diol		-604.14399	-379106.1	-41.2	-604.100455	-379078.8	-56.6
2-(1H-imidazol-2-yl) -2.5-dihydro-1H-imidazol-5-ol		-527.69788	-331135.4	-37.0	-527.656217	-331109.3	-47.4
	PreBI	-451.257169	-283168.2	-36.2	-451.218891	-283144.1	-42.6

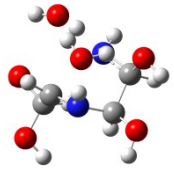
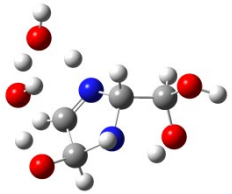
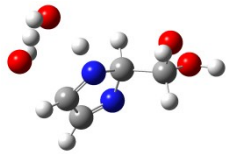
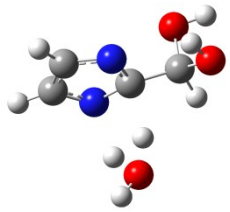
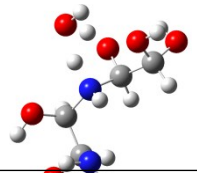
Table S2. Transition states with the participation of one water molecule

Reagents, TS, products	**TS**	G, a.u	G, kcal/mol	$\Delta G^{\#}$, kcal/mol Forward	$\Delta G^{\#}$, kcal/mol Back	H, a.u	H, kcal/mol	$\Delta H^{\#}$, kcal/mol Forward	$\Delta H^{\#}$, kcal/mol Back
Glyoxal trans		-227.879412	-142996.5	14.5	13.3	-227.851613	-142979.1	3.0	11.1
Monohydrate		-304.326221	-190967.6			-304.294176	-190947.5		
GLYOXAL_TRANS_H_2O_TS		-380.741682	-238919.0			-380.706046	-238896.7		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Glyoxal cis		-227.875282	-142993.9	13.1	14.5	-227.847284	-142976.3	1.3	12.1
Monohydrate		-304.326221	-190967.6			-304.294176	-190947.5		
GLYOXAL_CIS_H_2O_TS		-380.739752	-238917.8			-380.704437	-238895.7		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Monohydrate		-304.326221	-190967.6	14.4	13.7	-304.294176	-190947.5	1.5	10.5
Dihydrate		-380.773717	-238939.1			-380.73804	-238916.7		
MONOHYDRATE_H_2O_TS		-457.18861	-286890.2			-457.150938	-286866.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Glyoxal trans		-227.879412	-142996.5	4.9	4.9	-227.851613	-142979.1	-7.3	1.9
Bt_OHC-CHOHNH_2		-284.442632	-178490.5			-284.40967	-178469.8		
GLYOXAL_TRANS_NH_3_TS		-360.871546	-226450.3			-360.836251	-226428.2		
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Glyoxal cis		-227.875282	-142993.9			-227.847284	-142976.3		
Bc_OHC-CHOHNH_2		-284.440698	-178489.2			-284.408123	-178468.8		

GLYOXAL_CIS_NH_3_TS		-360.871544	-226450.3	2.4	3.7	-360.83625	-226428.2	-10.0	0.9
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Monohydrate		-304.326221	-190967.6			-304.294176	-190947.5		
$HOHOHC\text{-}CHOHNH_2$		-360.887994	-226460.6			-360.852274	-226438.2		
MONOHYDRATE_NH_3_TS		-437.329851	-274428.6	-2.3	-3.2	-437.285935	-274401.1	-11.7	-2.5
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Bt\_OHC\text{-}CHOHNH_2$		-284.442632	-178490.5			-284.40967	-178469.8		
$HOHOHC\text{-}CHOHNH_2$		-360.887994	-226460.6			-360.852274	-226438.2		
Bt_H_2O_TS		-437.303735	-274412.2	15.2	13.2	-437.265008	-274387.9	2.4	10.6
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Bc\_OHC\text{-}CHOHNH_2$		-284.440698	-178489.2			-284.408123	-178468.8		
$HOHOHC\text{-}CHOHNH_2$		-360.887994	-226460.6			-360.852274	-226438.2		
Bc_H_2O_TS		-437.299312	-274409.5	16.8	15.9	-437.260695	-274385.2	4.2	13.3
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Bt\_OHC\text{-}CHOHNH_2$		-284.442632	-178490.5			-284.40967	-178469.8		
$Dt\_NH_2HOHC\text{-}CHOHNH_2$		-340.998213	-213979.6			-340.962186	-213957.0		
Bt_NH_3_TS		-417.431199	-261942.0	7.2	2.3	-417.392444	-261917.7	-6.1	-0.4
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Bc\_OHC\text{-}CHOHNH_2$		-284.440698	-178489.2			-284.408123	-178468.8		
$Dc\_NH_2HOHC\text{-}CHOHNH_2$		-341.006158	-213984.6			-340.97102	-213962.6		

$Bc\_NH_3\_TS$		-417.429137	-261940.7	7.3	8.6	-417.390504	-261916.5	-5.9	6.3
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Bt\_OHC\text{-}CHOHNH_2$		-284.442632	-178490.5	20.0	18.1	-284.40967	-178469.8	17.7	6.8
Ct_OHC-CHNH		-207.991031	-130516.3			-207.962707	-130498.6		
$Bt\_\_\_H_2O\_TS$		-360.847536	-226435.3			-360.811087	-226412.4		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Bc\_OHC\text{-}CHOHNH_2$		-284.440698	-178489.2	19.5	20.3	-284.408123	-178468.8	17.6	9.1
Cc_OHC-CHNH		-207.993268	-130517.8			-207.964896	-130499.9		
$Bc\_\_\_H_2O\_TS$		-360.846324	-226434.5			-360.809654	-226411.5		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Ct_OHC-CHNH		-207.991031	-130516.3	12.3	15.8	-207.962707	-130498.6	9.3	9.3
HOHOHC-CHNH		-284.434161	-178485.1			-284.401101	-178464.4		
$Ct\_H_2O\_TS$		-360.851222	-226437.6			-360.815945	-226415.4		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Cc_OHC-CHNH		-207.993268	-130517.8	12.1	17.0	-207.964896	-130499.9	9.0	9.0
HOHOHC-CHNH		-284.434161	-178485.1			-284.401101	-178464.4		
$Cc\_H_2O\_TS$		-360.851614	-226437.8			-360.816332	-226415.7		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Ct_OHC-CHNH		-207.991031	-130516.3	8.4	3.1	-207.962707	-130498.6		
$Et\_NH_2HOHC\text{-}CHNH$		-264.545815	-166005.0			-264.513167	-165984.5		
$Ct\_NH_3\_TS$		-340.97765	-213966.7			-340.942603	-213944.7	-4.3	0.1
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		

Water		-76.448667	-47972.3			-76.4296	-47960.3		
Cc_OHC-CHNH		-207.993268	-130517.8			-207.964896	-130499.9		
Ec_NH_2HOHC-CHNH		-264.549056	-166007.0			-264.516326	-165986.5		
Cc_NH_3_TS		-340.97819	-213967.1	9.5	4.8	-340.942898	-213944.9	-3.1	1.9
Ammonia		-56.563306	-35494.0			-56.543448	-35481.6		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Dt_NH_2HOHC-CHOHNH_2		-340.998213	-213979.6			-340.962186	-213957.0		
Et_NH_2HOHC-CHNH		-264.545815	-166005.0			-264.513167	-165984.5		
Dt___H_2O_TS		-417.402519	-261924.0	20.3	18.0	-417.36268	-261899.0	18.3	6.1
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Dc_NH_2HOHC-CHOHNH_2		-341.006158	-213984.6			-340.97102	-213962.6		
Ec_NH_2HOHC-CHNH		-264.549056	-166007.0			-264.516326	-165986.5		
Dc___H_2O_TS		-417.413233	-261930.8	18.6	13.3	-417.373299	-261905.7	17.1	1.4
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Et_NH_2HOHC-CHNH		-264.545815	-166005.0			-264.513167	-165984.5		
Ft_HNHC-CHNH		-188.102608	-118036.2			-188.074205	-118018.4		
Et___H_2O_TS		-340.956089	-213953.2	16.6	20.0	-340.919151	-213930.0	14.8	8.9
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Ec_NH_2HOHC-CHNH		-264.549056	-166007.0			-264.516326	-165986.5		
Fc_HNHC-CHNH		-188.099923	-118034.5			-188.071189	-118016.5		
Ec____H_2O_TS		-340.956583	-213953.5	18.3	18.0	-340.919662	-213930.3	16.5	6.7
Water		-76.448667	-47972.3			-76.4296	-47960.3		
Bc_OHC-CHOHNH_2		-284.440698	-178489.2			-284.408123	-178468.8		

