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SUPPORTING INFORMATION

Catalyzing Epoxy Oxygen Migration on the Basal Surface of Graphene Oxide using Strong Hydrogen-Bond Donors

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Full Computational Details and Discussion, Tables S1–S4

[Total 57 pages]

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Full Computational Details and Discussion

Density functional theory (DFT) and double-hybrid DFT (DHDFT) calculations were performed to gain insight into the mechanism of the catalytic movement of the epoxy functional group by hydrogen-bond-donor (HBD) catalysts. The geometries and harmonic vibrational frequencies of all structures have been calculated at the PW6B95-D3BJ/def2-SVP level of theory.[1,2] Empirical D3 dispersion corrections are included using the Becke–Johnson damping potential.[3,4] Zero-point vibrational energies (ZPVEs), enthalpic temperature corrections (H_{298}–H_0), and entropic corrections have been obtained from such calculations. The equilibrium structures were verified to have all real harmonic frequencies, and the transition structures to have only one imaginary frequency. The connectivities of the transition and equilibrium structures were confirmed via intrinsic reaction coordinate (IRC) calculations.[5] The electronic energies were refined using two DFT functionals the hybrid-meta generalized gradient approximation (GGA) PWB95-D3BJ method and the double-hybrid DSD-PBEP86-D3BJ method.[6,7] These calculations were carried out with the large quadruple-zeta def2-QZVPP basis set.[2] We note that the use of such a large basis set makes the basis set superposition errors (BSSE) negligible.[8,9,10] All calculations were carried out using the Gaussian 16 rev. C.01 program suite.[11] For both the PW6B95 and DSD-PBEP86 calculations, the convergence criterion of 10^{-8} a.u. was used for the self-consistent field (SCF) iterations. Cartesian coordinates and absolute energies for all the key species considered in the present work are given at the end of the Supplementary Information in Tables S3 and S4, respectively.

Table S1 gives the Gibbs free reaction barrier heights ($\Delta G^{\ddagger}_{298}$) for the uncatalyzed and catalyzed reaction pathways for the oxygen ring-walking calculated at the PW6B95-D3BJ/def2-QZVPP. We note that the results calculated with the PW6B95-D3BJ hybrid-meta GGA method (rung 4 of Jacob's Ladder) are expected to be less accurate than those calculated with the double-hybrid DSD-PBEP86-D3BJ method (rung 5 of Jacob's Ladder) provided in the main text. Nevertheless, there is reasonable agreement between the two sets of reaction barrier heights. For the uncatalyzed

reaction barrier height, the difference between the two methods is merely 2.5 kJ mol^{-1}. For the catalyzed reactions, larger differences ranging between 4.7 and 16.2 kJ mol^{-1} are observed. In all cases, the less accurate PW6B95-D3BJ barrier heights overestimate the DSD-PBEP86-D3BJ ones. However, both methods reflect the expected trends of increased catalytic enhancement with increasing hydrogen bond donor strength of the catalyst.

Table S1. PW6B95-D3BJ/def2-QZVPP Gibbs barrier heights ($\Delta G^{\ddagger}_{298}$) for the uncatalyzed and HBD-catalyzed ring-walking of oxygen on the graphene surface (in kJ mol^{-1}).

Catalyst	$\Delta G^{\ddagger}_{298}$
Uncat	119.2
NH_3	125.0
H_2O	115.6
$2H_2O$	116.6
HF	82.7
Ethylene glycol	85.3
Guanidine	91.5
Thiourea	67.2

The reaction barrier heights in Table S1 and in the main text are calculated relative to the free reactants (i.e., the separated $C_{54}H_{18}O$ GO model and the HBD catalyst). It is also of interest to briefly examine the reaction energies and barrier heights calculated relative to the reactant complex in which the HBD catalyst is hydrogen bonded to the $C_{54}H_{18}O$ GO model. These results calculated at the PW6B95-D3BJ/def2-QZVPP and DSD-PBEP86-D3BJ/def2-QZVPP levels of theory are provided in Table S2. The main difference between the barriers calculated relative to the free reactants and those calculated relative to the reactant complex is that entropic effects are much less pronounced in the latter. Therefore, the reaction barrier heights are lower when calculated relative to the reactant complex (Table S2). For example, at the PW6B95-D3BJ/def2-QZVPP//PW6B95-D3BJ/def2-SVP level of theory, the barriers calculated relative to the reactant complex are lower than those calculated relative to the free reactants by amounts ranging from 5.3 (HF) to 41.1 ($2H_2O$) kJ mol^{-1}. Where the large difference in the barriers for two water catalysts is due to the more pronounced entropic effects associated with three bodies coming together in the transition structure. Nevertheless, both sets of barrier heights reflect similar trends of increased catalytic enhancement with increasing hydrogen bond donor

strength of the catalyst. Finally, we note that the reaction energy relative to the free reactants is basically nil and reflects the movement of the epoxy group from one C=C bond to the next. The reaction energies relative to the reactant complex can reach up to a few kJ mol^{-1} due to the slightly different H-bonding in the reactant and product complexes.

Table S2. Gibbs free reaction energies (ΔG_{298}) and barrier heights ($\Delta G^{\ddagger}_{298}$) for the uncatalyzed and HBD-catalyzed oxygen ring walking calculated at the PW6B95-D3BJ/def2-QZVPP and DSD-PBEP86-D3BJ/def2-QZVPP levels of theory. All values are calculated relative to the reactant complex in kJ mol^{-1}.

Catalyst		PW6B95	DSD-PBEP86
Uncat	$\Delta G^{\ddagger}_{298}$	119.2	116.7
	ΔG_{298}	0.1	–0.4
NH_3	$\Delta G^{\ddagger}_{298}$	104.3	99.5
	ΔG_{298}	–2.5	–2.5
H_2O	$\Delta G^{\ddagger}_{298}$	90.2	85.7
	ΔG_{298}	–5.1	–6.5
HF	$\Delta G^{\ddagger}_{298}$	77.4	70.1
	ΔG_{298}	0.7	–3.9
$2H_2O$	$\Delta G^{\ddagger}_{298}$	75.5	72.7
	ΔG_{298}	–3.4	–3.0
Ethylene glycol	$\Delta G^{\ddagger}_{298}$	66.6	59.7
	ΔG_{298}	–4.8	–4.9
Guanidine	$\Delta G^{\ddagger}_{298}$	82.2	73.6
	ΔG_{298}	0.5	–4.6
Thiourea	$\Delta G^{\ddagger}_{298}$	69.0	59.4
	ΔG_{298}	–0.9	–2.0

It is of interest to explore the possibility of a strong HBD catalyst (namely, ethylene glycol, guanidine, and thiourea) abstracting the epoxy oxygen from the graphene surface. A homolytic abstraction results in $C_{54}H_{18}$ and HBD•••O fragments. At the DSD-PBEP86-D3BJ/def2-QZVPP level of theory, the Gibbs homolytic bond dissociation energies are ΔG_{298} = 148.4 (ethylene glycol), 149.7 (guanidine), and 160.7 (thiourea) kJ mol^{-1}. These bond dissociation energies are significantly higher than the catalyzed reaction barrier heights $\Delta G^{\ddagger}_{298}$ = 72.4 (ethylene glycol), 81.5 (guanidine), and 51.0 (thiourea) kJ mol^{-1}. Thus, we conclude that the abstraction of the epoxy oxygen by the strong HBD catalysts should not proceed at room temperature.

Finally, a comment is due on the adsorption energies of the larger HBDs (ethylene glycol, guanidine, and thiourea) on the graphitic domains of GO. At the DSD-PBEP86-D3BJ/def2-QZVPP level of theory, we obtain binding energies 24.4 (ethylene glycol), 33.9 (guanidine), and 44.1 (thiourea) kJ mol^{-1} on the enthalpic potential energy surface at 298 K.

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Table S3. PW6B95-D3BJ/def2-SVP optimized geometries for the species considered in this work (Cartesian coordinates, Å).

Uncat, Reactant

O	-1.231266	0.018821	1.690929
C	6.163621	0.586029	-0.055629
C	4.911692	-1.498606	-0.018736
C	3.671349	-3.598699	-0.073263
C	2.429224	-5.690734	-0.208140
C	-0.049074	-5.638502	-0.211511
C	-2.530078	-5.601799	-0.275631
C	-3.721100	-3.485591	-0.140090
C	-4.905020	-1.353356	-0.048446
C	-6.093099	0.770930	-0.133457
C	-4.819006	2.893822	-0.148287
C	-3.547416	5.022481	-0.271248
C	-1.113037	4.971761	-0.163328
C	1.330323	4.951189	-0.149006
C	3.764976	4.917283	-0.168521
C	4.957965	2.750687	-0.068621
C	3.718221	0.656177	0.052875
C	2.462045	-1.462363	0.091361
C	1.207195	-3.567674	-0.029147
C	-1.249644	-3.529872	-0.017138
C	-2.483652	-1.409459	0.177508
C	-3.645458	0.777746	0.116450
C	-2.395161	2.875288	0.008888
C	0.081563	2.845305	0.058507
C	2.529066	2.797605	0.006046
C	2.602451	5.614001	-0.207881
C	0.123763	5.637433	-0.211574
C	-2.357479	5.676382	-0.275851
C	-3.612795	3.597454	-0.140431
C	-4.861567	1.502367	-0.048848
C	-6.113635	-0.585147	-0.133174
C	-4.905121	-2.745458	-0.147698
C	-3.699452	-4.911921	-0.270922
C	-1.264794	-4.935345	-0.163221
C	1.177898	-4.989392	-0.149070
C	3.612537	-5.029945	-0.168938
C	4.871388	-2.900867	-0.069097
C	6.142868	-0.773815	-0.055812
C	4.955297	1.347856	-0.018435
C	3.779869	3.484888	-0.072901

C	3.696461	-0.769386	0.052794
C	2.442340	-2.873429	0.005906
C	-0.005365	-2.846269	0.058594
C	-1.218564	-0.738160	0.490354
C	-2.481836	-2.800870	0.008943
C	-3.667388	-0.666129	0.116501
C	-2.439580	1.484587	0.177563
C	-1.141109	3.566489	-0.017199
C	1.315866	3.529281	-0.029109
C	0.078936	1.441588	0.222898
C	2.505621	1.386589	0.091435
C	1.235236	-0.741680	0.206866
C	-1.195595	0.775084	0.490351
C	1.257249	0.703839	0.206823
C	0.035005	-1.443128	0.223010
H	4.719533	5.438489	-0.217954
H	2.614160	6.699660	-0.288442
H	0.133847	6.721830	-0.313950
H	-2.327798	6.759715	-0.379544
H	-4.479592	5.575895	-0.371451
H	-5.752604	3.444285	-0.257924
H	-7.020402	1.334103	-0.223793
H	-7.057385	-1.120397	-0.223291
H	-5.854966	-3.267435	-0.257111
H	-4.647915	-5.436903	-0.371008
H	-2.532921	-6.685563	-0.379285
H	-0.071674	-6.722712	-0.313852
H	2.408197	-6.776221	-0.288792
H	4.550902	-5.579798	-0.218616
H	5.808668	-3.452996	-0.126026
H	7.073622	-1.337111	-0.095648
H	7.110939	1.121068	-0.095291
H	5.911510	3.274247	-0.125333

Uncat, Transition Structure

O	-1.811261	-1.267119	-0.000000
C	0.129768	5.676053	2.477092
C	0.063165	3.570853	3.696275
C	0.011844	1.461710	4.919724
C	0.021679	-0.644667	6.143174
C	0.047879	-2.780455	4.884144
C	0.169043	-4.933099	3.651369
C	0.178210	-4.944792	1.218670
C	0.178210	-4.944792	-1.218670

C	0.169043	-4.933099	-3.651369
C	0.047879	-2.780455	-4.884144
C	0.021679	-0.644667	-6.143174
C	0.011844	1.461710	-4.919724
C	0.063165	3.570853	-3.696275
C	0.129768	5.676053	-2.477092
C	0.128671	5.660506	0.000000
C	0.059334	3.564510	1.229416
C	-0.011824	1.448492	2.464038
C	-0.033750	-0.673326	3.687400
C	-0.005907	-2.799598	2.453444
C	-0.041866	-2.847378	-0.000000
C	-0.005907	-2.799598	-2.453444
C	-0.033750	-0.673326	-3.687400
C	-0.011824	1.448492	-2.464038
C	0.059334	3.564510	-1.229416
C	0.109098	5.001107	-3.656329
C	0.046759	2.856096	-4.898547
C	0.020273	0.712413	-6.143878
C	0.007621	-1.390732	-4.917577
C	0.063102	-3.501793	-3.677923
C	0.232119	-5.619330	-2.482038
C	0.236743	-5.624403	-0.000000
C	0.232119	-5.619330	2.482038
C	0.063102	-3.501793	3.677923
C	0.007621	-1.390732	4.917577
C	0.020273	0.712413	6.143878
C	0.046759	2.856096	4.898547
C	0.109098	5.001107	3.656329
C	0.106684	4.985873	1.223166
C	0.106684	4.985873	-1.223166
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C	0.041990	-3.526820	-1.213424
C	-0.068880	-1.381181	-2.465021
C	-0.021592	0.745396	-3.689359
C	0.037230	2.860829	-2.462350
C	-0.051358	0.735009	-1.234558
C	0.035239	2.855441	0.000000
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C	-0.118680	-0.665088	-1.244971

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H	0.069366	3.402308	-5.840386
H	0.035799	1.261310	-7.083820
H	0.040290	-1.194999	-7.082379
H	0.087967	-3.330872	-5.823746
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H	0.324031	-6.704142	-2.486642
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H	0.211408	-5.462860	4.601542
H	0.087967	-3.330872	5.823746
H	0.040290	-1.194999	7.082379
H	0.035799	1.261310	7.083820
H	0.069366	3.402308	5.840386
H	0.127516	5.543830	4.599788
H	0.164761	6.764104	2.467103
H	0.164309	6.749581	0.000000

