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

Supplementary Information for:

Strong Bases Behave as Weak Bases in Nanoscale Chemical Environments: Implication in Humidity-swing CO_2 Air Capture

Yingying Han[1], Liangliang Zhu[1], Yutong Yao[2], Xiaoyang Shi[2], Yayun Zhang[3], Hang Xiao[1], Xi Chen[2]*

[1] Shaanxi Institute of Energy and Chemical Engineering, School of Chemical Engineering, Northwest University, Xi'an, 710069, China

[2] Earth Engineering Center, Center for Advanced Materials for Energy and Environment, Department of Earth and Environmental Engineering, Columbia University, New York, NY10027, USA

[3] State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai, 200237, China

* E-mail: xiaohang07@nwu.edu.cn (H. X.)

1. Model snapshots

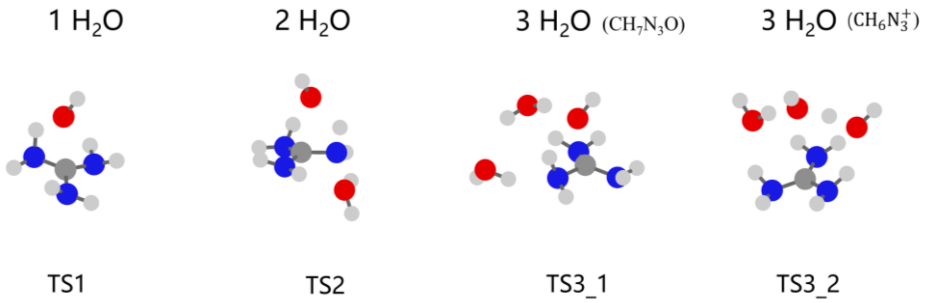

Figure S1: Model snapshots of transition states of the guanidine-H_2O reaction (n=1-3)