$HOHOHC\text{-}CHOHNH_2$		-360.887994	-226460.6	5.7	13.2	-360.852274	-226438.2		
Bc_1c_TS		-721.756371	-452909.0			-721.706197	-452877.5	-10.2	2.9
1c		-645.328713	-404949.9			-645.281251	-404920.1		
Water		-76.448667	-47972.3			-76.4296	-47960.3		
1c		-645.328713	-404949.9	31.7	43.0	-645.281251	-404920.1		
2c		-568.886083	-356981.4			-568.843681	-356954.8		
1c_2c_TS		-721.714902	-452883.0			-721.664147	-452851.1	29.3	24.3
Water		-76.448667	-47972.3			-76.4296	-47960.3		
2c		-568.886083	-356981.4	23.5	31.2	-568.843681	-356954.8		
3c		-492.43784	-309009.4			-492.397872	-308984.3		
2c_3c_TS		-645.285395	-404922.7			-645.24136	-404895.1	20.0	9.9
Water		-76.448667	-47972.3			-76.4296	-47960.3		
3c		-492.43784	-309009.4	15.7	30.1	-492.397872	-308984.3		
4c		-416.000138	-261044.0			-415.963334	-261020.9		
3c_4c_TS		-568.849566	-356958.5			-568.804558	-356930.3	14.4	11.3
Water		-76.448667	-47972.3			-76.4296	-47960.3		
4c		-416.000138	-261044.0	23.3	50.4	-415.963334	-261020.9		
HIC		-416.031375	-261063.6			-415.995213	-261040.9		
4c_HIC_TS		-492.399702	-308985.5			-492.358653	-308959.7	21.5	41.5
Water		-76.448667	-47972.3			-76.4296	-47960.3		
$Dc\_OHC\text{-}CHOHNH_2$		-341.006158	-213984.6	4.7	9.9	-340.97102	-213962.6		
Monohydrate		-304.326221	-190967.6			-304.294176	-190947.5		
Dc_1b_TS		-721.761598	-452912.3			-721.711189	-452880.6	1.7	11.8

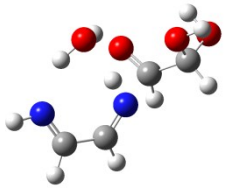
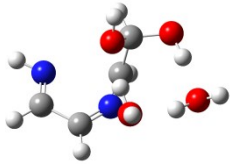
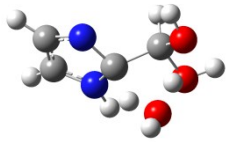
1b		-645.328713	-404949.9			-645.281251	-404920.1		
Water		-76.448667	-47972.3			-76.448667	-47972.3		
Fc_HNHC-CHNH		-188.099923	-118034.5			-188.071189	-118016.5		
Monohydrate		-304.326221	-190967.6			-304.294176	-190947.5		
1a		-492.426490	-309002.3			-492.384765	-308976.1		
Fc_1a_TS		-568.838934	-356951.8	15.0	22.7	-568.795241	-356924.4	11.8	24.0
Water		-76.448667	-47972.3			-76.448667	-47972.3		
1a		-492.426490	-309002.3			-492.384765	-308976.1		
2a		-416.424828	-261310.5			-416.387517	-261287.1		
H_3O^+		-76.830949	-48212.2			-76.812793	-48200.8		
1a_2a_TS		-569.287123	-357233.1	-26.1	22.0	-569.238068	-357202.3	-25.4	29.4
Water		-76.448667	-47972.3			-76.448667	-47972.3		
2a		-416.424828	-261310.5			-416.387517	-261287.1		
HIC		-416.031375	-261063.6			-415.995213	-261040.9		
H_3O^+		-76.830949	-48212.2			-76.812793	-48200.8		
2a_HIC_TS		-492.844235	-309264.4	10.9	11.4	-492.80582	-309240.3	19.1	1.4
Water		-76.448667	-47972.3			-76.448667	-47972.3		

Table S3. Cartesian coordinates of the most stable states for all structures

Structure	**Abbreviation**	Atom	X	Y	Z
trans-Glyoxal (trans-GO)	HOC-COHt	C	0.3291	0.6898	0.0000
		O	-0.3291	1.6986	-0.0001
		H	1.4356	0.6728	0.0001
		C	-0.3291	-0.6898	0.0000
		O	0.3291	-1.6986	-0.0001
		H	-1.4356	-0.6728	0.0001
Water	H_2O	O	0.0682	0.2921	-0.0000
		H	0.8072	-0.2921	-0.0000
		H	-0.8072	-0.0559	0.0000
Ammonia	NH_3	N	-0.0026	0.2314	-0.2007
		H	-0.8094	0.7032	0.2006
		H	0.8094	0.6942	0.2006
		H	-0.0078	-0.7032	0.2007
Hydronium	H_3O^+	O	0.0000	-0.2465	0.0000
		H	0.0000	0.7395	0.0000
		H	-0.8539	-0.7395	-0.0000
		H	0.8539	-0.7395	0.0000
Formic acid	HCOOH	C	0.1217	0.1808	0.0002
		O	1.1262	-0.4812	-0.0001
		O	-1.1262	-0.3075	0.0000
		H	0.0878	1.2781	-0.0002
		H	-1.0773	-1.2781	-0.0001
cis-Glyoxal (cis-GO)	$HOC\text{-}COH_c$	C	0.0000	-0.7730	0.0136
		O	0.0000	-1.4018	-1.0120
		H	0.0000	-1.2506	1.0120
		C	0.0000	0.7730	0.0136
		O	0.0000	1.4018	-1.0120
		H	0.0000	1.2506	1.0120
B from trans-GO	B_t_OHC-$CHOHNH_2$	C	-1.1022	-0.7589	-0.1158
		O	-2.0481	-0.1033	-0.4757
		H	-1.1804	-1.8467	0.0767
		O	1.1586	-1.0789	-0.5628
		H	2.0481	-0.7138	-0.4891
		N	0.4726	1.1827	-0.3574
		H	-0.0820	1.3434	-1.1941
		H	0.1593	1.8467	0.3422
		C	0.2938	-0.1690	0.1078
		H	0.4745	-0.1868	1.1941
B from cis-GO	B_c_OHC-$CHOHNH_2$	C	0.8417	-0.4904	0.1442
		O	1.7497	0.0596	-0.4283
		H	0.9531	-1.5070	0.5773
		O	-0.6004	1.3820	-0.1804
		H	-1.5319	1.6270	-0.2366
		N	-1.5234	-0.7741	-0.4390
		H	-1.1693	-1.0217	-1.3586
		H	-1.7497	-1.6270	0.0609
		C	-0.5749	0.0570	0.2934
		H	-0.8437	-0.0080	1.3586
Iminoacetaldehyde from cis-GO	C_c_OHC-CHNH	C	-0.2369	0.3880	0.0000
		H	-0.1424	1.4785	0.0000
		C	1.0481	-0.3784	-0.0001
		O	2.1322	0.1573	0.0001
		H	0.9206	-1.4785	0.0001
		N	-1.3235	-0.2695	0.0000
		H	-2.1322	0.3560	0.0001
Iminoacetaldehyde from trans-GO	C_t_OHC-CHNH	C	0.6930	0.4404	0.0001
		H	1.1538	1.4293	-0.0001
		C	-0.8211	0.3865	0.0000
		O	-1.4200	-0.6635	0.0000

		H	-1.3460	1.3587	0.0000
		N	1.4200	-0.5994	0.0000
		H	0.8115	-1.4293	-0.0001
Imino-aminoethanol from cis-GO	E_c_NH_2HOHC-CHNH	C	0.5183	-0.0316	0.3327
		H	0.4736	-0.0114	1.4295
		C	-0.8325	-0.0075	-0.3457
		H	-0.6782	-0.0019	-1.4295
		O	-1.4420	1.2181	0.0890
		H	-2.2921	1.2964	-0.3590
		N	1.5921	-0.0723	-0.3388
		H	2.4023	-0.0947	0.2841
		N	-1.5601	-1.2053	0.0041
		H	-1.8415	-1.1706	0.9803
		H	-2.4023	-1.2964	-0.5552
Imino-aminoethanol from trans-GO	E_t_NH_2HOHC-CHNH	C	0.4009	-0.4652	0.1467
		H	0.5066	-1.4831	0.5446
		C	-1.0119	0.0664	0.2881
		N	1.3422	0.1800	-0.4061
		H	2.1913	-0.3889	-0.4220
		N	-1.9802	-0.7533	-0.4379
		H	-1.6186	-1.0076	-1.3533
		H	-2.1913	-1.6100	0.0633
		O	-1.0667	1.3987	-0.1759
		H	-2.0057	1.6100	-0.2399
		H	-1.2836	0.0048	1.3533
Diiminoethane from cis-GO	F_c_HNHC-CHNH	C	-0.2922	0.4439	0.0003
		H	-0.7698	1.4286	0.0000
		C	1.2077	0.4398	-0.0003
		H	1.6905	1.4189	-0.0002
		N	-0.9257	-0.6569	0.0000
		H	-1.9345	-0.5022	-0.0002
		N	1.9345	-0.6026	-0.0003
		H	1.3224	-1.4286	-0.0001
Diiminoethane from trans-GO	F_t_HNHC-CHNH	C	0.7804	0.3847	0.0000
		H	0.6820	1.4803	0.0000
		C	-0.3131	-0.3847	-0.0000
		H	-0.2147	-1.4803	0.0000
		N	1.9957	0.0520	0.0000
		H	2.2549	-0.9365	0.0000
		N	-1.5284	-0.0520	-0.0000
		H	-2.2549	-0.7708	-0.0000
Diaminoethanediol from cis-GO	D_c_NH_2HOHC-$CHOHNH_2$	C	-0.6299	-0.3627	-0.4534
		H	-0.7285	-1.0530	-1.2997
		C	0.7616	0.2819	-0.5174
		H	0.8624	0.8347	-1.4568
		O	1.6663	-0.8420	-0.5066
		H	2.5645	-0.5002	-0.4413
		O	-0.7423	-1.1070	0.7781
		H	0.0216	-1.6993	0.8067
		N	-1.6500	0.6365	-0.5438
		H	-2.5645	0.2108	-0.4339
		H	-1.5206	1.3091	0.2072
		N	0.9321	1.2023	0.5761
		H	0.8970	0.6985	1.4568
		H	1.8136	1.6993	0.5179
Diaminoethanediol from trans-GO	D_t_NH_2HOHC-$CHOHNH_2$	C	0.7033	-0.0449	0.3076
		H	0.5973	-0.0517	1.4010
		C	-0.7033	0.0449	-0.3076
		H	-0.5973	0.0515	-1.4010
		O	-1.2542	1.2898	0.1433
		H	-2.1371	1.3602	-0.2352
		O	1.2542	-1.2898	-0.1434