Uncat, Product

O	1.231297	0.015348	1.690985
C	-3.751058	4.927865	-0.168518
C	-1.316316	4.954929	-0.148999
C	1.127074	4.968611	-0.163314
C	3.561565	5.012492	-0.271187
C	4.827118	2.880247	-0.148270
C	6.095201	0.753798	-0.133487
C	4.901131	-1.367135	-0.048506
C	3.711232	-3.496042	-0.140062
C	2.514270	-5.608903	-0.275584
C	0.033145	-5.638645	-0.211507
C	-2.445285	-5.683898	-0.208165
C	-3.681490	-3.588351	-0.073269
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C	-4.950127	2.764645	-0.068621
C	-2.521126	2.804711	0.006039
C	-0.073540	2.845518	0.058522
C	2.403249	2.868537	0.008901
C	3.647585	0.767487	0.116369
C	2.479642	-1.416448	0.177496
C	1.239665	-3.533404	-0.017071

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C	-1.191980	-4.986087	-0.149059
C	1.250855	-4.938898	-0.163167
C	3.685573	-4.922307	-0.270861
C	4.897328	-2.759237	-0.147717
C	6.111914	-0.602321	-0.133226
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C	2.373486	5.669744	-0.275803
C	-0.107845	5.637777	-0.211571
C	-2.586594	5.621311	-0.207878
C	-3.769987	3.495513	-0.072904
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C	-1.305882	3.532974	-0.029106
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C	2.443730	1.477729	0.177525
C	1.216457	-0.741529	0.490336
C	3.665439	-0.676453	0.116427
C	2.473913	-2.807845	0.008986
C	-0.002676	-2.846297	0.058630
C	-2.450434	-2.866553	0.005911
C	-3.698588	-0.758978	0.052788
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C	-2.501662	1.393632	0.091400
C	-0.074883	1.441796	0.222871
C	-0.039079	-1.443047	0.222973
C	-1.255227	0.707369	0.206747
C	1.197771	0.771649	0.490350
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H	-7.077310	-1.317202	-0.095636
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H	-4.566634	-5.566966	-0.218635
H	-2.427294	-6.769445	-0.288814
H	0.052710	-6.722914	-0.313851
H	2.514062	-6.692670	-0.379233
H	4.632572	-5.449934	-0.370949
H	5.845700	-3.283891	-0.257120
H	7.054139	-1.140249	-0.223337
H	7.024074	1.314390	-0.223799

H	5.762270	3.428074	-0.257878
H	4.495306	5.563272	-0.371332
H	2.346840	6.753166	-0.379431
H	-0.114848	6.722204	-0.313895
H	-2.595244	6.707000	-0.288423
H	-4.704159	5.451737	-0.217955
H	-5.902201	3.290879	-0.125348

NH_3 catalyst, Reactant

O	1.240774	0.000568	1.600798
H	-0.867151	-0.000271	2.732540
C	-6.101432	-0.683101	-0.194762
C	-4.882131	1.420290	-0.161021
C	-3.675885	3.540425	-0.211217
C	-2.466274	5.653548	-0.326569
C	0.013670	5.641533	-0.297303
C	2.497471	5.643350	-0.315426
C	3.718830	3.544833	-0.166072
C	4.934520	1.430660	-0.055867
C	6.157316	-0.675118	-0.113397
C	4.917100	-2.818291	-0.151076
C	3.682189	-4.967881	-0.290709
C	1.244873	-4.956339	-0.232003
C	-1.198918	-4.973695	-0.258150
C	-3.633957	-4.976714	-0.299309
C	-4.861614	-2.828418	-0.209588
C	-3.655132	-0.714340	-0.094416
C	-2.433978	1.423067	-0.059455
C	-1.212030	3.549339	-0.150754
C	1.244507	3.550931	-0.095662
C	2.508380	1.448504	0.114254
C	3.705022	-0.720448	0.078330
C	2.490342	-2.838207	-0.047540
C	0.013325	-2.847610	-0.051206
C	-2.433102	-2.836557	-0.133077
C	-2.460671	-5.656096	-0.326125
C	0.019273	-5.641598	-0.297175
C	2.503090	-5.640930	-0.315586
C	3.722364	-3.541200	-0.166272
C	4.935956	-1.425828	-0.055976
C	6.156631	0.681189	-0.113336
C	4.914283	2.823113	-0.150873
C	3.677238	4.971481	-0.290462
C	1.239945	4.957503	-0.231969

C	-1.203848	4.972411	-0.258399
C	-3.638880	4.972999	-0.299796
C	-4.864396	2.823507	-0.209881
C	-6.102097	0.676977	-0.194828
C	-4.880735	-1.425213	-0.160898
C	-3.672390	-3.544165	-0.210889
C	-3.655821	0.710622	-0.094449
C	-2.435902	2.834045	-0.133278
C	0.010495	2.847534	-0.051253
C	1.246711	0.753875	0.388898
C	2.487508	2.840616	-0.047431
C	3.704300	0.724052	0.078372
C	2.509828	-1.446082	0.114211
C	1.248053	-3.549779	-0.095708
C	-1.208508	-3.550638	-0.150587
C	-0.009386	-1.441535	0.094416
C	-2.432580	-1.425587	-0.059363
C	-1.197086	0.721910	0.050502
C	1.247466	-0.752725	0.388899
C	-1.196383	-0.723221	0.050527
C	-0.010825	1.441417	0.094402
H	-4.580011	-5.513037	-0.352347
H	-2.455645	-6.742266	-0.400479
H	0.027449	-6.726801	-0.391101
H	2.493094	-6.725226	-0.413373
H	4.624766	-5.507080	-0.368750
H	5.861364	-3.354598	-0.237471
H	7.095139	-1.223838	-0.181763
H	7.093893	1.230876	-0.181657
H	5.858006	3.360380	-0.237211
H	4.619271	5.511640	-0.368426
H	2.486377	6.727637	-0.413200
H	0.020748	6.726740	-0.391264
H	-2.462342	6.739714	-0.401029
H	-4.585481	5.508346	-0.352982
H	-5.810412	3.360870	-0.265111
H	-7.041578	1.225956	-0.231418
H	-7.040365	-1.233020	-0.231291
H	-5.807088	-3.366742	-0.264713
N	-1.844628	0.000205	3.021354
H	-1.951756	-0.807875	3.629119
H	-1.952414	0.812119	3.623874

NH_3 catalyst, Transition Structure

O	-1.195887	-0.551562	1.749932
H	0.588398	-0.128787	2.534811
C	6.147682	0.064468	-0.224180
C	4.726973	-1.909239	-0.170844
C	3.306100	-3.890876	-0.137249
C	1.884976	-5.869591	-0.148378
C	-0.579833	-5.594799	-0.149319
C	-3.050466	-5.350036	-0.222656
C	-4.056076	-3.134788	-0.203027
C	-5.053537	-0.912041	-0.180216
C	-6.039056	1.311953	-0.160567
C	-4.577587	3.318743	-0.079125
C	-3.144950	5.342817	-0.085151
C	-0.722076	5.089499	-0.105181
C	1.702459	4.833542	-0.173199
C	4.120840	4.581211	-0.240963
C	5.118616	2.315423	-0.233806
C	3.708790	0.337148	-0.173810
C	2.287045	-1.656365	-0.120283
C	0.853628	-3.640853	-0.091521
C	-1.591363	-3.384452	-0.075274
C	-2.635483	-1.164058	-0.005249
C	-3.599722	1.092571	-0.031738
C	-2.164721	3.090448	-0.040302
C	0.270030	2.842652	-0.092956
C	2.703774	2.578284	-0.176240
C	3.023490	5.382372	-0.220855
C	0.557970	5.639275	-0.150016
C	-1.907510	5.899201	-0.101255
C	-3.323802	3.918984	-0.064221
C	-4.742089	1.922187	-0.083378
C	-6.186996	-0.036026	-0.214694
C	-5.176481	-2.301856	-0.236133
C	-4.155684	-4.563347	-0.259800
C	-1.731806	-4.788745	-0.143040
C	0.702080	-5.057121	-0.127260
C	3.123252	-5.314617	-0.148285
C	4.568443	-3.299651	-0.161588
C	6.016004	-1.287544	-0.204569
C	5.003122	0.923757	-0.211155
C	4.002485	3.155077	-0.218467
C	3.573326	-1.075395	-0.152923
C	2.148023	-3.061152	-0.109116

C	-0.291276	-2.814606	-0.042256
C	-1.313348	-0.575652	0.365005
C	-2.761941	-2.549520	-0.092768
C	-3.754989	-0.336128	-0.069926
C	-2.308600	1.684741	0.002265
C	-0.872141	3.672479	-0.070787
C	1.558456	3.417702	-0.149320
C	0.121433	1.427860	-0.054457
C	2.559802	1.167756	-0.156930
C	1.131728	-0.828533	-0.086618
C	-1.156145	0.866518	0.034895
C	1.269306	0.587891	-0.101812
C	-0.135467	-1.408988	0.001412
H	5.118256	5.016267	-0.274354
H	3.132992	6.465288	-0.238603
H	0.671633	6.722142	-0.172250
H	-1.792311	6.981520	-0.120055
H	-4.031956	5.974129	-0.092594
H	-5.465650	3.949713	-0.106017
H	-6.912265	1.961550	-0.188652
H	-7.179978	-0.476893	-0.285349
H	-6.168230	-2.746336	-0.308095
H	-5.145480	-5.010994	-0.332130
H	-3.146020	-6.433707	-0.265949
H	-0.698584	-6.677363	-0.186977
H	1.767830	-6.951857	-0.167034
H	4.008960	-5.947371	-0.165046
H	5.453529	-3.933945	-0.180140
H	6.897859	-1.925681	-0.215744
H	7.135749	0.520851	-0.250558
H	6.112483	2.761349	-0.263506
N	1.558415	0.055037	2.819593
H	1.503019	0.753300	3.556867
H	1.867831	-0.797400	3.280494

NH_3 catalyst, Product

O	-0.917605	-0.831910	1.593455
H	1.057872	-0.358418	2.941544
C	6.024399	-1.155195	-0.320967
C	4.230749	-2.802220	-0.297242
C	2.420408	-4.444261	-0.299800
C	0.636528	-6.103165	-0.381994
C	-1.728442	-5.361138	-0.223333
C	-4.092520	-4.625332	-0.155779

C	-4.619121	-2.248926	-0.055435
C	-5.157986	0.130970	-0.125594
C	-5.681826	2.503515	-0.243235
C	-3.853342	4.183395	-0.220725
C	-2.039080	5.872801	-0.251148
C	0.283240	5.138625	-0.162777
C	2.608099	4.397059	-0.142256
C	4.929931	3.674670	-0.195820
C	5.471951	1.256158	-0.220574
C	3.691434	-0.395417	-0.150220
C	1.897574	-2.060847	-0.091559
C	0.070013	-3.732771	-0.107982
C	-2.256756	-3.000549	0.045893
C	-2.845877	-0.595371	0.130617
C	-3.341657	1.809835	-0.044557
C	-1.533955	3.474253	-0.095439
C	0.805678	2.738653	-0.028004
C	3.152893	1.993958	-0.094512
C	4.009009	4.675622	-0.185888
C	1.643249	5.416766	-0.174582
C	-0.715739	6.167761	-0.235109
C	-2.504719	4.516152	-0.188572
C	-4.291645	2.848967	-0.164889
C	-6.094439	1.209941	-0.230467
C	-5.548451	-1.209834	-0.127247
C	-5.010535	-3.627239	-0.132181
C	-2.685053	-4.351260	-0.105983
C	-0.360027	-5.083195	-0.242223
C	1.959676	-5.798950	-0.402139
C	3.786484	-4.117570	-0.355217
C	5.621070	-2.449226	-0.357857
C	5.082147	-0.076136	-0.226930
C	4.536041	2.301319	-0.165734
C	3.273574	-1.749777	-0.180988
C	1.465118	-3.413846	-0.153103
C	-0.886216	-2.724713	0.072543
C	-1.446192	-0.254954	0.403787
C	-3.234744	-1.937773	0.073692
C	-3.774476	0.444838	-0.010339
C	-1.957220	2.128280	-0.003557
C	-0.150031	3.778617	-0.087099
C	2.187305	3.043386	-0.079783
C	0.371814	1.383363	0.080903
C	2.734331	0.641857	-0.066516

C	0.962522	-1.014022	0.069607
C	-0.989255	1.107549	0.130221
C	1.349708	0.319959	0.051365
C	-0.425076	-1.365283	0.368090
H	5.992545	3.907458	-0.237302
H	4.328150	5.715911	-0.219597
H	1.973572	6.453438	-0.226606
H	-0.383703	7.203351	-0.284783
H	-2.779342	6.668661	-0.313260
H	-4.594812	4.977073	-0.302781
H	-6.408778	3.309521	-0.327058
H	-7.153688	0.969606	-0.304310
H	-6.606973	-1.453349	-0.209754
H	-6.072673	-3.857516	-0.195257
H	-4.411221	-5.663098	-0.237572
H	-2.059754	-6.394139	-0.321873
H	0.309471	-7.137501	-0.473045
H	2.702334	-6.587768	-0.508968
H	4.516112	-4.919938	-0.456133
H	6.353468	-3.250785	-0.436187
H	7.083526	-0.908109	-0.369936
H	6.531787	1.501296	-0.276207
N	2.031306	-0.285155	3.230145
H	2.536269	-0.922845	2.618665
H	2.324160	0.642700	2.933603