		H	2.1372	-1.3602	0.2351
		N	1.5007	1.1070	-0.0460
		H	2.3890	1.0838	0.4448
		H	1.7075	1.0843	-1.0414
		N	-1.5006	-1.1069	0.0461
		H	-1.7076	-1.0842	1.0415
		H	-2.3890	-1.0838	-0.4448
Glyoxal monohydrate	Monohydrate	C	-0.7094	-0.5667	-0.0107
		O	-1.6559	0.0878	-0.3621
		H	-0.7737	-1.6586	0.1695
		O	0.7617	1.2868	-0.2795
		H	1.6143	1.6586	-0.0248
		O	1.6559	-0.8852	-0.3465
		H	1.5350	-0.8677	-1.3053
		C	0.6997	-0.0134	0.2256
		H	0.8978	-0.0550	1.3053
Glyoxal dihydrate	Dihydrate	C	-0.6993	-0.0247	0.3073
		H	-0.5964	-0.0067	1.4028
		C	0.6993	0.0247	-0.3073
		H	0.5964	0.0066	-1.4028
		O	-1.3741	1.1103	-0.1578
		H	-2.1467	1.2592	0.3973
		O	-1.4007	-1.1774	-0.1163
		H	-0.8308	-1.9345	0.0720
		O	1.3741	-1.1103	0.1578
		H	2.1467	-1.2592	-0.3973
		O	1.4007	1.1774	0.1163
		H	0.8308	1.9345	-0.0720
Aminoethanetriol	HOHOHC-CHOHNH$_2$	C	0.6373	-0.3495	-0.3109
		H	0.5222	-0.3978	-1.3987
		C	-0.7681	-0.3661	0.3043
		H	-0.6829	-0.4724	1.3987
		O	-1.4652	-1.4460	-0.2468
		H	-2.2979	-1.5318	0.2299
		O	1.1719	0.9391	0.0672
		H	1.9256	1.1330	-0.4997
		N	1.4163	-1.4724	0.1258
		H	2.2979	-1.5156	-0.3744
		H	1.6303	-1.3853	1.1156
		O	-1.4575	0.8330	-0.0052
		H	-0.7882	1.5318	0.0206
Iminoethanediol	HOHOHC-CHNH	C	-0.4384	-0.0038	0.3286
		H	-0.3977	-0.0049	1.4241
		C	0.9165	-0.0029	-0.3350
		H	0.7937	-0.0022	-1.4241
		O	1.5710	-1.1773	0.1021
		H	2.3219	-1.3445	-0.4785
		N	-1.5002	-0.0027	-0.3612
		H	-2.3219	-0.0031	0.2468
		O	1.5706	1.1712	0.1035
		H	2.3160	1.3445	-0.4821
	HNHC-CHN-HOHC-CHOHOH$_t$	C	1.7040	-0.4471	-0.4412
		H	1.1212	-0.9938	-1.1867
		C	1.0446	0.6479	0.3118
		H	1.7141	1.1614	1.0052
		N	2.9255	-0.6989	-0.1824
		H	3.2663	-1.4670	-0.7640
		N	-0.1633	1.0444	0.2515
		C	-1.7541	-0.8336	0.0327
		H	-0.9924	-1.5990	0.2139
		O	-2.6959	-1.4153	-0.8273
		H	-3.2663	-0.6942	-1.1319

		O	-2.3437	-0.3910	1.2382
		H	-2.8509	-1.1280	1.5981
		O	-2.1693	1.3416	-0.9215
		H	-2.5508	1.5990	-0.0705
		C	-1.1340	0.4191	-0.6259
		H	-0.7307	0.1272	-1.5981
	HNHC-CHN-HOHC-CHOHOH$_c$	C	-1.9451	0.0802	-0.1928
		H	-3.0303	-0.0606	-0.1388
		C	-1.1633	-1.1271	0.1960
		H	-1.7455	-1.8689	0.7470
		N	-1.3999	1.1751	-0.5466
		H	-2.1109	1.8689	-0.7849
		N	0.0482	-1.4312	-0.0519
		C	1.6656	0.4197	0.1375
		H	0.9524	1.0878	0.6226
		O	2.5335	1.2341	-0.6067
		H	3.0303	0.6384	-1.1868
		O	2.3729	-0.3753	1.0741
		H	2.9480	0.2166	1.5726
		O	1.9098	-1.3642	-1.4649
		H	2.3845	-1.8450	-0.7724
		C	0.9383	-0.5698	-0.7979
		H	0.4364	0.0117	-1.5726
	HNHC-CHN-HOHC-CHOHOH$^+$	C	1.9180	0.5729	-0.2880
		H	2.7184	1.2339	-0.5897
		C	1.8676	-0.8924	-0.2723
		H	2.6762	-1.5446	-0.5720
		N	0.7698	0.9833	0.1310
		H	0.4649	1.9493	0.2133
		N	0.7203	-1.3081	0.1343
		C	-1.4060	-0.1238	-0.4132
		H	-1.1520	-0.1873	-1.4780
		O	-1.9740	1.0980	-0.0702
		H	-2.7184	1.2697	-0.6598
		O	-2.2390	-1.1686	-0.0158
		H	-2.0485	-1.9493	-0.5499
		C	-0.0862	-0.1674	0.4248
		H	-0.3827	-0.1492	1.4780
Imidazole	I	C	0.5049	0.6163	0.0000
		H	0.9489	1.5974	0.0001
		C	1.0407	-0.6461	-0.0000
		H	2.0840	-0.9221	-0.0001
		N	-0.8579	0.4286	0.0001
		H	-1.5586	1.1546	0.0003
		N	0.0394	-1.5974	-0.0003
		C	-1.0870	-0.9129	-0.0000
		H	-2.0840	-1.3257	-0.0001
Hydrated N-glyoxal substituted imidazole	HGI	C	1.4552	-0.5816	0.7443
		H	1.1121	-1.2391	1.5246
		C	2.6538	-0.4603	0.0928
		H	3.5560	-1.0300	0.2547
		N	0.6318	0.3721	0.1833
		N	2.5890	0.5425	-0.8548
		C	1.3620	1.0148	-0.7775
		H	0.9469	1.8229	-1.3571
		C	-0.7732	0.5853	0.4838
		H	-0.9594	0.1917	1.4902
		C	-1.6745	-0.1877	-0.4927
		H	-1.4114	0.0740	-1.5246
		O	-1.4755	-1.5507	-0.2403
		H	-1.7534	-2.0575	-1.0107
		O	-2.9912	0.2400	-0.1947

		H	-3.5560	0.0873	-0.9600
		O	-1.0195	1.9672	0.4019
		H	-1.9728	2.0575	0.2631
Hydrated imidazole-2-carboxaldehyde	HIC	C	-2.1080	0.3662	-0.3185
		H	-2.8993	1.0876	-0.4326
		C	-2.0990	-1.0050	-0.2719
		H	-2.9412	-1.6761	-0.3429
		N	-0.7909	0.7376	-0.1896
		H	-0.4201	1.6761	-0.1796
		N	-0.8116	-1.4752	-0.1170
		C	1.4390	-0.3375	0.1501
		H	1.6572	-0.3810	1.2234
		O	1.9624	0.9144	-0.2611
		H	1.8773	0.9576	-1.2234
		O	2.0250	-1.4148	-0.5315
		H	2.9412	-1.4789	-0.2365
		C	-0.0499	-0.3999	-0.0777
1H-imidazole-2-carboxaldehyde	IC	C	-1.4755	0.8001	0.4166
		H	-2.2823	1.5477	0.4166
		C	-1.6973	-0.5184	0.4166
		H	-2.6737	-1.0250	0.4166
		N	-0.1259	1.0735	0.4166
		H	0.1370	1.5997	-0.4166
		N	-0.6121	-1.1588	0.4166
		C	1.7986	-0.5178	0.4166
		H	2.0599	-1.5997	0.4166
		O	2.6737	0.3149	0.4166
		C	0.4955	-0.2322	0.4166
	$OHC\text{-}CN\text{-}HOHC\text{-}CHOHOH_t$	C	-1.9197	0.5310	-0.1968
		H	-3.0168	0.5075	-0.0556
		C	-1.2174	-0.7356	0.2141
		H	-1.8399	-1.4358	0.7745
		N	-0.0245	-1.0890	-0.0482
		C	1.6027	0.7569	0.1234
		H	0.8798	1.4448	0.5653
		O	2.4943	1.5414	-0.6205
		H	3.0168	0.9270	-1.1568
		O	2.2719	-0.0121	1.1056
		H	2.8286	0.5905	1.6125
		O	1.8790	-1.0888	-1.4058
		H	2.3376	-1.5414	-0.6840
		C	0.8987	-0.2637	-0.8007
		H	0.4243	0.2882	-1.6125
		O	-1.3639	1.5058	-0.6527
	$OHC\text{-}CN\text{-}HOHC\text{-}CHOHOH_c$	C	1.9243	-0.4742	-0.4610
		H	1.3273	-0.9877	-1.2349
		C	1.2684	0.6201	0.3305
		H	1.9472	1.1050	1.0352
		N	0.0648	1.0232	0.2746
		C	-1.5466	-0.8298	0.0235
		H	-0.7894	-1.6059	0.1775
		O	-2.5014	-1.3811	-0.8389
		H	-3.0768	-0.6519	-1.1135
		O	-2.1158	-0.4063	1.2441
		H	-2.6289	-1.1434	1.5957
		O	-1.9447	1.3762	-0.8706
		H	-2.3252	1.6059	-0.0110
		C	-0.9214	0.4339	-0.6134
		H	-0.5301	0.1636	-1.5957
		O	3.0768	-0.7791	-0.2532
	$OHC\text{-}CN\text{-}HOHC\text{-}CHOHOH^+$	C	1.9198	0.6705	-0.2601
		H	2.6781	1.3974	-0.5266

		C	1.9441	-0.7830	-0.3027
		H	2.7714	-1.3974	-0.6271
		N	0.8093	-1.2315	0.1109
		C	-1.3362	-0.0441	-0.4314
		H	-1.0605	-0.0838	-1.4882
		O	-1.9585	1.1768	-0.2277
		H	-2.3826	1.1683	0.6421
		O	-2.0729	-1.1408	-0.0033
		H	-2.7714	-1.3151	-0.6465
		C	-0.0190	-0.1456	0.4259
		H	-0.2744	-0.1091	1.4882
		O	0.7984	1.0766	0.1605
1.3-oxazole	oxazole	C	-1.1554	-0.6468	-0.0002
		H	-1.9264	-1.3969	-0.0003
		C	-1.1309	0.7054	-0.0000
		H	-1.9576	1.3969	0.0001
		N	0.1955	1.1366	0.0006
		C	0.8862	0.0439	-0.0007
		H	1.9576	-0.0771	-0.0005
		O	0.1427	-1.0890	0.0007
	$HNHC\text{-}CHN\text{-}CHOH\text{-}(CNHCHCHN)_t$	C	3.5475	-0.7732	-0.8180
		H	4.2882	-1.5323	-1.0034
		C	3.5031	0.5662	-1.1050
		H	4.2477	1.1669	-1.6030
		N	2.3580	-1.0499	-0.1790
		H	2.0274	-1.9516	0.1309
		N	2.3151	1.1077	-0.6539
		C	0.2855	0.2579	0.5084
		H	0.3655	0.1919	1.6030
		O	-0.2170	1.5407	0.1830
		C	1.6573	0.1077	-0.1067
		C	-2.6016	0.1995	-0.6680
		H	-2.2984	1.2163	-0.4315
		C	-1.6611	-0.9102	-0.3550
		H	-2.0920	-1.8892	-0.5822
		N	-3.7168	-0.1291	-1.1928
		H	-4.2882	0.7019	-1.3593
		N	-0.4857	-0.9075	0.1289
		H	0.4473	1.9516	-0.3953
	$HNHC\text{-}CHN\text{-}CHOH\text{-}(CNHCHCHN)_c$	C	-2.0852	-1.5193	-0.1280
		H	-2.3603	-2.5590	-0.0730
		C	-2.8016	-0.3626	0.0600
		H	-3.8441	-0.2590	0.3182
		N	-0.8106	-1.1134	-0.4473
		H	0.0283	-1.6597	-0.6508
		N	-1.9903	0.7363	-0.1364
		C	0.4140	1.0867	-0.6965
		H	0.9603	0.7189	-1.5701
		O	0.0295	2.4121	-0.9734
		C	-0.8070	0.2409	-0.4425
		C	2.7541	-0.7734	-0.2506
		H	3.8441	-0.8773	-0.2379
		C	2.2326	0.2875	0.6582
		H	2.8232	0.4062	1.5701
		N	1.9984	-1.5259	-0.9462
		H	2.5411	-2.1953	-1.4932
		N	1.2450	1.0769	0.5135
		H	-0.7993	2.5590	-0.4929
	$HNHC\text{-}CHN\text{-}CHOH\text{-}(CNHCHCHN)^+$	C	-2.5600	-0.6330	-0.7272
		C	-0.5422	0.0037	-0.1487
		C	-2.4711	0.7360	-0.6989
		H	-3.3671	-1.3054	-0.9625

		H	-3.2411	1.4577	-0.9200
		C	0.8900	-0.0630	0.3018
		H	0.9769	-0.0365	1.3965
		C	2.6570	0.6592	-0.9037
		C	2.6088	-0.8107	-0.8582
		H	3.3671	1.3088	-1.3965
		H	3.3225	-1.4678	-1.3358
		N	1.5941	-1.2187	-0.1881
		N	1.6455	1.0855	-0.2357
		H	1.3629	2.0546	-0.1110
		N	-1.1999	1.1257	-0.3345
		N	-1.3122	-1.0905	-0.3725
		H	-1.0188	-2.0546	-0.3055
2.2’-bisimidazole	BI	C	2.8233	-0.6307	0.0002
		C	2.7509	0.7413	0.0004
		C	0.7220	0.0415	-0.0001
		N	1.5195	-1.0636	-0.0001
		H	1.1920	-2.0186	-0.0003
		H	3.6543	-1.3153	0.0003
		H	3.5674	1.4467	0.0006
		C	-0.7220	-0.0415	-0.0003
		N	-1.5195	1.0636	-0.0005
		C	-2.7509	-0.7413	-0.0004
		C	-2.8233	0.6307	-0.0006
		H	-1.1920	2.0186	-0.0006
		H	-3.5674	-1.4467	-0.0004
		H	-3.6543	1.3153	-0.0006
		N	1.4384	1.1555	-0.0001
		N	-1.4384	-1.1555	-0.0005
N-glyoxal substituted hydrated 1H-imidazole-2-carbaldehyde	GHIC	C	-0.7441	0.9211	0.5620
		H	-1.7556	1.2209	0.7786
		C	0.4211	1.6235	0.4347
		H	0.5665	2.6894	0.5178
		N	-0.4013	-0.4065	0.3787
		N	1.4721	0.7697	0.1744
		C	1.7013	-1.7275	-0.1124
		H	1.3233	-2.2083	-1.0218
		O	1.4575	-2.6894	0.9046
		H	1.7065	-2.2921	1.7501
		O	3.0596	-1.4147	-0.2306
		H	3.5113	-2.2231	-0.4999
		C	0.9556	-0.4395	0.1484
		C	-1.3583	-1.5177	0.4314
		H	-0.7845	-2.4378	0.3074
		C	-2.3238	-1.3598	-0.7498
		O	-3.5113	-1.2510	-0.5721
		H	-1.8602	-1.3328	-1.7501
		O	-2.0479	-1.5412	1.6418
		H	-2.9728	-1.3264	1.4392
Hydrated N-glyoxal substituted hydrated 1H-imidazole-2-carbaldehyde	HGHIC	C	0.7963	0.8780	-0.5417
		H	1.8412	1.0528	-0.7157
		C	-0.3144	1.6689	-0.6505
		H	-0.3640	2.7027	-0.9563
		N	0.3404	-0.3483	-0.0946
		N	-1.4485	0.9649	-0.3017
		C	-1.8846	-1.4234	0.3797
		H	-1.5007	-1.9352	1.2680
		O	-1.8008	-2.4324	-0.6460
		H	-2.1776	-2.0461	-1.4500
		O	-3.1937	-0.9866	0.5572
		H	-3.7052	-1.7346	0.8877
		C	-1.0273	-0.2370	0.0242

		C	1.0999	-1.5882	0.1053
		H	0.7057	-2.0584	1.0105
		O	0.9982	-2.4434	-1.0079
		H	0.0631	-2.7027	-1.0796
		C	2.6029	-1.3684	0.3176
		H	3.0226	-2.3472	0.5887
		O	3.2384	-0.8875	-0.8547
		H	2.9578	-1.4566	-1.5844
		O	2.7730	-0.4389	1.3396
		H	3.7052	-0.4305	1.5844
N-glyoxal substituted 2.2'-bisimidazole	GBI	C	2.9603	-1.0835	0.0496
		C	2.1469	-2.1795	0.2008
		C	0.8366	-0.4780	0.0773
		N	2.1111	-0.0071	-0.0276
		H	2.3602	0.9644	-0.1441
		H	4.0298	-0.9751	-0.0098
		H	2.4364	-3.2141	0.2960
		C	-0.3022	0.4148	0.0194
		N	-1.6045	0.0449	0.2557
		C	-1.5015	2.1787	-0.2422
		C	-2.3777	1.1740	0.0781
		H	-1.7289	3.2141	-0.4432
		H	-3.4429	1.1528	0.2242
		N	0.8251	-1.7975	0.2137
		N	-0.2143	1.7024	-0.2793
		C	-2.1319	-1.2936	0.6107
		H	-1.3678	-1.7916	1.2086
		C	-2.3284	-2.0583	-0.7075
		O	-3.4290	-2.4101	-1.0539
		H	-1.4194	-2.2282	-1.3044
		O	-3.3276	-1.1842	1.3044
		H	-4.0298	-1.4638	0.6936
Hydrated glyoxal dimer substituted imidazole	HGGI	C	-1.9592	-1.0539	0.4696
		C	-3.2854	-1.3836	0.5025
		C	-3.0988	0.0892	-1.0419
		N	-1.8430	-0.0972	-0.5237
		H	-1.1114	-1.3816	1.0418
		H	-3.7727	-2.0971	1.1492
		H	-3.2825	0.7842	-1.8473
		O	0.3222	-0.4290	-1.3532
		O	1.4333	1.3657	-0.4722
		C	0.1057	1.4477	0.0129
		H	-0.1943	2.4949	-0.0467
		O	-0.0362	0.9316	1.3051
		H	0.4167	1.5230	1.9176
		C	2.2721	-0.9085	-0.0376
		H	1.7247	-0.8766	0.9136
		O	2.2607	-2.2170	-0.5844
		H	1.3382	-2.4949	-0.6503
		O	3.5975	-0.5025	0.1065
		H	3.9925	-1.0164	0.8197
		N	-3.9925	-0.6619	-0.4433
		C	-0.6483	0.5512	-0.9929
		H	-0.9255	1.1492	-1.8644
		C	1.6171	0.0688	-1.0190
		H	2.2338	0.1548	-1.9176
2-(2-amino-1,2-dihydroxyethylamino)ethane-1,1,2-triol		C	1.2030	0.6280	0.1301
		C	2.2916	-0.4118	0.4660
		C	-0.7903	-0.5152	-0.9215
		H	0.5517	0.7715	0.9970
		H	2.9446	0.0190	1.2391
		N	0.3890	0.3257	-1.0273