H_2O catalyst, Reactant

O	-0.615481	-1.042886	1.593712
H	-1.819694	0.613564	2.831390
C	2.785086	5.560160	-0.086388
C	3.911766	3.406238	-0.029238
C	5.059757	1.253674	-0.062796
C	6.201750	-0.896221	-0.174960
C	4.866851	-2.985382	-0.197816
C	3.543993	-5.085027	-0.279280
C	1.114924	-4.999434	-0.188914
C	-1.324083	-4.898843	-0.144330
C	-3.754281	-4.806394	-0.272945
C	-4.901603	-2.612398	-0.317761
C	-6.054325	-0.419047	-0.471115
C	-4.743892	1.631751	-0.347336
C	-3.455552	3.707231	-0.307310
C	-2.158430	5.768349	-0.298632
C	0.309828	5.658029	-0.148067

C	1.449942	3.509244	-0.004820
C	2.603466	1.333561	0.055181
C	3.750016	-0.834368	-0.040490
C	2.438118	-2.912274	-0.048146
C	-0.018725	-2.861447	0.096829
C	-2.489720	-2.711778	-0.010652
C	-3.626978	-0.551663	-0.146798
C	-2.313507	1.545224	-0.076919
C	-0.996322	3.609054	-0.101325
C	-3.357202	5.138559	-0.363339
C	-4.667511	3.034429	-0.395103
C	-5.991668	0.936870	-0.480586
C	-4.874027	-1.215873	-0.315435
C	-3.738661	-3.373792	-0.194489
C	-2.608047	-5.530678	-0.249280
C	-0.133792	-5.624070	-0.217983
C	2.346108	-5.724027	-0.294208
C	3.632607	-3.657283	-0.169931
C	4.950681	-1.599806	-0.137055
C	6.252617	0.458030	-0.136374
C	5.088531	2.641379	-0.058158
C	3.935038	4.834540	-0.065046
C	1.504922	4.925350	-0.074355
C	-0.930105	5.034939	-0.178035
C	2.655294	2.748231	0.018041
C	3.799261	0.581682	-0.006766
C	2.501306	-1.494087	0.024673
C	0.060317	-1.429880	0.399952
C	1.173426	-3.584644	-0.044055
C	-1.268943	-3.483565	0.014240
C	-2.466712	-1.314285	0.042978
C	-3.563021	0.877375	-0.177184
C	-2.251999	2.953939	-0.162671
C	-1.119401	0.813038	0.109797
C	0.194375	2.854690	0.008200
C	1.347039	0.661293	0.144490
C	-1.217371	-0.622538	0.372508
C	0.124217	1.433176	0.121005
C	1.321655	-0.728233	0.162214
H	-2.104804	6.854696	-0.345985
H	-4.275833	5.714393	-0.462155
H	-5.585818	3.607877	-0.514841
H	-6.898486	1.526975	-0.601832
H	-7.010544	-0.926633	-0.585580

H	-5.856195	-3.122366	-0.441648
H	-4.716694	-5.304396	-0.377962
H	-2.641924	-6.615420	-0.335041
H	-0.181541	-6.707200	-0.323869
H	2.301910	-6.807465	-0.391423
H	4.468964	-5.652872	-0.364206
H	5.782083	-3.569927	-0.282207
H	7.118784	-1.479531	-0.238586
H	7.211518	0.972517	-0.169411
H	6.049064	3.153676	-0.097303
H	4.901408	5.335436	-0.086257
H	2.822727	6.647495	-0.124812
H	0.361013	6.744727	-0.203114
O	-2.724379	0.287894	2.872284
H	-2.589116	-0.663618	2.822754

H_2O catalyst, Transition Structure

O	-0.068458	-1.298673	1.744178
H	-1.380377	-0.345210	2.456212
C	2.853483	5.527987	-0.145109
C	3.953884	3.359459	-0.084879
C	5.059408	1.185965	-0.030407
C	6.161645	-0.986090	-0.023028
C	4.784127	-3.047518	-0.052353
C	3.434068	-5.129037	-0.171735
C	1.005354	-5.003927	-0.218811
C	-1.426549	-4.867338	-0.272618
C	-3.854320	-4.719716	-0.317062
C	-4.965698	-2.499550	-0.226567
C	-6.104673	-0.297238	-0.206290
C	-4.765519	1.736427	-0.163882
C	-3.426442	3.773819	-0.173643
C	-2.089972	5.806967	-0.197781
C	0.380216	5.649019	-0.169049
C	1.490756	3.488289	-0.107037
C	2.606152	1.308200	-0.037811
C	3.707405	-0.876618	-0.000796
C	2.355027	-2.931640	-0.029541
C	-0.097098	-2.837752	-0.033642
C	-2.541481	-2.655347	-0.136825
C	-3.655362	-0.462104	-0.131828
C	-2.317581	1.585185	-0.117840
C	-0.965129	3.625643	-0.139659
C	-3.305350	5.200133	-0.198904

C	-4.666381	3.127927	-0.180351
C	-6.029549	1.057621	-0.192498
C	-4.922078	-1.109674	-0.185576
C	-3.802182	-3.288305	-0.221103
C	-2.724280	-5.470339	-0.350967
C	-0.247683	-5.615176	-0.298144
C	2.229014	-5.748655	-0.247166
C	3.538678	-3.700605	-0.076978
C	4.895820	-1.662491	-0.021491
C	6.239271	0.368520	-0.024255
C	5.115344	2.578042	-0.059954
C	3.994087	4.789287	-0.119097
C	1.564564	4.907115	-0.140982
C	-0.878339	5.045095	-0.169276
C	2.682945	2.718249	-0.077778
C	3.789186	0.538218	-0.014478
C	2.445255	-1.513825	0.021664
C	-0.027977	-1.396565	0.355293
C	1.077350	-3.586717	-0.090768
C	-1.344131	-3.450600	-0.146762
C	-2.475071	-1.237453	-0.087207
C	-3.577683	0.952201	-0.128087
C	-2.235281	2.993350	-0.143799
C	-1.131508	0.803147	-0.070969
C	0.222647	2.848503	-0.104461
C	1.338604	0.662098	-0.015577
C	-1.221106	-0.591960	-0.022117
C	0.141847	1.435062	-0.064234
C	1.270108	-0.731784	0.053061
H	-2.016887	6.892935	-0.217380
H	-4.216307	5.795679	-0.219061
H	-5.575931	3.726283	-0.204451
H	-6.937091	1.658476	-0.210640
H	-7.072817	-0.794277	-0.237353
H	-5.934219	-2.996396	-0.278141
H	-4.831732	-5.195712	-0.375153
H	-2.787578	-6.553879	-0.435778
H	-0.306731	-6.699428	-0.382757
H	2.173576	-6.832695	-0.331254
H	4.353450	-5.711571	-0.196027
H	5.691272	-3.650764	-0.076499
H	7.068465	-1.588558	-0.028107
H	7.208937	0.863161	-0.028678
H	6.085999	3.071670	-0.068735

H	4.966080	5.279297	-0.123038
H	2.903233	6.615184	-0.169956
H	0.441904	6.736734	-0.192015
O	-2.216109	0.104392	2.712221
H	-2.783632	-0.637693	2.934553

H_2O catalyst, Product

O	-1.231756	0.148764	1.599823
H	0.507014	-0.019149	2.670115
C	3.018968	-5.387905	-0.272242
C	0.602255	-5.090664	-0.232449
C	-1.821581	-4.778452	-0.213420
C	-4.242063	-4.496823	-0.283231
C	-5.208909	-2.212943	-0.163335
C	-6.181443	0.064593	-0.144453
C	-4.714148	2.007689	-0.085814
C	-3.251606	3.960006	-0.187530
C	-1.785227	5.896339	-0.324877
C	0.680119	5.594993	-0.289294
C	3.143643	5.307706	-0.305896
C	4.088612	3.063617	-0.193374
C	5.030126	0.812381	-0.147709
C	5.985830	-1.422888	-0.182074
C	4.496281	-3.403255	-0.191124
C	2.084597	-3.118224	-0.111981
C	-0.345175	-2.833298	-0.035450
C	-2.802997	-2.525143	-0.045141
C	-3.753724	-0.275775	0.061971
C	-2.305257	1.733316	0.099712
C	-0.795546	3.668012	-0.099099
C	1.643342	3.370326	-0.139581
C	2.599405	1.111064	-0.047303
C	3.553816	-1.159121	-0.080388
C	6.151241	-0.072890	-0.182286
C	5.181348	2.207723	-0.193418
C	4.225312	4.490489	-0.277605
C	1.807852	4.784256	-0.244695
C	-0.620246	5.063742	-0.233282
C	-3.037352	5.371236	-0.309908
C	-4.525307	3.387481	-0.181383
C	-6.017340	1.410885	-0.149217
C	-5.060049	-0.827839	-0.076134
C	-4.110225	-3.074962	-0.167140
C	-3.152649	-5.307089	-0.298797

C	-0.687308	-5.606804	-0.271805
C	1.772383	-5.920667	-0.296625
C	3.229420	-3.970137	-0.188974
C	4.684788	-2.012613	-0.146373
C	0.783117	-3.678821	-0.129176
C	-1.655342	-3.381415	-0.083210
C	-2.655447	-1.140256	0.108907
C	-1.138520	0.891534	0.381498
C	-3.579082	1.158171	0.057067
C	-2.115218	3.112511	-0.060694
C	0.344394	2.821050	-0.047380
C	2.771957	2.512505	-0.119082
C	3.726983	0.255791	-0.082412
C	1.285980	0.564137	0.059894
C	2.254195	-1.717317	-0.041392
C	-0.153141	-1.440178	0.105778
C	0.195211	1.422693	0.097167
C	1.112067	-0.870917	0.066958
C	-1.319846	-0.602667	0.386163
H	6.851589	-2.081911	-0.218134
H	7.150097	0.358499	-0.218659
H	6.185308	2.627078	-0.246335
H	5.229704	4.907719	-0.326397
H	3.271287	6.386514	-0.377103
H	0.804267	6.673203	-0.381318
H	-1.643074	6.971418	-0.420724
H	-3.906868	6.020910	-0.393982
H	-5.396846	4.034381	-0.273922
H	-6.881182	2.069063	-0.224811
H	-7.178154	-0.367395	-0.216226
H	-6.210461	-2.632045	-0.252013
H	-5.242345	-4.919058	-0.362535
H	-3.272775	-6.385262	-0.390280
H	-0.825970	-6.683486	-0.361079
H	1.636429	-6.998560	-0.366153
H	3.893566	-6.034309	-0.322437
H	5.369855	-4.051732	-0.244617
O	1.409585	-0.026480	3.015010
H	1.724977	0.854764	2.797760

HF catalyst, Reactant

O	-1.168104	-0.003834	1.580320
H	-2.659184	0.000161	2.438732
C	6.248275	0.700541	0.011042

C	5.034836	-1.406418	0.018320
C	3.836392	-3.530279	-0.061473
C	2.637973	-5.646257	-0.216838
C	0.159483	-5.640809	-0.273593
C	-2.320712	-5.650965	-0.393236
C	-3.552609	-3.555590	-0.301868
C	-4.777099	-1.444173	-0.257729
C	-6.001840	0.657075	-0.369937
C	-4.767612	2.802851	-0.349328
C	-3.535279	4.957018	-0.425424
C	-1.104252	4.952231	-0.257634
C	1.338580	4.977138	-0.187298
C	3.773500	4.987855	-0.151908
C	5.003049	2.842893	-0.029662
C	3.800297	0.725390	0.058548
C	2.583565	-1.416612	0.067062
C	1.371774	-3.546124	-0.073204
C	-1.085312	-3.554636	-0.117109
C	-2.363608	-1.455137	0.023992
C	-3.561384	0.709272	-0.074602
C	-2.349400	2.831248	-0.129044
C	0.124970	2.847803	-0.017875
C	2.573054	2.844895	-0.013233
C	2.599724	5.663156	-0.215217
C	0.121321	5.640788	-0.274224
C	-2.358714	5.633956	-0.396601
C	-3.576247	3.530207	-0.305491
C	-4.786472	1.410696	-0.259904
C	-5.997510	-0.698513	-0.368729
C	-4.748880	-2.836299	-0.345617
C	-3.501926	-4.982189	-0.421057
C	-1.070748	-4.960651	-0.255718
C	1.372297	-4.968955	-0.187650
C	3.807056	-4.962833	-0.153879
C	5.021905	-2.809639	-0.030658
C	6.252659	-0.659478	0.010883
C	5.025483	1.439726	0.018698
C	3.812662	3.555484	-0.060410
C	3.805057	-0.700381	0.058395
C	2.592029	-2.828258	-0.013585
C	0.144030	-2.847913	-0.017024
C	-1.117970	-0.756394	0.356794
C	-2.330510	-2.848088	-0.126698
C	-3.556628	-0.734143	-0.073523

C	-2.373136	1.438358	0.022664
C	-1.109059	3.546235	-0.118888
C	1.347975	3.554368	-0.073267
C	0.145899	1.443673	0.137167
C	2.574099	1.433296	0.067127
C	1.340967	-0.719407	0.147587
C	-1.123074	0.747980	0.356286
C	1.336057	0.727586	0.147457
C	0.155589	-1.443634	0.137839
H	4.719368	5.526274	-0.177807
H	2.593865	6.749089	-0.291712
H	0.113891	6.725638	-0.371520
H	-2.347008	6.718277	-0.492792
H	-4.475051	5.493343	-0.544870
H	-5.708667	3.336685	-0.475458
H	-6.937296	1.203670	-0.475426
H	-6.929644	-1.250873	-0.473317
H	-5.686617	-3.376138	-0.470916
H	-4.438347	-5.524632	-0.539422
H	-2.302176	-6.735194	-0.489133
H	0.158799	-6.725676	-0.371034
H	2.639054	-6.732187	-0.293959
H	4.756371	-5.495057	-0.180678
H	5.970398	-3.344241	-0.063772
H	7.194131	-1.205842	-0.005678
H	7.186420	1.252552	-0.005337
H	5.948131	3.383533	-0.062303
F	-3.519449	0.004848	2.806609