		H	0.9833	-0.0306	-1.7704
		N	1.6883	-1.6718	0.8888
		H	2.4069	-2.3905	0.8903
		C	-1.7271	-0.0955	0.2249
		H	-1.3242	-0.4503	1.1829
		O	-1.8469	1.3120	0.2242
		H	-2.3777	1.5634	0.9886
		O	-2.9651	-0.7265	-0.0270
		H	-3.4272	-0.8413	0.8093
		O	3.0510	-0.7129	-0.6943
		H	3.4272	0.1242	-0.9949
		O	1.9459	1.8197	-0.1371
		H	1.3487	2.3905	-0.6353
		H	-1.3603	-0.3861	-1.8462
		H	1.3568	-1.5909	1.8462
		O	-0.5066	-1.9036	-0.8263
		H	0.2464	-1.9869	-0.1939
2-(dihydroxymethyl) imidazolidine-4,5-diol		C	-1.5553	-0.7354	0.5468
		C	-1.3936	0.8173	0.5656
		C	0.4623	-0.0800	-0.5409
		H	-1.6817	-1.1445	1.5503
		H	-0.9942	1.1404	1.5303
		H	0.8584	-0.2199	-1.5503
		N	-0.3833	-1.2164	-0.1293
		H	0.1272	-1.9449	0.3529
		N	-0.3866	1.1016	-0.4869
		H	-0.8810	1.2249	-1.3657
		C	1.6718	0.1220	0.3817
		H	1.3393	0.2031	1.4291
		O	2.4950	-0.9999	0.2176
		H	3.1589	-0.9970	0.9156
		O	2.3740	1.2892	0.0023
		H	1.6840	1.9449	-0.1852
		O	-2.5958	1.4888	0.3361
		H	-3.1589	0.8371	-0.1164
		O	-2.7547	-1.0749	-0.1816
		H	-2.4496	-1.3459	-1.0570
2-(dihydroxymethyl)5-hydroxy-2,5-dihydro-1H-imidazol		C	-1.6920	1.1395	-0.5148
		C	-2.1044	-0.3218	-0.4909
		C	0.0639	0.1084	0.3538
		H	-2.3538	1.9257	-0.8673
		H	-2.5065	-0.6854	-1.4384
		H	0.2240	0.0709	1.4384
		N	-0.5556	1.3851	-0.0011
		N	-0.8352	-0.9418	-0.1525
		H	-0.9478	-1.7306	0.4718
		C	1.4394	-0.0310	-0.3145
		H	1.3398	0.2149	-1.3832
		O	2.3217	0.8305	0.3370
		H	3.1623	0.8055	-0.1340
		O	1.9232	-1.3572	-0.1651
		H	1.3367	-1.9257	-0.6812
		O	-3.1623	-0.5478	0.4439
		H	-2.8971	-0.1774	1.2957
(2H-imidazol-2-yl) methanediol	PreHIC	C	1.9717	-1.0101	-0.2885
		C	1.9311	0.4674	-0.2470
		C	0.0216	-0.3502	0.4159
		H	2.8116	-1.6201	-0.6023
		H	2.7315	1.1425	-0.5286
		H	-0.2685	-0.3868	1.4721
		N	0.8502	-1.5031	0.0955
		N	0.7848	0.8706	0.1652

		C	-1.2875	-0.3056	-0.4017
		H	-1.0362	-0.3460	-1.4721
		O	-2.0620	-1.3967	-0.0163
		H	-2.8116	-1.4564	-0.6195
		O	-2.0011	0.8784	-0.1045
		H	-1.3962	1.6201	-0.2402
1-amino-2-(hydroxy(1H-imidazol-2-yl) methylamino) ethane-1,2-diol		C	-1.3853	0.6040	-0.4807
		C	-2.3409	-0.4783	-1.0248
		C	0.0593	-0.5265	1.2584
		H	-0.4920	0.6414	-1.1132
		H	-2.6770	-0.1484	-2.0195
		N	-0.9642	0.4596	0.9019
		H	-1.7838	0.2995	1.4828
		N	-1.6871	-1.7747	-1.0575
		H	-2.2927	-2.4588	-1.4990
		O	-3.4635	-0.6190	-0.1646
		H	-3.8925	0.2459	-0.1399
		O	-2.1388	1.8089	-0.5926
		H	-1.6898	2.4588	-0.0387
		H	0.4186	-0.2514	2.2545
		H	-0.8149	-1.7284	-1.5807
		O	-0.4220	-1.8468	1.3826
		H	-0.9165	-2.0360	0.5474
		C	1.2235	-0.4313	0.2948
		C	3.0433	0.3841	-0.6695
		C	2.5722	-0.6996	-1.3629
		H	3.8925	1.0302	-0.8134
		H	2.9817	-1.1484	-2.2545
		N	1.4374	-1.2007	-0.7568
		N	2.1711	0.5425	0.3849
		H	2.2218	1.2591	1.0937
2-(1H-imidazol-2-yl) imidazolidine-4,5-diol		C	2.0874	-0.6574	-0.8008
		C	1.7962	0.8718	-0.7029
		C	0.3494	-0.2046	0.7585
		H	1.9951	-1.0265	-1.8235
		H	1.1150	1.1725	-1.5039
		H	0.2245	-0.4186	1.8235
		N	1.1610	-1.2714	0.1169
		H	0.5754	-1.9805	-0.3088
		N	1.0928	1.0361	0.5924
		H	1.7973	1.1139	1.3214
		O	2.9519	1.6502	-0.7800
		H	3.6697	1.0536	-0.5068
		O	3.4506	-0.9024	-0.4005
		H	3.3929	-1.2308	0.5057
		C	-1.0118	-0.0878	0.1143
		C	-2.8956	-0.5069	-0.8301
		C	-2.8938	0.8406	-0.5754
		H	-3.6697	-1.0928	-1.3013
		H	-3.6112	1.6198	-0.7698
		N	-1.6829	1.0902	0.0319
		H	-1.3099	1.9805	0.3274
		N	-1.7156	-1.0793	-0.3962
2-(1H-imidazol-2-yl) -2,5-dihydro-1H-imidazol-5-ol		C	-2.1641	0.9408	-0.9020
		C	-2.5260	-0.5060	-0.6138
		C	-0.6091	0.2707	0.5266
		H	-2.7530	1.5639	-1.5696
		H	-2.5165	-1.1206	-1.5183
		H	-0.5984	0.6108	1.5696
		N	-1.1511	1.3847	-0.2795
		N	-1.5017	-0.8808	0.3435
		H	-0.9716	-1.6957	0.0563

		O	-3.8567	-0.6317	-0.1149
		H	-3.8695	-0.2155	0.7564
		C	0.7995	-0.0423	0.0953
		N	1.7914	0.8870	0.0583
		N	1.2387	-1.2270	-0.2772
		C	2.9379	0.2555	-0.3735
		H	1.6909	1.8692	0.2667
		C	2.5766	-1.0509	-0.5725
		H	3.8695	0.7811	-0.4969
		H	3.1945	-1.8692	-0.9071
	PreBI	C	2.7568	-0.3290	-0.5754
		C	2.7788	0.5785	0.5960
		C	1.0348	-0.7332	0.7129
		H	3.4893	-0.3596	-1.3744
		H	3.5293	1.3314	0.8099
		H	1.0574	-1.6061	1.3744
		N	1.7347	-1.1002	-0.5326
		N	1.7704	0.3613	1.3571
		C	-0.4073	-0.3952	0.4774
		N	-0.8197	0.8084	-0.0093
		N	-1.4235	-1.2138	0.6591
		C	-2.1873	0.7541	-0.1443
		H	-0.2336	1.6061	-0.2067
		C	-2.5411	-0.5037	0.2714
		H	-2.7607	1.5921	-0.5031
		H	-3.5293	-0.9338	0.3197

Table S4. Cartesian coordinates of the transition states

TS	Atom	X	Y	Z
GLYOXAL_TRANS_H_2O_TS	C	-1.7890	-0.4525	-0.3683
	O	-2.8357	-0.1684	0.1597
	H	-1.6976	-0.6893	-1.4480
	C	-0.4637	-0.5692	0.3708
	O	0.2771	-1.5557	-0.0147
	H	-0.5704	-0.3587	1.4480
	O	0.2551	0.8672	-0.1528
	H	0.0918	1.5557	0.5065
	H	1.4523	0.4831	-0.1401
	O	2.3294	-0.2926	-0.1266
	H	1.5990	-1.0800	-0.0195
	H	2.8357	-0.2194	0.6934
	H	-0.3474	0.1487	-0.2426
	H	0.8498	0.1966	-0.3239
	H	1.6458	-0.9363	-0.2022
	H	0.9438	-1.1503	-0.2306
GLYOXAL_CIS_H_2O_TS	C	-0.6232	0.6802	0.3253
	O	0.0142	-0.0997	1.1232
	H	-0.8750	1.6895	0.6840
	C	-1.7495	0.0913	-0.5390
	O	-1.9809	-1.0904	-0.5879
	H	-2.3279	0.8342	-1.1232
	O	0.3565	1.0814	-1.0306
	H	1.0491	0.0177	-1.0063
	H	0.8994	1.8313	-0.7539
	O	1.3873	-1.0311	-0.6268
	H	2.3279	-1.0207	-0.4072
	H	0.8117	-0.8721	0.2854
	H	-0.3502	0.7841	-0.4833
	H	0.3920	-0.1980	-1.0290
	H	0.8955	-1.8313	-0.5540

	H	0.1816	-0.9160	0.0027
MONOHYDRATE_H_2O_TS	C	0.1048	-0.5375	-0.6938
	O	0.9175	-1.5367	-0.4886
	H	-0.3443	-0.4715	-1.6961
	O	-1.9378	-1.2704	0.1957
	H	-2.5373	-1.2566	0.9509
	O	-1.5152	1.0250	0.3197
	H	-2.0555	1.0677	-0.4816
	C	-0.9637	-0.2855	0.3904
	H	-0.4902	-0.3482	1.3758
	O	0.9790	0.8524	-0.6536
	H	0.3893	1.5367	-0.2950
	H	1.8281	0.5290	0.1152
	O	2.5373	-0.2636	0.7445
	H	1.8784	-1.0541	0.3306
	H	2.3953	-0.1923	1.6961
	H	0.6525	-0.0178	-0.8066
	H	1.2425	0.2519	-0.1278
	H	2.0353	-0.8791	0.2382
	H	1.2526	-1.1225	0.0434
GLYOXAL_TRANS_NH_3_TS	C	1.7427	0.0843	-0.8566
	O	2.2817	-0.9494	-0.5406
	H	1.9727	0.6130	-1.8002
	C	0.6439	0.7777	-0.0390
	O	-0.4047	1.1463	-0.8287
	H	1.0935	1.6312	0.4866
	N	0.1829	-0.2363	1.0069
	H	-0.5656	-0.8313	0.4192
	H	-0.2599	0.2210	1.8002
	H	0.9563	-0.8195	1.3275
	O	-1.4499	-1.0142	-0.7574
	H	-1.0592	-1.6312	-1.3857
	H	-0.9892	0.1444	-0.9781
	H	-1.1486	1.5831	-0.4502
	H	-0.8085	-1.0510	-0.1903
	H	-2.2817	-1.2094	-0.3605
	H	-1.1478	-0.4668	-1.2611
GLYOXAL_CIS_NH_3_TS	C	1.7424	0.0840	-0.8565
	O	2.2816	-0.9493	-0.5398
	H	1.9722	0.6122	-1.8006
	C	0.6437	0.7780	-0.0391
	O	-0.4051	1.1461	-0.8288
	H	1.0933	1.6318	0.4859
	N	0.1829	-0.2354	1.0074
	H	-0.5656	-0.8308	0.4202
	H	-0.2597	0.2222	1.8006
	H	0.9565	-0.8183	1.3282
	O	-1.4497	-1.0146	-0.7565
	H	-1.0588	-1.6318	-1.3845
	H	-0.9893	0.1443	-0.9778
	H	-1.1489	1.5831	-0.4504
	H	-0.8083	-1.0506	-0.1894
	H	-2.2816	-1.2097	-0.3599
	H	-1.1478	-0.4669	-1.2609
MONOHYDRATE_NH_3_TS	O	-1.8734	0.4495	-0.5007
	H	-2.3049	0.3277	-1.3538
	O	-1.4188	-1.8445	-0.3598
	H	-2.0314	-1.9138	0.3843
	C	-0.8828	-0.5362	-0.3725
	H	-0.1747	-0.5379	-1.2023
	C	-0.1429	-0.2290	0.9409
	O	0.6839	-0.9898	1.4142

	H	-0.5318	0.6371	1.4988
	N	1.2313	1.4215	-0.2649
	H	1.8996	0.7224	-0.5847
	H	1.7243	2.0798	0.3300
	H	0.8950	1.9292	-1.0772
	O	2.3049	-1.5373	-0.8601
	H	1.8304	-2.0798	-1.4988
	H	1.7815	-1.6127	-0.0466
Bt_H_2O_TS	C	-0.1025	0.0764	-0.7126
	O	0.6508	1.1321	-0.6214
	H	0.0544	-0.5952	-1.5741
	O	-2.1895	-1.0014	-0.4996
	H	-3.0716	-0.9131	-0.1201
	N	-1.8622	0.8783	0.8805
	H	-1.2810	0.4122	1.5741
	H	-1.5754	1.8526	0.8669
	C	-1.5858	0.2823	-0.4100
	H	-1.9729	0.9571	-1.1868
	O	0.3812	-0.9566	0.5232
	H	0.0927	-1.8526	0.3050
	H	1.5615	-0.7550	0.4363
	O	2.5582	-0.0972	0.1615
	H	1.8552	0.6320	-0.3150
	H	3.0716	-0.5315	-0.5305
	H	-0.2117	-0.3616	0.9498
	H	0.9412	-0.9020	0.1671
	H	1.7550	-0.4844	0.4654
	H	1.2528	0.3283	-0.4689
Bc_H_2O_TS	C	-0.1027	-0.6119	0.3161
	O	0.6123	-1.5970	-0.1304
	H	-0.1375	-0.4515	1.4100
	O	-2.2407	-1.5354	0.1298
	H	-3.1560	-1.3399	-0.1051
	N	-2.1825	0.8005	0.0162
	H	-2.1470	0.9711	1.0182
	H	-1.7691	1.5970	-0.4563
	C	-1.4826	-0.4218	-0.3223
	H	-1.3345	-0.4447	-1.4100
	O	0.6933	0.8123	-0.1445
	H	0.5641	1.4797	0.5425
	H	1.8265	0.3858	-0.1063
	O	2.7085	-0.4466	-0.0810
	H	1.8818	-1.1983	-0.0411
	H	3.1560	-0.4293	0.7740
	H	0.0820	0.1009	-0.2309
	H	1.2017	0.1372	-0.2698
	H	2.0136	-1.0634	-0.2364
	H	1.2160	-1.2510	-0.2220
Bt_NH_3_TS	C	0.3496	0.0289	0.5634
	O	-0.4747	-1.0504	0.6272
	H	0.8727	0.2227	1.5087
	O	2.0948	1.1588	-0.5809
	H	2.7584	1.1083	-1.2784
	N	2.3082	-1.1806	-0.4084
	H	2.7199	-1.1411	0.5223
	H	1.7886	-2.0523	-0.4626
	C	1.3864	-0.0740	-0.5715
	H	0.8344	-0.2279	-1.5087
	N	-0.5043	1.2821	0.2558
	H	0.0741	2.0523	-0.0785
	H	-1.0285	1.5750	1.0773
	H	-1.1965	0.8975	-0.5008

	O	-1.8116	-0.3312	-1.2465
	H	-2.7584	-0.3887	-1.0819
	H	-1.1845	-0.8894	-0.2774
	H	-0.9736	-1.3074	-0.1294
	H	-1.5065	0.3120	-0.7008
	H	-1.3262	-1.1042	-1.4794
	H	-1.6556	-1.2375	-0.6459
$Bc\_NH_3\_TS$	C	-0.0406	-0.5730	-0.5362
	O	0.4302	-1.2421	0.5500
	H	0.0987	-1.1001	-1.4931
	O	-2.2418	-1.3901	-0.6153
	H	-3.1111	-1.2515	-0.2220
	N	-1.8416	0.3542	0.9176
	H	-1.2115	-0.0419	1.6104
	H	-1.7929	1.3651	0.9478
	C	-1.5230	-0.1826	-0.3851
	H	-1.7841	0.5668	-1.1453
	N	0.8050	0.7089	-0.6917
	H	0.5421	1.3901	0.0207
	H	0.7343	1.1423	-1.6104
	H	1.8231	0.3303	-0.4670
	O	2.7418	-0.6887	0.1778
	H	3.1111	-1.2624	-0.5025
	H	1.5840	-1.1373	0.4622
	H	0.3512	-0.8618	1.4082
	H	1.1847	0.1077	-0.6149
	H	1.9304	-0.9180	0.5978
	H	0.9518	-1.1713	0.1831
$Bt\_\_\_H_2O\_TS$	C	-0.6452	-0.4851	0.2493
	H	-0.2059	-0.1431	1.1780
	C	-1.9934	0.0504	-0.1535
	O	-2.6381	-0.4650	-1.0339
	H	-2.3342	0.9436	0.3931
	N	-0.1404	-1.5309	-0.3371
	H	-0.6447	-1.8079	-1.1780
	O	0.3402	1.1238	-0.7215
	H	0.5168	1.8079	-0.0634
	H	1.2691	0.4313	-0.7440
	O	2.0978	-0.5510	-0.7254
	H	0.9937	-1.3895	-0.4385
	H	2.6381	-0.4774	0.0695
	H	-0.3679	0.5163	-0.5910
	H	0.6714	0.0888	-0.8104
	H	1.4184	-1.2016	-0.7745
	H	0.3198	-1.4671	-0.5757
$Bc\_\_\_H_2O\_TS$	C	0.5040	-0.6186	-0.3460
	H	0.3739	-0.2643	-1.3616
	C	1.8329	-0.3554	0.2936
	O	2.7564	0.1277	-0.3117
	H	1.8966	-0.6384	1.3616
	N	-0.3253	-1.5155	0.1125
	H	-0.1338	-1.8490	1.0542
	O	-0.3324	1.1633	0.3824
	H	-0.1756	1.8490	-0.2791
	H	-1.3642	0.6910	0.1566
	O	-2.3469	-0.1036	-0.0812
	H	-1.3979	-1.1558	-0.0770
	H	-2.6401	0.0379	-0.9886
	H	-1.0381	0.5501	0.2669
	H	-1.6382	0.1456	-0.1694
	H	-2.7564	-0.7665	0.4481
	H	-1.8464	-1.4061	-0.5408