HF catalyst, Transition Structure

O	-0.100849	-1.292027	1.747594
H	-1.274013	-0.516759	2.287969
C	2.980079	5.459853	-0.141019
C	4.028121	3.265189	-0.093701
C	5.081196	1.065296	-0.044683
C	6.129886	-1.132785	-0.033988
C	4.702654	-3.160151	-0.050143
C	3.302714	-5.209131	-0.153141
C	0.877643	-5.024463	-0.200083
C	-1.549581	-4.829440	-0.261036
C	-3.972670	-4.622942	-0.307150
C	-5.029039	-2.375731	-0.219953
C	-6.114849	-0.147893	-0.181692
C	-4.728478	1.852850	-0.137169

C	-3.340346	3.857762	-0.142308
C	-1.955824	5.858280	-0.162670
C	0.510159	5.640314	-0.151387
C	1.568802	3.453321	-0.106442
C	2.631855	1.247210	-0.048856
C	3.679135	-0.963441	-0.009213
C	2.277083	-2.985554	-0.023636
C	-0.171865	-2.830555	-0.027723
C	-2.609799	-2.591345	-0.143058
C	-3.670366	-0.371392	-0.133748
C	-2.284318	1.642691	-0.113941
C	-0.883499	3.649996	-0.126976
C	-3.185551	5.280706	-0.158178
C	-4.595494	3.241350	-0.143706
C	-6.008123	1.204943	-0.159626
C	-4.951973	-0.987664	-0.176719
C	-3.884974	-3.192915	-0.219083
C	-2.861383	-5.401164	-0.337254
C	-0.389259	-5.605772	-0.278065
C	2.082710	-5.799123	-0.223562
C	3.441679	-3.783176	-0.068235
C	4.848089	-1.778133	-0.027560
C	6.240758	0.219640	-0.039216
C	5.170399	2.455575	-0.073510
C	4.102727	4.693676	-0.122771
C	1.676766	4.870145	-0.133793
C	-0.762770	5.067131	-0.147820
C	2.742247	2.655039	-0.085204
C	3.795519	0.448491	-0.026878
C	2.401622	-1.569576	0.018229
C	-0.070526	-1.387306	0.352976
C	0.984142	-3.608535	-0.079496
C	-1.432764	-3.414367	-0.144615
C	-2.508183	-1.174410	-0.105529
C	-3.558321	1.039356	-0.119258
C	-2.168126	3.048763	-0.127668
C	-1.117511	0.831882	-0.082120
C	0.285650	2.844119	-0.101594
C	1.349442	0.631923	-0.024440
C	-1.243047	-0.559388	-0.048488
C	0.170990	1.433231	-0.068458
C	1.247157	-0.759027	0.047310
H	-1.857090	6.942272	-0.175487
H	-4.082264	5.897733	-0.166890

H	-5.490713	3.861284	-0.155264
H	-6.901463	1.826817	-0.164399
H	-7.094563	-0.622109	-0.204821
H	-6.009375	-2.849506	-0.263754
H	-4.961352	-5.075515	-0.360146
H	-2.950607	-6.483391	-0.414813
H	-0.473925	-6.688854	-0.355197
H	2.000690	-6.881969	-0.300495
H	4.207769	-5.813763	-0.174136
H	5.595005	-3.785123	-0.072042
H	7.021896	-1.756913	-0.038481
H	7.222055	0.690716	-0.046275
H	6.152497	2.925968	-0.083457
H	5.086009	5.160506	-0.128261
H	3.055644	6.545649	-0.161227
H	0.597589	6.726381	-0.168189
F	-2.066725	0.008075	2.519210

HF catalyst, Product

O	-1.249799	0.001501	1.607322
H	0.203002	0.002767	2.526670
C	3.654820	-4.979960	-0.263023
C	1.220062	-4.975195	-0.225955
C	-1.223515	-4.956223	-0.218331
C	-3.659915	-4.966741	-0.305304
C	-4.893783	-2.815199	-0.192579
C	-6.133012	-0.670838	-0.177856
C	-4.909545	1.433779	-0.103450
C	-3.691498	3.548166	-0.187392
C	-2.467648	5.646237	-0.312419
C	0.015572	5.642284	-0.271358
C	2.494761	5.652547	-0.289796
C	3.701523	3.538165	-0.180363
C	4.906416	1.416820	-0.140292
C	6.123939	-0.687401	-0.179576
C	4.882544	-2.831952	-0.183837
C	2.454294	-2.839058	-0.100366
C	0.007676	-2.848092	-0.028340
C	-2.468842	-2.837378	-0.056089
C	-3.683188	-0.718046	0.043257
C	-2.486447	1.450759	0.097629
C	-1.218178	3.552369	-0.085495
C	1.238121	3.548664	-0.120368
C	2.457971	1.421643	-0.027586

C	3.677973	-0.717207	-0.069539
C	6.125533	0.672723	-0.179858
C	4.889160	2.820174	-0.184979
C	3.666546	4.971019	-0.264467
C	1.231835	4.972037	-0.226582
C	-1.211699	4.958923	-0.217996
C	-3.648033	4.975310	-0.304317
C	-4.886994	2.826677	-0.192010
C	-6.131331	0.685358	-0.177690
C	-4.913042	-1.422286	-0.103719
C	-3.700003	-3.539531	-0.187982
C	-2.481136	-5.640508	-0.313313
C	0.002169	-5.642518	-0.271349
C	2.481399	-5.658702	-0.288697
C	3.693209	-3.547186	-0.179145
C	4.903073	-1.428627	-0.139697
C	1.229679	-3.551914	-0.119631
C	-1.226730	-3.549759	-0.085533
C	-2.489972	-1.445027	0.097681
C	-1.228641	0.752548	0.380753
C	-3.681438	0.726596	0.043334
C	-2.462004	2.843070	-0.055904
C	0.014475	2.847757	-0.028822
C	2.460978	2.832923	-0.101335
C	3.679637	0.708243	-0.069879
C	1.220927	0.721059	0.081982
C	2.454606	-1.427819	-0.026927
C	0.031140	-1.442296	0.114269
C	0.034651	1.441817	0.113735
C	1.219216	-0.724360	0.082491
C	-1.230503	-0.749881	0.380986
H	7.062283	-1.237929	-0.218981
H	7.065208	1.220956	-0.219484
H	5.835393	3.356896	-0.241015
H	4.613791	5.505261	-0.315186
H	2.491699	6.738876	-0.360611
H	0.010111	6.727637	-0.362787
H	-2.454462	6.730868	-0.405208
H	-4.588715	5.516375	-0.390815
H	-5.829220	3.364862	-0.287867
H	-7.067180	1.235828	-0.257019
H	-7.070250	-1.218915	-0.257302
H	-5.837310	-3.351065	-0.288664
H	-4.601910	-5.505473	-0.392131

H	-2.470635	-6.725140	-0.406384
H	-0.005960	-6.727837	-0.362995
H	2.475706	-6.745028	-0.359467
H	4.600734	-5.516577	-0.313403
H	5.827470	-3.370991	-0.239615
F	1.050867	0.002538	2.923540

2H_2O catalyst, Reactant

O	-0.330205	-1.155438	1.502387
H	-1.971647	-1.319192	2.683297
C	1.411435	6.034155	-0.191301
C	3.024429	4.216009	-0.122972
C	4.659002	2.403307	-0.116718
C	6.287771	0.590997	-0.172846
C	5.496856	-1.759061	-0.167884
C	4.720083	-4.117030	-0.220821
C	2.340727	-4.617931	-0.168305
C	-0.051010	-5.107325	-0.168994
C	-2.429311	-5.605092	-0.340223
C	-4.070652	-3.752917	-0.438995
C	-5.719409	-1.902399	-0.619128
C	-4.945996	0.407349	-0.486892
C	-4.196315	2.731857	-0.428381
C	-3.436411	5.043955	-0.402481
C	-1.014759	5.532124	-0.256795
C	0.609510	3.721988	-0.121231
C	2.254705	1.890246	-0.038446
C	3.891388	0.061574	-0.074416
C	3.119824	-2.271304	-0.051321
C	0.720504	-2.811667	0.055791
C	-1.709966	-3.263871	-0.103665
C	-3.332410	-1.443038	-0.291549
C	-2.564592	0.910525	-0.218083
C	-1.787375	3.229107	-0.221169
C	-4.448335	4.144594	-0.471912
C	-5.211013	1.786763	-0.523934
C	-5.986413	-0.571016	-0.626556
C	-4.382165	-2.391222	-0.456096
C	-2.760086	-4.209889	-0.290528
C	-1.142985	-6.030718	-0.283456
C	1.280158	-5.525536	-0.206149
C	3.711987	-5.026258	-0.239839
C	4.460608	-2.708245	-0.140976
C	5.242902	-0.393238	-0.137230

C	6.009623	1.917935	-0.159771
C	4.351392	3.756846	-0.130382
C	2.702651	5.607733	-0.163110
C	0.322009	5.109547	-0.185380
C	-2.067265	4.627567	-0.288339
C	1.963172	3.274714	-0.087501
C	3.597214	1.447846	-0.068611
C	2.837657	-0.878915	-0.010943
C	0.445185	-1.397371	0.325400
C	2.054539	-3.228342	-0.050554
C	-0.340278	-3.718180	-0.039263
C	-2.023301	-1.901359	-0.079787
C	-3.615631	-0.039135	-0.321375
C	-2.846492	2.292008	-0.289291
C	-1.230226	0.488596	-0.037889
C	-0.450450	2.784814	-0.119259
C	1.195883	0.936074	0.038736
C	-0.983351	-0.921295	0.250107
C	-0.175115	1.390191	-0.018158
C	1.505999	-0.417803	0.089823
H	-3.647010	6.111434	-0.439561
H	-5.479217	4.481882	-0.564567
H	-6.240715	2.122060	-0.640443
H	-7.009254	-0.219072	-0.749561
H	-6.524269	-2.625811	-0.736773
H	-4.872284	-4.480041	-0.562386
H	-3.240913	-6.322234	-0.450018
H	-0.913050	-7.092853	-0.347783
H	1.497125	-6.589662	-0.290622
H	3.932017	-6.089735	-0.315396
H	5.756025	-4.446413	-0.280539
H	6.527456	-2.106566	-0.226837
H	7.319509	0.245872	-0.212195
H	6.816561	2.648216	-0.188859
H	5.160283	4.485787	-0.161697
H	3.519339	6.327411	-0.177265
H	1.185754	7.098543	-0.227851
H	-1.228082	6.599207	-0.305045
O	-2.788112	-0.844039	2.883049
H	-3.413413	-1.162743	2.226152
H	-0.755328	1.368041	2.660732
O	-1.632298	1.753669	2.742068
H	-2.189363	0.962739	2.821449

$2H_2O$ catalyst, Transition Structure

O	-0.107370	-1.291274	1.662813
H	-1.471089	-0.407129	2.384744
C	2.443415	5.696744	-0.217043
C	3.678229	3.601361	-0.188519
C	4.920465	1.502362	-0.166658
C	6.156857	-0.595069	-0.183130
C	4.911202	-2.737625	-0.212729
C	3.692793	-4.901881	-0.300428
C	1.260888	-4.930360	-0.303523
C	-1.175146	-4.945480	-0.305209
C	-3.608117	-4.953525	-0.312271
C	-4.854858	-2.807214	-0.225192
C	-6.129128	-0.680484	-0.207203
C	-4.920261	1.433167	-0.186986
C	-3.714082	3.552258	-0.207980
C	-2.508493	5.665709	-0.233264
C	-0.033055	5.662158	-0.224226
C	1.212828	3.575253	-0.193001
C	2.465217	1.468959	-0.164951
C	3.701526	-0.638993	-0.160149
C	2.480838	-2.776198	-0.165132
C	0.029330	-2.834838	-0.105665
C	-2.424863	-2.809311	-0.165339
C	-3.673666	-0.690821	-0.160686
C	-2.468566	1.438082	-0.171211
C	-1.247583	3.558433	-0.199264
C	-3.683091	4.983887	-0.227542
C	-4.909460	2.829344	-0.203455
C	-6.139340	0.676627	-0.199541
C	-4.897786	-1.416766	-0.195274
C	-3.644600	-3.521189	-0.228383
C	-2.432985	-5.630411	-0.357661
C	0.047299	-5.618673	-0.349765
C	2.528286	-5.597051	-0.349349
C	3.708782	-3.468758	-0.220261
C	4.935490	-1.348692	-0.183534
C	6.149549	0.761516	-0.172723
C	4.887756	2.894017	-0.178947
C	3.628598	5.030446	-0.204847
C	1.196938	4.995460	-0.211999
C	-1.250593	4.981436	-0.219657
C	2.451351	2.880648	-0.182974
C	3.692398	0.774784	-0.155984