$Ct\_H_2O\_TS$	C	-1.9556	0.3108	-0.0135
	H	-2.3203	1.2628	0.3770
	C	-0.5163	-0.0507	0.3116
	O	-0.0962	-1.1922	-0.1404
	H	-0.2367	0.2384	1.3367
	N	-2.7168	-0.4287	-0.7048
	H	-2.1777	-1.2646	-0.9708
	O	2.1380	-0.3642	-0.4979
	H	1.2641	-0.9894	-0.2911
	H	2.7168	-0.3586	0.2755
	O	0.3402	1.2016	-0.4277
	H	1.4171	0.5805	-0.4972
	H	0.0113	1.2646	-1.3367
	H	1.4490	-1.0029	-0.5658
	H	0.5963	-1.0356	-0.4665
	H	-0.0331	0.5724	0.1658
	H	0.7958	0.3032	-0.6233
$Cc\_H_2O\_TS$	C	1.6483	0.4519	-0.4233
	H	2.1495	1.3809	-0.7060
	C	0.3202	0.6375	0.3028
	O	-0.5443	1.3466	-0.4025
	H	0.4688	0.9552	1.3474
	N	2.0513	-0.7133	-0.7141
	H	2.9147	-0.7209	-1.2556
	O	-2.0975	-0.4413	-0.8359
	H	-1.5530	0.5056	-0.7839
	H	-2.9147	-0.3456	-0.3318
	O	-0.1851	-0.8551	0.5157
	H	-1.1860	-0.8717	-0.1062
	H	0.5163	-1.3809	0.0595
	H	-1.9477	-1.2179	-1.3474
	H	-1.9499	-0.0443	-0.9214
	H	-1.0276	-1.2408	0.6855
	H	-1.7457	-1.0365	-0.4783
$Ct\_NH_3\_TS$	C	-1.7908	0.2421	-0.7065
	H	-2.2305	1.0203	-1.3382
	C	-0.6277	0.6585	0.2031
	O	-0.0875	-0.3699	0.9071
	H	-0.9716	1.4765	0.8501
	N	-2.2740	-0.9264	-0.7290
	H	-1.7315	-1.4969	-0.0652
	O	1.3575	-1.0890	-0.8762
	H	0.6350	-0.8874	0.1452
	H	2.2740	-1.1546	-0.5874
	H	1.0174	0.3179	-1.0375
	N	0.4625	1.2528	-0.7172
	H	1.0940	1.8402	-0.1763
	H	0.0971	1.8020	-1.4935
	H	0.6326	-0.2123	1.4935
	H	0.7916	-1.8402	-0.8217
	H	0.0418	-1.0117	-0.1889
	H	0.4158	-0.0138	-1.1208
$Cc\_NH_3\_TS$	C	1.4529	0.3577	-0.8206
	H	1.6974	1.1987	-1.4765
	C	0.2888	0.6461	0.1220
	O	-0.7490	1.2768	-0.5015
	H	0.6684	1.2286	0.9734
	N	2.0401	-0.7646	-0.8238
	H	2.7873	-0.8046	-1.5175
	O	-1.8839	-0.7249	-1.2061
	H	-1.3809	0.4154	-0.9689
	H	-2.7873	-0.7098	-0.8720

	H	-0.9649	-1.0041	-0.0469
	N	-0.1678	-0.7119	0.6715
	H	-0.5432	-0.6359	1.6127
	H	0.6157	-1.3704	0.6436
	H	-1.5228	1.5042	-0.0147
	H	-1.5451	-1.5042	-1.6127
	H	-1.7971	-0.1131	-1.1312
	H	-1.4970	-1.1111	-0.4762
Dt___H_2O_TS	C	0.3519	0.0624	0.5845
	H	0.6932	0.4852	1.5249
	C	1.2836	0.2014	-0.6142
	H	0.6805	0.2537	-1.5249
	O	2.1061	-0.9853	-0.6296
	H	1.5253	-1.7552	-0.6805
	O	-0.8619	1.6505	-0.0023
	H	-1.4351	1.7552	0.7671
	N	-0.4968	-0.9414	0.5903
	H	-0.9972	-1.0895	1.4587
	H	-1.1295	-0.9070	-0.3336
	N	2.1119	1.3616	-0.5121
	H	2.7622	1.2509	0.2620
	H	2.6690	1.4545	-1.3550
	O	-1.8077	-0.1348	-1.3927
	H	-2.7622	-0.2384	-1.3187
	H	-1.3969	0.9567	-0.6721
	H	-1.0193	0.9528	-0.6154
	H	-1.6450	-1.1748	-0.7097
	H	-1.2591	-0.8921	-1.5063
	H	-1.6965	0.3617	-0.8592
Dc___H_2O_TS	C	1.3054	-0.0309	-0.2703
	H	1.4185	0.6356	-1.1314
	C	0.0087	-0.7964	-0.4472
	H	-0.4153	-0.9040	-1.4376
	O	-1.2817	1.0613	-0.1697
	H	-1.4281	1.5367	-0.9946
	O	1.2141	0.7206	0.9369
	H	0.3662	1.2002	0.8452
	N	2.4015	-0.9579	-0.2743
	H	3.2828	-0.4550	-0.2788
	H	2.3801	-1.5367	0.5605
	N	-0.5255	-1.4797	0.5131
	H	-0.1412	-1.3007	1.4376
	H	-1.6278	-1.4972	0.4326
	O	-2.9002	-0.7091	0.2087
	H	-2.1506	0.2945	-0.0181
	H	-3.2828	-0.9749	-0.6348
	H	-1.8353	0.3346	0.0598
	H	-2.0864	-1.5081	-0.0856
	H	-3.1939	-1.1132	1.0074
	H	-2.4545	-0.1969	-0.3990
Et___H_2O_TS	C	-1.3478	-0.3709	0.2663
	H	-1.4945	-0.7184	1.2939
	C	-0.0031	-0.5827	-0.3042
	H	0.1777	-0.1842	-1.2939
	N	-2.2369	0.1795	-0.4530
	H	-3.1189	0.2544	0.0572
	N	0.8125	-1.5001	0.1395
	H	0.6195	-1.8876	1.0574
	O	0.9775	1.1834	0.4493
	H	1.9583	0.6768	0.1487
	H	0.8174	1.8876	-0.1904
	O	2.9217	-0.1400	-0.1798

	H	1.8542	-1.2347	-0.0888
	H	3.1189	0.0090	-1.1113
	H	0.3678	0.4695	0.5264
	H	1.3596	0.3744	-0.0214
	H	2.2728	-0.7761	0.0683
	H	1.1871	-1.3223	-0.2504
Ec____H_2O_TS	C	1.5152	0.0822	-0.0086
	H	1.7985	0.9891	0.5281
	C	0.1599	-0.4477	0.2928
	H	-0.3404	-0.1064	1.1883
	N	2.2382	-0.5256	-0.8546
	H	3.1357	-0.0561	-0.9805
	N	-0.3132	-1.5057	-0.2981
	H	0.2054	-1.8093	-1.1183
	O	-0.9832	1.1258	-0.6884
	H	-1.8581	0.3946	-0.6459
	H	-1.1711	1.8093	-0.0335
	O	-2.6710	-0.6306	-0.5614
	H	-1.4111	-1.4687	-0.3455
	H	-3.1357	-0.5609	0.2799
	H	-1.5725	0.3983	-0.7923
	H	-2.1993	-0.1940	-0.7721
	H	-2.9273	-1.2852	-1.1883
	H	-2.0325	-1.5914	-0.6240
Bc_1c_TS	C	-1.2873	0.4246	-1.1709
	H	-1.2845	0.1573	-2.2309
	C	-2.0031	-0.7008	-0.3842
	H	-1.9534	-0.4540	0.6884
	O	-1.4677	-1.9606	-0.6457
	H	-0.5759	-1.9986	-0.2284
	O	-1.9923	1.6128	-0.9148
	H	-1.9731	2.1802	-1.6935
	N	0.1240	0.6201	-0.7107
	H	0.4888	1.4802	-1.1167
	H	0.1542	0.7052	0.4425
	O	-3.3373	-0.7618	-0.8210
	H	-3.6907	0.1352	-0.7648
	C	1.0840	-0.5436	-0.9722
	O	1.0330	-1.4023	0.1154
	H	0.7424	-1.0578	-1.8758
	O	2.7470	0.9926	-0.2424
	H	3.6907	1.1854	-0.2849
	N	3.5110	-1.0046	-1.2270
	H	3.2750	-1.6893	-0.5126
	H	3.5647	-1.4849	-2.1191
	C	2.4940	0.0194	-1.2484
	H	2.4946	0.4853	-2.2437
	O	0.4407	0.2618	1.7468
	H	0.8344	-0.7344	1.0316
	H	-0.3487	0.0236	2.2437
	H	-0.3372	0.3596	0.0992
	H	1.5642	-2.1802	0.1267
	H	0.7173	-0.2689	1.0193
	H	0.2876	-0.8872	0.6359
1c_2c_TS	C	-0.8946	-1.4937	-0.2963
	C	-1.4650	-0.5579	0.8343
	C	0.7630	0.0421	-1.0879
	H	-0.0907	-2.1082	0.1250
	H	-1.7124	-1.2330	1.6744
	N	-0.3335	-0.6129	-1.3097
	H	-1.0727	-0.0433	-1.8456
	N	-0.5461	0.4375	1.1028