C	2.481393	-1.353453	-0.136408
C	0.017982	-1.386779	0.269584
C	1.246628	-3.509860	-0.190690
C	-1.179639	-3.525772	-0.187885
C	-2.447339	-1.390986	-0.124472
C	-3.685971	0.726163	-0.164936
C	-2.475175	2.848363	-0.194259
C	-1.234740	0.733914	-0.140619
C	-0.012949	2.857310	-0.182305
C	1.242185	0.742876	-0.137985
C	-1.235090	-0.666138	-0.082446
C	-0.004841	1.441189	-0.152636
C	1.266124	-0.648494	-0.087774
H	-2.503673	6.754207	-0.247006
H	-4.629728	5.521146	-0.236384
H	-5.855454	3.368594	-0.216310
H	-7.082927	1.219293	-0.209755
H	-7.064379	-1.237445	-0.225960
H	-5.791004	-3.363847	-0.260825
H	-4.554135	-5.490765	-0.352367
H	-2.427939	-6.716386	-0.433960
H	0.053855	-6.705246	-0.424278
H	2.539522	-6.683238	-0.421972
H	4.646400	-5.425982	-0.333548
H	5.854159	-3.282927	-0.240631
H	7.099371	-1.139908	-0.191687
H	7.086089	1.316257	-0.172935
H	5.824985	3.448582	-0.184492
H	4.567942	5.580483	-0.207144
H	2.424717	6.785089	-0.229665
H	-0.039138	6.751775	-0.237803
O	-2.297523	0.040087	2.664023
H	-2.863748	-0.699747	2.896748
H	1.399011	-0.659892	2.423192
O	2.194475	-0.147751	2.680866
H	1.812907	0.692729	2.947333

2H_2O catalyst, Product

O	0.498936	-1.111019	1.521798
H	0.131041	0.496643	2.633150
C	2.659462	5.509995	-0.435171
C	3.761687	3.337903	-0.440187
C	4.853535	1.152365	-0.474855
C	5.969983	-1.009909	-0.584555

C	4.624454	-3.086302	-0.390307
C	3.283584	-5.165561	-0.307319
C	0.856392	-5.034980	-0.170328
C	-1.581987	-4.914192	-0.211444
C	-4.009276	-4.780176	-0.296912
C	-5.135506	-2.567510	-0.237226
C	-6.274774	-0.364885	-0.231366
C	-4.941442	1.673367	-0.146216
C	-3.602041	3.713223	-0.134912
C	-2.283319	5.755262	-0.207813
C	0.191193	5.626273	-0.277351
C	1.305491	3.467191	-0.223807
C	2.428783	1.291024	-0.187634
C	3.543765	-0.916484	-0.239635
C	2.216329	-2.960904	-0.066020
C	-0.257849	-2.885090	0.043245
C	-2.709779	-2.714202	-0.096633
C	-3.827120	-0.525157	-0.109917
C	-2.487858	1.530861	-0.042467
C	-1.140984	3.591947	-0.121751
C	-3.494603	5.137495	-0.178811
C	-4.843555	3.058039	-0.152760
C	-6.202090	0.988726	-0.206131
C	-5.092899	-1.179318	-0.192088
C	-3.967588	-3.348959	-0.205518
C	-2.874206	-5.525177	-0.305613
C	-0.395159	-5.649708	-0.233417
C	2.076828	-5.782626	-0.269384
C	3.398363	-3.736623	-0.248482
C	4.723260	-1.693231	-0.408952
C	6.031761	0.345608	-0.609789
C	4.905643	2.555963	-0.532007
C	3.794593	4.771924	-0.502625
C	1.369411	4.892968	-0.306991
C	-1.066148	5.006693	-0.196979
C	2.495241	2.698616	-0.284532
C	3.610547	0.511199	-0.289393
C	2.321618	-1.567282	-0.026303
C	-0.205615	-1.448011	0.322225
C	0.930519	-3.618540	-0.030323
C	-1.511429	-3.498225	-0.086145
C	-2.643858	-1.295487	-0.042483
C	-3.747190	0.889930	-0.090774
C	-2.410609	2.943931	-0.089570

C	-1.297446	0.747685	0.046530
C	0.050209	2.825568	-0.110326
C	1.174300	0.674096	0.013585
C	-1.398772	-0.638305	0.080020
C	-0.008713	1.403449	0.006512
C	1.140575	-0.760977	0.295314
H	-2.221989	6.841288	-0.251106
H	-4.411083	5.724673	-0.198642
H	-5.753676	3.655341	-0.190517
H	-7.110433	1.587913	-0.239023
H	-7.241583	-0.862551	-0.284119
H	-6.100639	-3.067027	-0.310782
H	-4.982175	-5.262765	-0.372561
H	-2.928906	-6.609287	-0.388653
H	-0.446248	-6.733957	-0.325112
H	2.011451	-6.866973	-0.340061
H	4.196366	-5.750095	-0.409157
H	5.527752	-3.682644	-0.512836
H	6.874584	-1.604474	-0.699551
H	6.987650	0.848986	-0.743933
H	5.871926	3.041867	-0.660913
H	4.761792	5.260377	-0.608063
H	2.705921	6.596392	-0.486925
H	0.239435	6.712807	-0.337200
O	0.427846	1.254864	3.156520
H	0.322578	2.001019	2.558888
H	2.607328	-0.867822	2.800639
O	2.940710	0.027229	2.690809
H	2.184708	0.570817	2.968217

Ethylene glycol catalyst, Reactant

O	-0.409433	1.190971	1.381529
C	2.173115	-5.702207	-0.507365
C	-0.178990	-5.103684	-0.356765
C	-2.547856	-4.521993	-0.283499
C	-4.913673	-3.935810	-0.278296
C	-5.576626	-1.546229	-0.240142
C	-6.256653	0.842970	-0.255017
C	-4.566330	2.591897	-0.211953
C	-2.860021	4.339363	-0.197800
C	-1.170254	6.090077	-0.318931
C	1.229937	5.481583	-0.421057
C	3.631468	4.880750	-0.618011
C	4.282395	2.531522	-0.600449

C	4.961669	0.185406	-0.675432
C	5.625320	-2.156635	-0.756468
C	3.896566	-3.923295	-0.604608
C	1.540937	-3.340180	-0.385742
C	-0.844554	-2.748714	-0.230983
C	-3.225313	-2.153849	-0.205841
C	-3.894176	0.210036	-0.144651
C	-2.209541	2.001930	-0.041175
C	-0.451372	3.743852	-0.156917
C	1.913762	3.152162	-0.345941
C	2.594446	0.772393	-0.390869
C	3.246182	-1.584502	-0.505342
C	5.958366	-0.842681	-0.784567
C	5.272334	1.538965	-0.706963
C	4.597921	3.928994	-0.676392
C	2.251135	4.529808	-0.463637
C	-0.112743	5.120544	-0.294679
C	-2.474230	5.719342	-0.274695
C	-4.197095	3.938692	-0.228849
C	-5.931931	2.161362	-0.263887
C	-5.250504	-0.179027	-0.208175
C	-4.600201	-2.534917	-0.239739
C	-3.938802	-4.877989	-0.295292
C	-1.534662	-5.469292	-0.331245
C	0.866487	-6.074149	-0.440661
C	2.555286	-4.325396	-0.496360
C	4.261019	-2.584125	-0.621296
C	0.171631	-3.729965	-0.315334
C	-2.203549	-3.135756	-0.232454
C	-2.879925	-0.785257	-0.138695
C	-1.183336	0.980184	0.186874
C	-3.548325	1.600043	-0.131444
C	-1.839996	3.349071	-0.104093
C	0.573328	2.792924	-0.157920
C	2.933524	2.150681	-0.430762
C	3.598509	-0.211243	-0.530517
C	1.253981	0.366475	-0.203806
C	1.893040	-1.969562	-0.372733
C	-0.502778	-1.366865	-0.151222
C	0.257779	1.388876	0.118324
C	0.886134	-0.971541	-0.218467
C	-1.516367	-0.422071	-0.067005
H	6.396520	-2.920524	-0.839998
H	6.999226	-0.541539	-0.890026

H	6.311436	1.842956	-0.826370
H	5.641553	4.214759	-0.796187
H	3.892490	5.935059	-0.691384
H	1.486605	6.536671	-0.507988
H	-0.901223	7.142178	-0.395424
H	-3.260446	6.471215	-0.315767
H	-4.974743	4.699482	-0.284811
H	-6.711925	2.919216	-0.312944
H	-7.300206	0.535565	-0.296610
H	-6.625923	-1.836058	-0.277412
H	-5.961971	-4.229017	-0.294550
H	-4.197543	-5.935071	-0.325729
H	-1.795573	-6.526324	-0.366181
H	0.593934	-7.127970	-0.459094
H	2.955618	-6.455660	-0.579521
H	4.669644	-4.686004	-0.689799
H	1.243567	1.194435	2.460191
O	2.121737	1.175732	2.852344
C	2.506386	-0.158704	3.053010
C	1.428067	-1.016064	3.679580
H	2.819736	-0.637364	2.109012
H	3.383696	-0.138442	3.713427
O	0.376300	-1.314066	2.800533
H	1.066081	-0.517894	4.597076
H	1.865944	-1.976892	3.980686
H	-0.010860	-0.493057	2.472298

Ethylene glycol catalyst, Transition Structure

O	-0.739313	1.089933	1.549823
C	0.009759	-6.139133	-0.402088
C	-1.974808	-4.734106	-0.324304
C	-3.963936	-3.324135	-0.256889
C	-5.953074	-1.918764	-0.219794
C	-5.697782	0.548367	-0.206103
C	-5.474459	3.021558	-0.240298
C	-3.264935	4.041106	-0.260807
C	-1.051353	5.058230	-0.290015
C	1.164139	6.061638	-0.320153
C	3.184931	4.614524	-0.338409
C	5.218249	3.199055	-0.419456
C	4.982233	0.775521	-0.467234
C	4.739450	-1.650693	-0.528136
C	4.505866	-4.070967	-0.555227
C	2.249457	-5.088444	-0.474827

C	0.262241	-3.695475	-0.383067
C	-1.738999	-2.291854	-0.298589
C	-3.732435	-0.870774	-0.218435
C	-3.494474	1.575105	-0.178048
C	-1.277202	2.634326	-0.148896
C	0.967485	3.620513	-0.249374
C	2.974746	2.200530	-0.356442
C	2.742306	-0.231313	-0.430969
C	2.495508	-2.669952	-0.463731
C	5.298266	-2.965755	-0.569000
C	5.538204	-0.497804	-0.523991
C	5.783274	1.966745	-0.463960
C	3.793443	3.366389	-0.368344
C	1.786128	4.768213	-0.296502
C	-0.185946	6.199661	-0.327036
C	-2.442602	5.169154	-0.296417
C	-4.695362	4.131915	-0.275840
C	-4.901834	1.706291	-0.203430
C	-5.149532	-0.730283	-0.213889
C	-5.388380	-3.153024	-0.234726
C	-3.363107	-4.584780	-0.287474
C	-1.341922	-6.018823	-0.357161
C	0.860370	-4.986540	-0.420060
C	3.081342	-3.962589	-0.498855
C	-1.149008	-3.572803	-0.334858
C	-3.143760	-2.161667	-0.253059
C	-2.916909	0.281082	-0.182834
C	-0.664415	1.306853	0.164252
C	-2.666599	2.750392	-0.191090
C	-0.461338	3.762490	-0.228583
C	1.568723	2.331085	-0.281269
C	3.561721	0.915539	-0.412789
C	3.324964	-1.516337	-0.482394
C	1.328181	-0.090830	-0.351802
C	1.083673	-2.538552	-0.400723
C	-0.917517	-1.133184	-0.295681
C	0.766997	1.176361	-0.243069
C	0.492722	-1.253581	-0.348616
C	-1.508429	0.133925	-0.181680
H	4.948636	-5.065031	-0.583258
H	6.381437	-3.066733	-0.606803
H	6.621289	-0.604966	-0.561665
H	6.865888	1.859695	-0.500770
H	5.842576	4.090928	-0.420713

H	3.808098	5.508087	-0.358885
H	1.805579	6.940832	-0.346190
H	-0.636852	7.190054	-0.358563
H	-2.897754	6.158002	-0.332131
H	-5.150267	5.120173	-0.315207
H	-6.559404	3.110390	-0.251016
H	-6.781872	0.658264	-0.210751
H	-7.036284	-1.810284	-0.210977
H	-6.014402	-4.043552	-0.235749
H	-3.992165	-5.473684	-0.284976
H	-1.972300	-6.906118	-0.345091
H	0.474424	-7.123295	-0.426427
H	2.704977	-6.078016	-0.500890
H	0.902051	0.973392	2.251452
O	1.816799	0.842648	2.577366
C	1.992181	-0.488694	2.962094
C	0.751809	-1.144229	3.534893
H	2.326903	-1.117851	2.114450
H	2.797592	-0.518151	3.712501
O	-0.231710	-1.386708	2.571008
H	0.369234	-0.520580	4.363881
H	1.036771	-2.114827	3.966421
H	-0.539886	-0.522624	2.226869

Ethylene glycol catalyst, Product

O	-1.160748	-0.521287	1.393818
C	5.268191	-3.019148	-0.621907
C	3.052164	-4.024088	-0.526556
C	0.821701	-5.020681	-0.455422
C	-1.392133	-6.042466	-0.460540
C	-3.404109	-4.595242	-0.288760
C	-5.419852	-3.157427	-0.194284
C	-5.178289	-0.734137	-0.127450
C	-4.951507	1.695880	-0.208654
C	-4.713696	4.114015	-0.326303
C	-2.452240	5.140746	-0.378697
C	-0.202567	6.179157	-0.483960
C	1.775442	4.755152	-0.474646
C	3.752289	3.324198	-0.521580
C	5.731840	1.914090	-0.614505
C	5.494333	-0.553911	-0.588256
C	3.290312	-1.567611	-0.445549
C	1.071106	-2.589307	-0.320370
C	-1.185458	-3.608083	-0.252764

C	-3.164674	-2.183386	-0.076653
C	-2.973537	0.285938	-0.022495
C	-2.700831	2.725803	-0.205585
C	-0.466930	3.742470	-0.334095
C	1.527023	2.312458	-0.344963
C	3.522852	0.871366	-0.453020
C	5.168562	3.152207	-0.602325
C	3.152956	4.594071	-0.533711
C	1.146251	6.045132	-0.517378
C	-1.066670	5.035746	-0.397072
C	-3.282889	4.009434	-0.298747
C	-5.508174	3.013549	-0.290914
C	-5.739241	0.543096	-0.183901
C	-5.980863	-1.922829	-0.168922
C	-3.996208	-3.335333	-0.182234
C	-2.017977	-4.759359	-0.337957
C	-0.040752	-6.166033	-0.508200
C	2.220256	-5.136978	-0.538457
C	4.481986	-4.123654	-0.614291
C	4.709722	-1.698325	-0.549179
C	4.931436	0.732092	-0.549334
C	2.472609	-2.723886	-0.431873
C	0.238637	-3.740257	-0.330495
C	-1.776581	-2.349016	-0.087423
C	-1.527126	0.172062	0.188233
C	-3.762075	-0.868282	-0.046183
C	-3.535507	1.563712	-0.143551
C	-1.285850	2.596380	-0.220740
C	0.942131	3.598506	-0.377087
C	2.932546	2.169759	-0.436448
C	0.695545	1.160694	-0.218984
C	2.706474	-0.282470	-0.384162
C	0.512194	-1.300315	-0.188828
C	-0.680519	1.324927	-0.122025
C	1.293099	-0.154657	-0.243606
C	-0.906387	-1.193237	0.148221
H	6.812866	1.803823	-0.680739
H	5.794720	4.040986	-0.658861
H	3.788889	5.475765	-0.603025
H	1.783555	6.925261	-0.584071
H	-0.658154	7.167134	-0.523161
H	-2.911198	6.126740	-0.438539
H	-5.155933	5.106738	-0.390403
H	-6.591405	3.115937	-0.327106

H	-6.823158	0.641716	-0.229254
H	-7.063323	-1.811405	-0.200345
H	-6.048097	-4.045040	-0.245803
H	-4.043128	-5.475260	-0.351290
H	-2.026900	-6.925234	-0.514552
H	0.416446	-7.149829	-0.599880
H	2.661743	-6.129128	-0.623258
H	4.926847	-5.115310	-0.676725
H	6.350415	-3.115545	-0.691403
H	6.576496	-0.652543	-0.664405
H	0.113585	0.791332	2.355990
O	0.552169	1.389385	2.972492
C	1.887313	0.989058	3.107968
C	2.018120	-0.429232	3.620636
H	2.437030	1.074430	2.155027
H	2.362018	1.679855	3.817650
O	1.497138	-1.373235	2.719974
H	1.528389	-0.502124	4.607175
H	3.079470	-0.674347	3.757741
H	0.553687	-1.206945	2.614906

Guanidine catalyst, Reactant

O	-1.115160	-0.638282	1.438757
C	5.509903	-2.294612	-0.643096
C	3.437541	-3.572333	-0.598557
C	1.348774	-4.841935	-0.516427
C	-0.719796	-6.132942	-0.481655
C	-2.892083	-4.952953	-0.228380
C	-5.067888	-3.781315	-0.048109
C	-5.129783	-1.347331	0.042050
C	-5.212183	1.091784	-0.029575
C	-5.284223	3.521070	-0.146831
C	-3.172129	4.824960	-0.256483
C	-1.072317	6.139807	-0.396985
C	1.070939	4.977809	-0.413878
C	3.213937	3.806843	-0.457857
C	5.354284	2.654277	-0.526427
C	5.426315	0.176623	-0.549027
C	3.365420	-1.104787	-0.494388
C	1.292737	-2.399818	-0.368183
C	-0.815403	-3.693951	-0.248121
C	-2.950297	-2.532237	0.014663
C	-3.067653	-0.058805	0.093597
C	-3.110429	2.397012	-0.088269

C	-1.026398	3.688475	-0.267442
C	1.131173	2.521328	-0.323577
C	3.291285	1.342746	-0.443823
C	4.641836	3.813647	-0.509730
C	2.458560	4.991418	-0.462465
C	0.282604	6.177804	-0.442124
C	-1.785092	4.896261	-0.306796
C	-3.851471	3.597522	-0.160323
C	-5.932085	2.329016	-0.091234
C	-5.848271	-0.150874	0.012056
C	-5.778036	-2.627263	0.010907
C	-3.633535	-3.778823	-0.083206
C	-1.498653	-4.940475	-0.323664
C	0.634958	-6.085820	-0.563927
C	2.750015	-4.780678	-0.616532
C	4.869326	-3.489658	-0.670842
C	4.790292	-1.055912	-0.559584
C	4.706895	1.380891	-0.504897
C	2.699354	-2.355011	-0.497732
C	0.611158	-3.646343	-0.368617
C	-1.553578	-2.520713	-0.043778
C	-1.612375	0.010029	0.262865
C	-3.706107	-1.303116	0.081356
C	-3.789675	1.138244	-0.005631
C	-1.691434	2.447394	-0.142756
C	0.389373	3.724012	-0.331340
C	2.544721	2.556144	-0.406655
C	0.452910	1.272449	-0.203232
C	2.624937	0.095293	-0.421121
C	0.579342	-1.192547	-0.205163
C	-0.928621	1.260831	-0.067048
C	1.210258	0.042660	-0.265093
C	-0.827640	-1.267819	0.183423
H	6.441925	2.680553	-0.563839
H	5.154125	4.773831	-0.536637
H	2.979160	5.946966	-0.512747
H	0.802439	7.132282	-0.505188
H	-1.648894	7.062863	-0.423907
H	-3.753289	5.745209	-0.299080
H	-5.849868	4.449957	-0.195446
H	-7.020183	2.294181	-0.095903
H	-6.936832	-0.189107	-0.001436
H	-6.866369	-2.652437	0.013700
H	-5.581350	-4.740262	-0.092483

H	-3.417429	-5.905608	-0.284050
H	-1.239876	-7.088010	-0.531435
H	1.208883	-7.003842	-0.678435
H	3.311803	-5.709133	-0.710352
H	5.436672	-4.416153	-0.739723
H	6.596807	-2.254022	-0.687186
H	6.514026	0.214555	-0.586763
N	3.900110	0.158897	2.628112
C	2.635128	-0.019251	2.711312
N	1.667751	0.964130	2.803569
N	2.124814	-1.294366	2.777921
H	1.938089	1.874615	2.463996
H	0.721818	0.703545	2.554805
H	2.782982	-2.016120	2.528372
H	1.173956	-1.443806	2.475550
H	4.123030	1.151407	2.641031

Guanidine catalyst, Transition Structure

O	1.089305	-0.847170	1.618615
C	-2.606773	5.531549	-0.392054
C	-0.211547	5.123488	-0.290649
C	2.192294	4.716699	-0.191780
C	4.592666	4.305932	-0.124057
C	5.425544	1.969935	-0.107572
C	6.292483	-0.358301	-0.152632
C	4.743435	-2.233726	-0.201186
C	3.184233	-4.104735	-0.248298
C	1.618393	-5.966152	-0.292385
C	-0.827808	-5.532011	-0.315116
C	-3.273198	-5.133000	-0.418320
C	-4.107199	-2.844690	-0.473510
C	-4.936656	-0.552194	-0.544723
C	-5.772220	1.730526	-0.569583
C	-4.175350	3.617347	-0.477726
C	-1.781401	3.221550	-0.367012
C	0.632936	2.820047	-0.247623
C	3.041046	2.401511	-0.140652
C	3.883086	0.089585	-0.102108
C	2.342571	-1.821103	-0.102383
C	0.742058	-3.678029	-0.208790
C	-1.680822	-3.263536	-0.327789
C	-2.524291	-0.968000	-0.417473
C	-3.353157	1.333404	-0.461958
C	-6.010003	0.393436	-0.589651

C	-5.159827	-1.934865	-0.541971
C	-4.314754	-4.265067	-0.473366
C	-1.916480	-4.668981	-0.349529
C	0.499504	-5.067485	-0.265507
C	2.895759	-5.507680	-0.294023
C	4.488357	-3.605735	-0.247247
C	6.072007	-1.696560	-0.201517
C	5.206646	0.579692	-0.114938
C	4.381025	2.886265	-0.121607
C	3.551835	5.176110	-0.152835
C	1.108249	5.590320	-0.237592
C	-1.334722	6.008065	-0.335764
C	-2.875172	4.126782	-0.412337
C	-4.439097	2.247111	-0.504905
C	-0.453849	3.720852	-0.302807
C	1.954968	3.310125	-0.187602
C	2.798284	1.008877	-0.109511
C	1.216268	-0.894888	0.233448
C	3.645965	-1.327326	-0.134255
C	2.093592	-3.190265	-0.184851
C	-0.357085	-2.775970	-0.232691
C	-2.768336	-2.357123	-0.402306
C	-3.603530	-0.062229	-0.485193
C	-1.189341	-0.483585	-0.320426
C	-2.023929	1.822649	-0.388370
C	0.395834	1.417079	-0.234126
C	-0.128819	-1.383081	-0.193237
C	-0.939293	0.918360	-0.315954
C	1.469604	0.533706	-0.117188
H	-6.599603	2.437227	-0.597932
H	-7.030207	0.016730	-0.634163
H	-6.182327	-2.306427	-0.590059
H	-5.336798	-4.636169	-0.524456
H	-3.451408	-6.206928	-0.427002
H	-1.004542	-6.606885	-0.342852
H	1.418651	-7.035767	-0.325929
H	3.729548	-6.206847	-0.328119
H	5.325013	-4.302039	-0.283559
H	6.910629	-2.389688	-0.240168
H	7.309100	0.031083	-0.152720
H	6.451347	2.337402	-0.102511
H	5.616655	4.674986	-0.102066
H	3.733105	6.249424	-0.152463
H	1.289474	6.664097	-0.234381

H	-1.149795	7.080597	-0.322231
H	-3.450131	6.219110	-0.423210
H	-5.011887	4.314954	-0.506863
N	-3.105271	0.548542	2.601332
C	-1.911022	0.077125	2.693459
N	-1.548053	-1.251103	2.788204
N	-0.836423	0.925480	2.752544
H	-2.234920	-1.908191	2.450670
H	-0.587271	-1.448185	2.501815
H	-1.056130	1.889167	2.555457
H	0.050890	0.548939	2.414536
H	-3.783365	-0.210517	2.623355

Guanidine catalyst, Product

O	0.429871	-1.180361	1.415328
C	-2.032382	5.771547	-0.401139
C	0.309902	5.136045	-0.249293
C	2.669725	4.515204	-0.177134
C	5.026009	3.890904	-0.177922
C	5.651138	1.490675	-0.163995
C	6.293579	-0.908805	-0.198318
C	4.576050	-2.631440	-0.165469
C	2.842583	-4.351975	-0.160795
C	1.126502	-6.074996	-0.306805
C	-1.261217	-5.427292	-0.443118
C	-3.648317	-4.785051	-0.687557
C	-4.262536	-2.424944	-0.661569
C	-4.902180	-0.066748	-0.708537
C	-5.532510	2.284013	-0.736827
C	-3.781660	4.020249	-0.534826
C	-1.437803	3.398724	-0.306776
C	0.938254	2.768952	-0.142243
C	3.309592	2.135451	-0.122545
C	3.940975	-0.239864	-0.084655
C	2.228221	-2.005590	0.005216
C	0.443201	-3.718496	-0.132669
C	-1.907794	-3.086840	-0.367970
C	-2.548612	-0.694223	-0.407164
C	-3.166180	1.671669	-0.477144
C	-5.884367	0.976576	-0.799910
C	-5.234824	-1.415119	-0.765882
C	-4.598258	-3.817067	-0.755898
C	-2.265434	-4.458487	-0.501791
C	0.084562	-5.088609	-0.289202

C	2.435801	-5.725136	-0.247656
C	4.185999	-3.972319	-0.187575
C	5.948146	-2.222017	-0.214515
C	5.303736	0.128642	-0.144526
C	4.690396	2.494936	-0.153375
C	4.066233	4.848890	-0.185284
C	1.671270	5.479069	-0.216590
C	-0.720557	6.123366	-0.325177
C	-2.436152	4.400905	-0.410808
C	-4.163689	2.686744	-0.580954
C	-0.062680	3.767120	-0.223429
C	2.304073	3.134188	-0.139052
C	2.942323	0.771451	-0.068427
C	1.219954	-0.970301	0.243644
C	3.573804	-1.624239	-0.081624
C	1.837596	-3.346737	-0.065056
C	-0.566358	-2.750187	-0.141295
C	-2.908878	-2.067130	-0.469765
C	-3.535599	0.306455	-0.543133
C	-1.207866	-0.314349	-0.172572
C	-1.810994	2.033540	-0.316120
C	0.573387	1.391082	-0.069175
C	-0.235893	-1.354719	0.161730
C	-0.821020	1.019094	-0.160291
C	1.573641	0.428399	0.004850
H	-6.291837	3.061064	-0.805299
H	-6.928535	0.692631	-0.919010
H	-6.277411	-1.700221	-0.900599
H	-5.643804	-4.085038	-0.898333
H	-3.925004	-5.834190	-0.776142
H	-1.533062	-6.477396	-0.543210
H	0.841622	-7.122087	-0.393934
H	3.210259	-6.489214	-0.286975
H	4.951649	-4.744982	-0.245712
H	6.716281	-2.991643	-0.267286
H	7.341887	-0.617766	-0.237793
H	6.704852	1.764322	-0.198813
H	6.078826	4.167544	-0.191752
H	4.342101	5.901865	-0.205599
H	1.949344	6.532024	-0.240386
H	-0.432078	7.173055	-0.329725
H	-2.802987	6.537764	-0.466163
H	-4.543452	4.795178	-0.609346
N	-3.457976	0.666743	2.614012