	H	-0.6583	1.8396	0.2188
	C	1.9464	-0.3602	-0.2314
	H	1.6259	-0.8540	0.6894
	O	2.8003	-1.2002	-1.0086
	H	2.5907	-2.1249	-0.8035
	O	2.6134	0.8367	0.0145
	H	3.3175	0.6594	0.6579
	O	-2.7695	-0.0479	0.3396
	H	-3.3175	-0.8266	0.1319
	O	-1.9270	-2.2780	-0.8262
	H	-1.5491	-2.9538	-1.4100
	H	0.9478	0.9003	-1.7291
	H	-0.5712	0.7125	2.0825
	O	-0.6459	2.6525	-0.4392
	H	0.2740	2.9538	-0.4275
	O	-2.0824	1.1930	-2.0825
	H	-1.5367	1.9041	-1.6519
	H	-2.6185	0.9037	-1.3058
	H	-1.4945	-0.5901	-1.8901
	H	-0.9678	1.2817	-0.0490
	H	-0.8398	1.7308	-0.4254
2c_3c_TS	C	1.7340	-0.1641	0.8144
	C	1.2837	-1.5199	0.2989
	C	-0.1020	0.3753	-0.4626
	H	2.5243	-0.0600	1.5418
	H	0.9301	-2.1567	1.1140
	H	0.0177	0.8985	-1.4123
	N	0.9313	0.8234	0.5188
	H	1.6025	1.8323	0.4152
	N	0.0916	-1.1082	-0.5516
	H	0.1982	-1.4586	-1.5079
	C	-1.5249	0.6281	0.0928
	H	-1.5580	1.5459	0.6873
	O	-2.3415	0.7234	-1.1063
	H	-3.2830	0.5857	-0.8137
	O	-1.9025	-0.4613	0.9175
	H	-1.3872	-1.2262	0.4655
	O	2.3225	-2.1830	-0.4024
	H	2.9764	-1.3950	-0.6187
	O	3.2830	0.1219	-0.6956
	H	2.7589	0.2321	-1.5418
	O	2.7707	2.3782	0.1415
	H	3.2147	1.3909	-0.2476
	H	2.7163	3.0354	-0.6001
	H	1.0918	1.4126	0.2107
	H	-2.7462	-0.4645	1.3366
	H	-1.8362	-1.4528	-0.0099
	H	2.1708	-3.0354	-0.7734
	H	2.2971	-1.4805	-0.7188
	H	3.0567	-0.5605	-0.0869
	H	2.1365	1.6845	0.2036
	H	2.6174	1.0624	-0.3666
3c_4c_TS	C	-0.7782	-1.6709	0.2948
	C	-1.3780	-0.4150	0.7793
	C	0.5046	-0.0134	-0.3678
	H	-1.1909	-2.6596	0.4521
	H	-2.1820	-0.3045	1.4871
	H	0.4065	0.3724	-1.3891
	N	0.2923	-1.4502	-0.3727
	N	-0.5347	0.5535	0.4952
	H	-1.0536	1.5080	0.2366
	C	1.9031	0.3861	0.1382

	H	2.0681	-0.0594	1.1291
	O	2.8150	-0.0756	-0.8068
	H	3.7020	0.1075	-0.4753
	O	1.9927	1.7965	0.2083
	H	1.6878	2.0808	1.0775
	O	-2.9600	-0.0784	-0.6487
	H	-2.6168	-0.4107	-1.4871
	O	-2.1715	2.2003	-0.4266
	H	-2.6699	1.0877	-0.6039
	H	-2.7017	2.6596	0.2341
	H	-1.3230	0.9190	-0.0070
	H	-3.7020	-0.4953	-0.2452
	H	-2.4666	1.3779	-0.7786
	H	-2.7219	0.4161	-0.7622
4c_HIC_TS	C	-1.4912	-1.6344	-0.4475
	H	-2.0143	-2.4155	-0.9820
	C	-1.9402	-0.8807	0.6565
	H	-2.9030	-0.9061	1.1490
	O	-0.8517	2.1820	-0.0708
	H	-1.1699	1.5731	0.7328
	C	0.0269	-0.2169	0.0699
	C	1.4909	0.0738	0.3406
	H	1.6385	1.0831	0.7444
	N	-0.9844	-0.0134	1.0151
	H	-0.3552	1.2213	-0.4564
	N	-0.2701	-1.2270	-0.7989
	H	-1.6109	2.4155	-0.6253
	O	2.2138	0.0266	-0.8625
	H	1.8579	-0.7353	-1.3455
	O	1.9498	-0.8889	1.2714
	H	2.9030	-0.7621	1.3455
	H	-0.8417	1.3621	0.3929
	H	-1.4187	1.0005	0.4344
	H	-0.7445	0.6656	-0.5923
Dc_1b_TS	C	-0.9171	0.4310	-0.2267
	H	-0.7495	0.7303	-1.2652
	C	-1.7795	-0.8425	-0.1645
	H	-1.3373	-1.6245	-0.7899
	O	-3.0296	-0.4110	-0.7154
	H	-3.6602	-1.1362	-0.6462
	O	-1.5181	1.4636	0.5242
	H	-2.4427	1.5001	0.2432
	N	0.3969	0.1980	0.3915
	H	0.9060	1.2009	0.6397
	H	0.2584	-0.3709	1.2308
	N	-1.8260	-1.3208	1.1914
	H	-2.3503	-0.6810	1.7801
	H	-2.2342	-2.2451	1.2593
	C	1.4302	-0.4114	-0.5520
	O	1.9996	0.5914	-1.2961
	H	0.9268	-1.1425	-1.1933
	O	2.8009	-0.3541	1.4134
	H	3.4661	-0.8195	1.9329
	O	3.5927	-1.4080	-0.5211
	H	3.6602	-0.6069	-1.0709
	C	2.4835	-1.1686	0.2931
	H	2.1062	-2.1416	0.6257
	O	1.8553	2.2451	0.4425
	H	2.5447	1.9902	1.0668
	H	2.0736	1.4908	-0.5425
	H	0.3828	0.8061	0.4179
	H	2.6629	0.3869	-1.9329

	H	1.1061	1.6887	0.3151
	H	1.4973	1.1154	-0.6182
Fc_1a_TS	C	2.5970	-0.5637	0.0561
	H	3.3991	-1.2922	-0.0697
	C	1.2156	-1.1279	0.0031
	H	1.1406	-2.1940	0.2148
	N	2.7792	0.6842	0.2894
	H	3.7745	0.9593	0.3330
	N	0.1599	-0.4361	-0.2048
	H	0.2629	0.6168	-0.3589
	C	-1.4532	-0.4119	0.8897
	O	-1.2132	0.5714	1.6704
	H	-1.3761	-1.4512	1.2431
	O	-2.1650	0.8979	-0.9787
	H	-2.8711	1.0146	-1.6704
	O	-3.7745	-0.1545	0.4386
	H	-3.6606	0.6063	1.0779
	C	-2.4868	-0.2738	-0.2229
	H	-2.5445	-1.1860	-0.8196
	O	0.3992	2.1940	0.1722
	H	-0.2644	1.8715	0.8651
	H	1.3166	1.8896	0.4736
	H	-0.7542	-0.8927	-0.2275
	H	-0.2858	0.2347	-0.5372
1a_2a_TS	C	-2.7187	-0.4999	-0.2500
	H	-3.4938	-1.2077	0.0382
	C	-1.4589	-1.0800	-0.8416
	H	-1.2993	-2.1433	-0.9634
	N	-2.7604	0.7536	-0.1303
	H	-3.6203	1.1063	0.2881
	N	-0.5870	-0.2387	-1.1733
	C	0.4235	1.5926	0.0943
	H	-0.0448	2.5507	0.3364
	O	1.7195	1.8461	-0.3176
	H	2.1427	0.9886	-0.5988
	O	0.3166	0.6835	1.1649
	H	0.6764	1.1029	1.9564
	O	2.6932	-0.5118	-1.1114
	H	2.2074	-1.1841	-0.5848
	C	-0.3501	1.0055	-1.0843
	H	-0.4924	1.6400	-1.9564
	O	1.0839	-1.9904	0.5419
	H	1.5108	-2.5507	1.1993
	H	0.8178	-1.1835	1.0145
	H	3.6203	-0.6245	-0.8740
2a_HIC_TS	C	1.9459	0.3451	0.2999
	H	2.8320	0.8580	0.6285
	C	1.8375	-0.8317	-0.5000
	H	2.6576	-1.3926	-0.9116
	N	0.7055	0.7141	0.5985
	H	0.4294	1.5006	1.1791
	N	0.5518	-1.1518	-0.6777
	C	-1.3225	0.4701	-0.8080
	H	-0.9317	0.8473	-1.7522
	O	-1.8298	1.4965	0.0208
	H	-2.5434	1.9865	-0.4580
	O	-2.4225	-0.4888	-1.0590
	H	-2.1543	-1.1550	-1.7428
	C	-0.2240	-0.2112	0.0218
	H	-1.1725	-0.9388	1.0084
	O	-2.2473	-1.1482	1.2699
	H	-2.4458	-1.9865	1.7522

	H	-2.5600	-1.0945	0.2800
	H	-0.8222	-0.7289	0.8047
	H	-1.4668	-1.1610	0.4229
	H	-2.8320	-0.8416	0.5980
	H	-2.5600	-1.3726	-0.3536