C	-2.358174	0.050823	2.838235
N	-2.184303	-1.318318	2.879050
N	-1.217221	0.763939	3.144892
H	-2.858988	-1.873046	2.376203
H	-1.241954	-1.679957	2.866398
H	-1.344325	1.752841	2.982328
H	-0.361579	0.395576	2.748323
H	-4.222588	0.005803	2.493781

Thiourea catalyst, Reactant

O	-1.167039	-0.619426	1.394126
C	5.379048	-2.393761	-0.829085
C	3.286568	-3.634991	-0.726593
C	1.177597	-4.867176	-0.598746
C	-0.912835	-6.121132	-0.518819
C	-3.058567	-4.901610	-0.226749
C	-5.209329	-3.690795	-0.002612
C	-5.225739	-1.255873	0.088737
C	-5.265553	1.184952	0.025805
C	-5.295884	3.615625	-0.081543
C	-3.163420	4.881485	-0.240812
C	-1.043872	6.158067	-0.432009
C	1.076499	4.956498	-0.506397
C	3.196011	3.746578	-0.607527
C	5.312105	2.557285	-0.736030
C	5.339852	0.080106	-0.752918
C	3.260417	-1.166116	-0.625701
C	1.167309	-2.423831	-0.460538
C	-0.960634	-3.679943	-0.293654
C	-3.069042	-2.479771	0.009761
C	-3.140221	-0.004597	0.092538
C	-3.142361	2.452367	-0.080939
C	-1.039750	3.705826	-0.309455
C	1.094874	2.499612	-0.420341
C	3.229800	1.283021	-0.588967
C	4.621402	3.728717	-0.699723
C	2.462253	4.944508	-0.592145
C	0.309918	6.170798	-0.512072
C	-1.776966	4.927559	-0.326435
C	-3.862660	3.666379	-0.130699
C	-5.964024	2.435412	-0.013949
C	-5.922752	-0.046266	0.078952
C	-5.897181	-2.524127	0.071982
C	-3.776269	-3.714130	-0.069591

C	-1.667377	-4.914415	-0.350281
C	0.440697	-6.098296	-0.627373
C	2.577439	-4.831145	-0.726627
C	4.717545	-3.577734	-0.832580
C	4.683664	-1.142136	-0.734442
C	4.642717	1.296770	-0.692781
C	2.572097	-2.404418	-0.613613
C	0.464047	-3.658042	-0.442578
C	-1.673972	-2.493256	-0.079412
C	-1.679942	0.036814	0.223728
C	-3.801119	-1.237187	0.093468
C	-3.842227	1.205762	0.014882
C	-1.724654	2.476882	-0.171602
C	0.374465	3.715292	-0.408597
C	2.505868	2.508752	-0.536836
C	0.395832	1.263409	-0.289960
C	2.543005	0.047550	-0.540213
C	0.478170	-1.203099	-0.292205
C	-0.982044	1.276286	-0.120617
C	1.129709	0.020174	-0.365356
C	-0.921614	-1.252018	0.125979
H	6.398537	2.563711	-0.802397
H	5.149382	4.679814	-0.740035
H	2.998671	5.890475	-0.655633
H	0.845599	7.115659	-0.586509
H	-1.603735	7.091674	-0.442026
H	-3.728441	5.812349	-0.266208
H	-5.845628	4.554748	-0.113027
H	-7.052357	2.420482	0.008119
H	-7.011845	-0.064738	0.091893
H	-6.985435	-2.529994	0.099783
H	-5.740834	-4.640354	-0.034540
H	-3.601674	-5.844999	-0.268274
H	-1.450508	-7.067024	-0.554986
H	0.995844	-7.026830	-0.749592
H	3.120679	-5.769637	-0.829451
H	5.266947	-4.514268	-0.910474
H	6.464935	-2.372305	-0.902548
H	6.426407	0.099606	-0.823720
C	2.391787	-0.109912	2.683132
N	1.472227	0.878720	2.684911
N	1.891275	-1.360931	2.614848
H	1.819700	1.822138	2.623644
H	0.512696	0.691441	2.419714

H	2.547184	-2.118251	2.518425
H	0.908342	-1.530476	2.454080
S	4.030826	0.185464	2.775836

Thiourea catalyst, Transition Structure

O	1.153224	-0.800928	1.577531
C	-2.412464	5.592426	-0.508237
C	-0.027840	5.139704	-0.356338
C	2.363829	4.684236	-0.193779
C	4.752889	4.227274	-0.062021
C	5.540404	1.875652	-0.025009
C	6.364129	-0.467814	-0.049756
C	4.780652	-2.312793	-0.143194
C	3.189584	-4.154639	-0.241737
C	1.589976	-5.985041	-0.335332
C	-0.847068	-5.504611	-0.424704
C	-3.282208	-5.059181	-0.576279
C	-4.070381	-2.754697	-0.643872
C	-4.851293	-0.446923	-0.717327
C	-5.645100	1.850065	-0.724863
C	-4.014461	3.706915	-0.620207
C	-1.630431	3.266987	-0.476536
C	0.770510	2.819397	-0.297003
C	3.166457	2.352765	-0.120988
C	3.962627	0.025647	-0.063141
C	2.385665	-1.855550	-0.111944
C	0.756082	-3.681805	-0.276956
C	-1.656001	-3.220190	-0.464258
C	-2.450497	-0.910267	-0.569493
C	-3.235032	1.406746	-0.609423
C	-5.905905	0.517142	-0.755869
C	-5.102104	-1.825069	-0.720087
C	-4.305162	-4.170692	-0.646099
C	-1.917710	-4.621717	-0.485699
C	0.488091	-5.065174	-0.340225
C	2.875540	-5.551664	-0.299000
C	4.501750	-3.679896	-0.200625
C	6.118891	-1.801239	-0.106723
C	5.295732	0.490430	-0.039880
C	4.514004	2.812086	-0.066081
C	3.730127	5.117429	-0.117677
C	1.297915	5.579916	-0.267619
C	-1.133520	6.045121	-0.424949
C	-2.706976	4.192553	-0.537448

C	-4.303715	2.341065	-0.653979
C	-0.296567	3.741125	-0.379638
C	2.099603	3.283435	-0.197857
C	2.897577	0.965246	-0.096926
C	1.266683	-0.907961	0.190575
C	3.698864	-1.386391	-0.103166
C	2.114399	-3.219672	-0.209322
C	-0.324821	-2.757007	-0.338392
C	-2.722002	-2.293494	-0.558377
C	-3.510622	0.016205	-0.648667
C	-1.108580	-0.453501	-0.440032
C	-1.897917	1.872157	-0.510968
C	0.504965	1.421505	-0.295950
C	-0.072588	-1.371912	-0.288298
C	-0.831679	0.948029	-0.420743
C	1.559607	0.515216	-0.144202
H	-6.459658	2.571596	-0.747511
H	-6.932770	0.159323	-0.800415
H	-6.131874	-2.175090	-0.771839
H	-5.333675	-4.521555	-0.708418
H	-3.481554	-6.129365	-0.584965
H	-1.043239	-6.576032	-0.454590
H	1.370843	-7.050625	-0.375871
H	3.696211	-6.266895	-0.309885
H	5.326230	-4.391368	-0.214899
H	6.944522	-2.510612	-0.124639
H	7.387662	-0.098088	-0.022468
H	6.572475	2.223668	0.007591
H	5.782881	4.576521	-0.013393
H	3.932092	6.187014	-0.111954
H	1.500579	6.649794	-0.257292
H	-0.929184	7.114015	-0.404953
H	-3.242186	6.295571	-0.554132
H	-4.838185	4.419362	-0.654913
C	-1.873086	-0.133666	2.662002
N	-1.445150	-1.409251	2.607269
N	-0.891482	0.786481	2.619343
H	-2.146062	-2.127757	2.538465
H	-0.467521	-1.582116	2.359972
H	-1.174711	1.751937	2.599579
H	0.045631	0.482367	2.327197
S	-3.497051	0.280105	2.774920

Thiourea catalyst, Product

O	0.187287	-1.199137	1.346531
C	-0.328060	6.158630	-0.361233
C	1.770874	4.942835	-0.180005
C	3.890637	3.737762	-0.056504
C	6.007447	2.530798	0.010734
C	5.997406	0.050512	0.020022
C	6.005840	-2.433246	-0.017096
C	3.904910	-3.658396	-0.079950
C	1.791895	-4.877672	-0.193222
C	-0.296444	-6.101723	-0.470417
C	-2.429417	-4.861833	-0.703659
C	-4.562517	-3.625719	-1.018327
C	-4.557599	-1.189299	-0.929134
C	-4.580985	1.252720	-0.895608
C	-4.596322	3.686688	-0.846287
C	-2.464845	4.915305	-0.563126
C	-0.360369	3.712311	-0.313854
C	1.770615	2.492441	-0.109615
C	3.898662	1.272705	-0.017888
C	3.899762	-1.185230	0.014917
C	1.788924	-2.453988	0.004842
C	-0.364004	-3.651384	-0.267981
C	-2.461647	-2.435328	-0.593346
C	-2.473663	0.039019	-0.564537
C	-2.469692	2.485289	-0.557081
C	-5.263444	2.512561	-0.965242
C	-5.238613	0.036522	-1.018232
C	-5.231690	-2.445537	-1.081803
C	-3.150550	-3.667166	-0.777746
C	-1.051905	-4.881828	-0.478108
C	1.053288	-6.099757	-0.336371
C	3.187060	-4.854467	-0.148240
C	5.336861	-3.613891	-0.066321
C	5.312692	-1.177346	0.011573
C	5.325675	1.267032	0.006284
C	5.325591	3.702641	-0.015270
C	3.173284	4.925370	-0.106229
C	1.028241	6.161399	-0.254335
C	-1.068722	4.937442	-0.409471
C	-3.174712	3.725444	-0.650458
C	1.060711	3.714599	-0.194420
C	3.183377	2.495780	-0.054537
C	3.193041	0.047701	0.004702

C	1.067683	-1.195748	0.216345
C	3.190263	-2.429069	-0.016996
C	1.073419	-3.649519	-0.119618
C	-1.090577	-2.457497	-0.300723
C	-3.167239	-1.194147	-0.688488
C	-3.171482	1.261556	-0.678920
C	-1.089073	0.060809	-0.291982
C	-1.068257	2.487258	-0.366024
C	1.064510	1.252650	-0.078896
C	-0.428892	-1.197761	0.049580
C	-0.373541	1.250387	-0.225494
C	1.780779	0.065703	0.016958
H	-5.132782	4.632293	-0.901035
H	-6.341811	2.506263	-1.112801
H	-6.315004	0.029357	-1.182672
H	-6.305618	-2.433992	-1.259155
H	-5.093911	-4.566961	-1.147587
H	-2.955055	-5.805677	-0.843577
H	-0.833815	-7.039625	-0.599985
H	1.608094	-7.036141	-0.358013
H	3.731906	-5.796800	-0.190522
H	5.883769	-4.554563	-0.101063
H	7.094404	-2.420535	-0.011474
H	7.086574	0.045058	0.027330
H	7.095817	2.528577	0.035849
H	5.862411	4.649767	-0.011488
H	3.711938	5.872182	-0.101393
H	1.575015	7.102472	-0.230072
H	-0.874971	7.097900	-0.422738
H	-3.001274	5.860738	-0.632731
C	-2.835150	-0.139117	2.634185
N	-2.456885	-1.433002	2.616106
N	-1.831633	0.763250	2.717131
H	-3.182914	-2.121530	2.508645
H	-1.487197	-1.715645	2.578234
H	-2.090630	1.727006	2.575847
H	-0.882714	0.486074	2.498060
S	-4.439695	0.312746	2.575834

C54H18···Diol

C	5.632868	-2.220335	-0.490585
C	4.991225	0.128038	-0.481170
C	4.352801	2.483875	-0.447950
C	3.720854	4.834482	-0.395482

C	1.324179	5.462578	-0.322120
C	-1.069306	6.102162	-0.240841
C	-2.781687	4.371583	-0.210715
C	-4.501580	2.640259	-0.167648
C	-6.220121	0.916838	-0.113187
C	-5.565613	-1.473722	-0.142598
C	-4.922225	-3.867375	-0.159662
C	-2.568551	-4.484368	-0.239580
C	-0.210143	-5.108260	-0.312287
C	2.141011	-5.736252	-0.376440
C	3.882642	-3.974436	-0.439619
C	3.254475	-1.623818	-0.447075
C	2.615796	0.748003	-0.440535
C	1.969641	3.117524	-0.383810
C	-0.398386	3.744128	-0.300879
C	-2.132423	2.004963	-0.264156
C	-3.859342	0.259458	-0.207544
C	-3.217692	-2.105596	-0.230861
C	-0.845546	-2.737715	-0.313041
C	1.528935	-3.360761	-0.383189
C	0.831008	-6.091775	-0.334682
C	-1.562469	-5.452188	-0.265511
C	-3.959064	-4.824417	-0.188831
C	-4.591805	-2.473800	-0.177636
C	-5.230927	-0.118331	-0.154696
C	-5.873128	2.229861	-0.119162
C	-4.122484	3.984031	-0.167920
C	-2.379532	5.746322	-0.204500
C	-0.028876	5.118880	-0.288893
C	2.329444	4.494898	-0.366742
C	4.683766	3.877574	-0.433307
C	5.326768	1.484142	-0.476692
C	5.981240	-0.907529	-0.499220
C	4.260590	-2.630370	-0.460512
C	2.541888	-4.361240	-0.401347
C	3.618355	-0.249957	-0.461891
C	2.977166	2.115175	-0.427320
C	0.604755	2.747975	-0.351600
C	-1.123654	1.001330	-0.314465
C	-1.769419	3.371880	-0.260334
C	-3.496176	1.633340	-0.214423
C	-2.857755	-0.738126	-0.248309
C	-2.209827	-3.106995	-0.262194
C	0.158142	-3.733430	-0.337440

C	-0.481602	-1.361250	-0.338059
C	1.890760	-1.994492	-0.408749
C	1.241933	0.374818	-0.408464
C	-1.484659	-0.365185	-0.304440
C	0.881414	-0.991174	-0.388983
C	0.240464	1.370964	-0.363472
H	2.916876	-6.499872	-0.391058
H	0.547751	-7.142834	-0.315687
H	-1.840534	-6.505247	-0.246692
H	-4.231846	-5.878268	-0.172511
H	-5.973514	-4.147516	-0.119784
H	-6.616083	-1.759094	-0.101598
H	-7.268705	0.626561	-0.074337
H	-6.641061	3.000839	-0.085172
H	-4.894351	4.751794	-0.130952
H	-3.154620	6.510004	-0.167792
H	-0.785450	7.153191	-0.233429
H	1.603273	6.515470	-0.311174
H	3.994577	5.888165	-0.384492
H	5.735658	4.157706	-0.452566
H	6.378013	1.769223	-0.492586
H	7.030505	-0.617759	-0.519162
H	6.401091	-2.991726	-0.503407
H	4.655320	-4.742184	-0.451226
H	0.914738	-1.400628	3.820259
O	0.270570	-0.760403	4.144315
C	0.301994	0.290444	3.223287
C	1.724033	0.705339	2.932143
H	-0.183382	0.013472	2.270544
H	-0.258023	1.135155	3.643639
O	2.376742	-0.461647	2.484650
H	2.191281	1.089780	3.854043
H	1.743736	1.506335	2.174707
H	3.291307	-0.263976	2.270756

C54H18···Guanidine

C	5.032909	-3.746191	-0.063622
C	5.074675	-1.312050	-0.077927
C	5.120593	1.128562	-0.080459
C	5.170917	3.562860	-0.069278
C	3.045932	4.837508	-0.146582
C	0.926698	6.121863	-0.208884
C	-1.200271	4.939466	-0.293530
C	-3.334559	3.758109	-0.365487

C	-5.466934	2.585129	-0.415354
C	-5.506518	0.106526	-0.433321
C	-5.559118	-2.371262	-0.433714
C	-3.470895	-3.621356	-0.384471
C	-1.383267	-4.881256	-0.307584
C	0.696598	-6.143558	-0.216476
C	2.861778	-4.939464	-0.145252
C	2.919000	-2.507328	-0.167870
C	2.970466	-0.051685	-0.180302
C	3.011909	2.404655	-0.171020
C	0.913423	3.669876	-0.244307
C	-1.236776	2.484978	-0.336699
C	-3.381912	1.292420	-0.399682
C	-3.427388	-1.157595	-0.408350
C	-1.328597	-2.428143	-0.344040
C	0.774690	-3.692271	-0.246789
C	-0.660352	-6.116958	-0.265705
C	-2.777468	-4.832719	-0.350214
C	-4.901552	-3.559342	-0.414562
C	-4.850494	-1.126383	-0.427377
C	-4.805435	1.314057	-0.417688
C	-4.766843	3.748776	-0.391672
C	-2.595898	4.942715	-0.330037
C	-0.430602	6.146906	-0.252443
C	1.651478	4.886350	-0.199884
C	3.741136	3.626633	-0.129752
C	5.827305	2.373983	-0.046009
C	5.775164	-0.104504	-0.049855
C	5.734179	-2.583251	-0.041000
C	3.602015	-3.755787	-0.125993
C	1.466664	-4.935905	-0.202633
C	3.652631	-1.290477	-0.143532
C	3.698809	1.160386	-0.145929
C	1.598888	2.432479	-0.232392
C	-0.548424	1.238154	-0.334644
C	-0.507079	3.695420	-0.293564
C	-2.649846	2.510048	-0.371194
C	-2.699240	0.054188	-0.399717
C	-2.740696	-2.400727	-0.383229
C	-0.644946	-3.664438	-0.301386
C	-0.594384	-1.209479	-0.338052
C	1.506048	-2.482083	-0.230620
C	1.548071	-0.025362	-0.248981
C	-1.276682	0.027711	-0.370904

C	0.817730	-1.235925	-0.276519
C	0.864516	1.212722	-0.278021
H	1.226499	-7.094014	-0.183636
H	-1.227874	-7.046081	-0.272025
H	-3.340462	-5.765267	-0.351516
H	-5.458573	-4.494782	-0.417251
H	-6.647424	-2.345198	-0.452356
H	-6.595657	0.127051	-0.447927
H	-6.555497	2.600020	-0.433443
H	-5.288855	4.704283	-0.390555
H	-3.123107	5.896040	-0.328480
H	-0.961712	7.097332	-0.256375
H	1.492585	7.051479	-0.177755
H	3.607618	5.770301	-0.114203
H	5.728164	4.497711	-0.040621
H	6.914714	2.348046	0.001449
H	6.863151	-0.125289	0.000110
H	6.821679	-2.599040	0.007535
H	5.553542	-4.701927	-0.033339
H	3.387240	-5.893120	-0.112045
C	-1.494334	-0.122553	2.780759
N	-2.012667	1.157836	2.727264
N	-0.115708	-0.138191	2.876586
H	-3.014872	1.240858	2.796175
H	-1.501012	1.882402	3.209424
H	0.259064	-1.065718	2.731271
H	0.363998	0.564348	2.329005
N	-2.147969	-1.217740	2.725848
H	-3.151072	-1.049347	2.751174

C54H18···Thiourea

C	-0.793354	-6.133097	-0.265676
C	1.309519	-4.910873	-0.350049
C	3.420924	-3.689250	-0.421697
C	5.531668	-2.474911	-0.468264
C	5.524128	0.004669	-0.482807
C	5.527063	2.484253	-0.469433
C	3.414104	3.694634	-0.423061
C	1.300570	4.912432	-0.351093
C	-0.804389	6.130917	-0.266292
C	-2.945852	4.885118	-0.219236
C	-5.092672	3.649566	-0.154561
C	-5.085269	1.215260	-0.175460
C	-5.083070	-1.225077	-0.175122

C	-5.086119	-3.659413	-0.153831
C	-2.937063	-4.891141	-0.218390
C	-0.828522	-3.681275	-0.314388
C	1.297329	-2.455470	-0.405878
C	3.421836	-1.222966	-0.464589
C	3.419553	1.228318	-0.465237
C	1.292851	2.456979	-0.406451
C	-0.835163	3.679009	-0.315146
C	-2.954389	2.452205	-0.256346
C	-2.956489	-0.003008	-0.274635
C	-2.950005	-2.458239	-0.255681
C	-5.765848	-2.483715	-0.137283
C	-5.762370	-0.005511	-0.148360
C	-5.770309	2.472682	-0.137816
C	-3.662016	3.686600	-0.211197
C	-1.550802	4.908531	-0.266999
C	0.553239	6.133454	-0.305543
C	2.696307	4.891744	-0.384298
C	4.846039	3.659275	-0.445501
C	4.844078	1.224641	-0.475239
C	4.846367	-1.216551	-0.474596
C	4.852820	-3.651195	-0.443952
C	2.705252	-4.887655	-0.382898
C	0.564301	-6.133229	-0.304765
C	-1.541970	-4.912066	-0.266206
C	-3.655403	-3.693897	-0.210405
C	0.591772	-3.680808	-0.357694
C	2.712022	-2.454599	-0.434795
C	2.712569	0.002013	-0.464773
C	0.581463	1.223585	-0.410187
C	2.707501	2.458659	-0.435700
C	0.585091	3.681058	-0.358441
C	-1.541440	2.454011	-0.313364
C	-3.663244	1.221238	-0.238188
C	-3.661045	-1.228518	-0.237810
C	-1.535334	-0.001722	-0.340776
C	-1.537043	-2.457535	-0.312591
C	0.583642	-1.223393	-0.410030
C	-0.830454	1.222362	-0.361456
C	-0.828268	-1.224574	-0.360763
C	1.288615	0.000742	-0.442746
H	-5.624021	-4.605381	-0.121172
H	-6.853584	-2.479022	-0.091198
H	-6.850594	-0.006472	-0.099549

H	-6.858028	2.466073	-0.091609
H	-5.632231	4.594592	-0.121909
H	-3.490465	5.827802	-0.182862
H	-1.353857	7.070163	-0.230740
H	1.101414	7.074055	-0.301873
H	3.240392	5.835394	-0.376570
H	5.384941	4.605277	-0.440031
H	6.615675	2.480587	-0.483277
H	6.613389	0.005662	-0.491286
H	6.620270	-2.469287	-0.482116
H	5.393491	-4.596181	-0.438217
H	3.251010	-5.830331	-0.375079
H	1.114101	-7.072874	-0.301318
H	-1.341160	-7.073329	-0.230481
H	-3.480007	-5.834791	-0.182119
C	1.350186	0.002001	2.759898
N	2.067766	1.143796	2.661468
N	2.053099	-1.149123	2.664080
H	1.540255	2.000879	2.610279
H	3.012077	1.151577	2.303776
H	1.514897	-1.999542	2.612648
H	2.998444	-1.169728	2.309784
S	-0.293744	0.012785	3.020804

Table S4. Absolute electronic (E_e), enthalpic at 0 K (H_0), enthalpic at 298 K (H_{298}), and Gibbs at 298 K (G_{298}) energies for the species considered in this work (in a.u.).

	PW6B95-D3BJ Def2-SVP E_e	PW6B95-D3BJ Def2-SVP H_0	PW6B95-D3BJ Def2-SVP H_{298}	PW6B95-D3BJ Def2-SVP G_{298}	PW6B95-D3BJ Def2-QZVPP E_e	DSD-PBEP86-D3BJ Def2-QZVPP E_e
Ethylene glycol	-230.340286	-230.253607	-230.247779	-230.280648	-230.635094	-230.016747
Guanidine	-205.465126	-205.388470	-205.383008	-205.414805	-205.724288	-205.145390
Thiourea	-548.492983	-548.431530	-548.425686	-548.459050	-548.830297	-547.776815
C54H18_d6h.log	-2070.390089	-2069.843968	-2069.814587	-2069.895866	-2072.644094	-2066.165342
Uncat, reac	-2145.537454	-2144.989412	-2144.959125	-2145.044258	-2147.887073	-2141.225412
Uncat, TS	-2145.483907	-2144.937247	-2144.906974	-2144.992271	-2147.840095	-2141.179385
Uncat, prod	-2145.537491	-2144.989407	-2144.959125	-2145.044249	-2147.887099	-2141.225611
NH3, reac	-2202.118427	-2201.533621	-2201.499292	-2201.594498	-2204.545449	-2197.728807
NH3, TS	-2202.072259	-2201.489085	-2201.455059	-2201.549099	-2204.504955	-2197.690136
NH3, prod	-2202.117661	-2201.533569	-2201.499120	-2201.595337	-2204.544810	-2197.728137
H2O, reac	-2221.989727	-2221.417446	-2221.383685	-2221.476391	-2224.443611	-2217.596700
H2O, TS	-2221.947629	-2221.376868	-2221.343498	-2221.435280	-2224.408254	-2217.563073
H2O, prod	-2221.990193	-2221.417674	-2221.383903	-2221.477180	-2224.445224	-2217.598870
HF, reac	-2246.013571	-2245.452988	-2245.420207	-2245.511503	-2248.500268	-2241.616601
HF, TS	-2245.978715	-2245.419838	-2245.387592	-2245.477314	-2248.470138	-2241.589241
HF, prod	-2246.013912	-2245.452872	-2245.420167	-2245.511471	-2248.500360	-2241.618475
2H2O, reac	-2298.448843	-2297.851423	-2297.814832	-2297.913301	-2301.005893	-2293.974479
2H2O, TS	-2298.413080	-2297.816199	-2297.779954	-2297.877925	-2300.976753	-2293.946398
2H2O, prod	-2298.451171	-2297.853455	-2297.817069	-2297.915263	-2301.007540	-2293.975996
Diol, reac	-2375.899793	-2375.263278	-2375.226528	-2375.326696	-2378.535306	-2371.257566
Diol, TS	-2375.873196	-2375.237771	-2375.201746	-2375.299859	-2378.510177	-2371.235075
Diol, prod	-2375.899663	-2375.263935	-2375.226961	-2375.327708	-2378.536007	-2371.258290
Guanidine, reac	-2351.027344	-2350.401735	-2350.365109	-2350.464260	-2353.627392	-2346.387330
Guanidine, TS	-2350.993006	-2350.368231	-2350.332296	-2350.429602	-2353.596416	-2346.359628
Guanidine, prod	-2351.027861	-2350.401465	-2350.365027	-2350.464463	-2353.627512	-2346.389377
Thiourea, reac	-2694.061152	-2693.449638	-2693.412926	-2693.513137	-2696.738951	-2689.026299
Thiourea, TS	-2694.029910	-2693.420113	-2693.383881	-2693.483038	-2696.711525	-2689.002551
Thiourea, prod	-2694.062595	-2693.451115	-2693.414423	-2693.514213	-2696.739679	-2689.027434
C54H18•••Diol	-2300.746844	-2300.112922	-2300.076842	-2300.176192	-2303.290500	-2296.193360
C54H18•••Guanidine	-2275.875813	-2275.252150	-2275.216621	-2275.313446	-2278.382209	-2271.325220
C54H18•••Thiourea	-2618.907349	-2618.298443	-2618.262523	-2618.360902	-2621.491668	-2613.960983