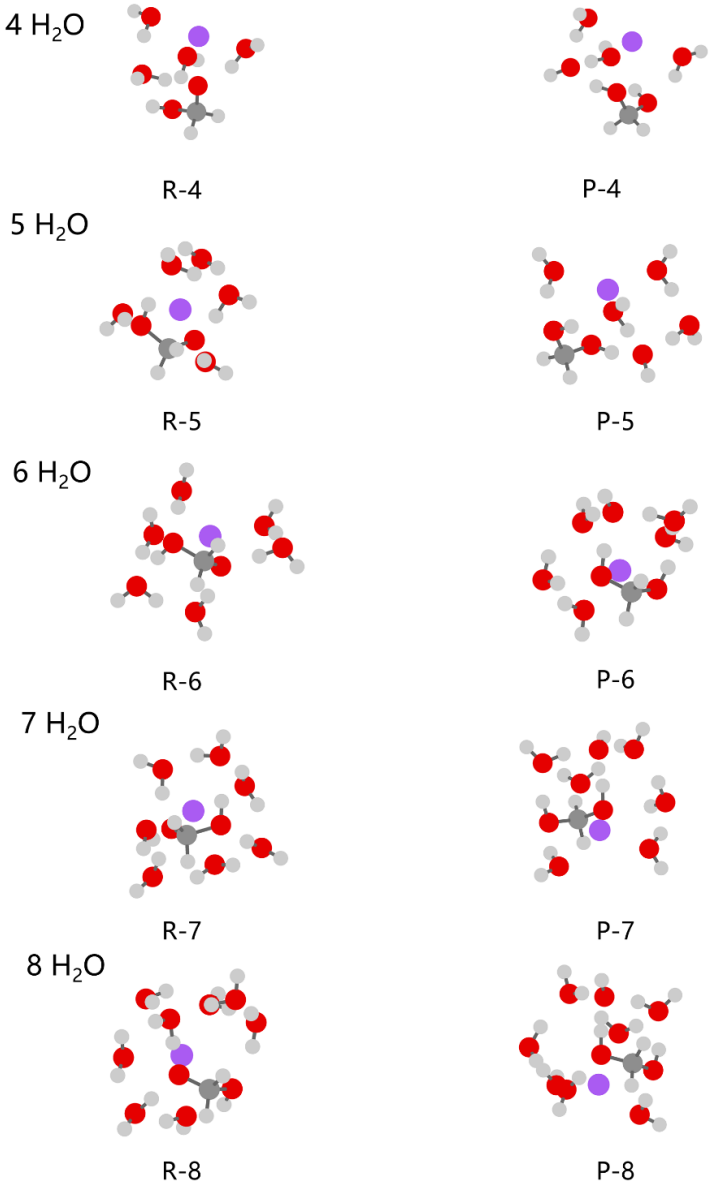

Figure S2: Model snapshots of reactants and products of the $CH_3O_2^-$-H_2O reaction (n = 4-8).

2. Structure files (xyz format)

2.1 Structure files (xyz format) of reactants and products of the guanidine-H_2O reaction (*n*=1-8)

Reactants: CH_5N_3+1H_2O

C	0.71856	-0.06791	0.02398
N	-0.02475	-1.11244	0.06416
H	0.51015	-1.97058	0.06945
N	0.16811	1.18571	0.13346
N	2.09564	-0.05836	-0.13672
H	-0.84382	1.18653	0.06769
H	0.61771	1.90485	-0.40700
H	2.57650	0.68541	0.34190
H	2.54284	-0.95084	-0.01891
O	-2.55612	0.02585	-0.14456
H	-3.12254	-0.14725	0.60566
H	-1.81621	-0.61191	-0.07248

Reactants:CH_5N_3+2H_2O

C	1.28169	0.03843	-0.02357
N	2.65874	-0.01952	0.14146
N	0.68002	-1.18303	-0.03034
N	0.60430	1.12467	-0.15158
H	3.14363	0.84281	-0.03632
H	3.10702	-0.81259	-0.28688
H	-0.33773	-1.20895	-0.02051
H	1.12562	-1.90504	0.50726
H	1.20124	1.93561	-0.24729
O	-2.12569	1.37585	0.00576
H	-1.13719	1.34321	-0.05943
H	-2.31903	1.82192	0.82907

O	-2.25085	-1.33665	0.04808
H	-2.37190	-0.36534	0.04842
H	-2.69089	-1.65075	-0.74045

Reactants:CH_5N_3+3H_2O

C	-0.15930	-1.29508	0.03859
N	0.96198	-1.77861	-0.59828
N	0.07735	-0.74187	1.26490
N	-1.37031	-1.38279	-0.40493
H	0.84937	-1.92638	-1.58568
H	1.82149	-1.29970	-0.36895
H	-0.70935	-0.24655	1.65033
H	0.96592	-0.27587	1.37608
H	-1.41720	-1.87639	-1.28630
O	2.39461	0.76958	0.22604
H	1.65096	1.32250	-0.08343
H	3.07762	1.37191	0.51552
O	-2.20084	1.08621	0.28409
H	-3.11331	1.35160	0.19001
H	-2.12132	0.14560	-0.02582
O	0.16893	2.18959	-0.59054
H	0.06144	2.29955	-1.53417
H	-0.69451	1.86410	-0.26771

Reactants:CH_5N_3+4H_2O

C	-0.40118	-1.35026	-0.12885
N	-1.68532	-1.70640	0.20976
N	-0.30779	-0.53570	-1.21886
N	0.66714	-1.78024	0.46017
H	-1.78989	-2.11575	1.12068
H	-2.40072	-1.02883	-0.01789
H	0.58369	-0.08661	-1.34303

H	-1.09923	0.06457	-1.39637
H	0.45759	-2.42844	1.20699
O	1.68766	1.83387	-0.45796
H	2.27313	1.07486	-0.23312
H	2.23761	2.61569	-0.46087
O	-0.55659	1.81652	1.15444
H	-0.34849	1.15216	1.81156
H	0.23738	1.86194	0.58651
O	-2.69791	1.02460	-0.36111
H	-2.00363	1.40583	0.21305
H	-3.34472	1.71105	-0.51245
O	2.96628	-0.43340	0.14598
H	2.16692	-1.02113	0.27899
H	3.52383	-0.88024	-0.48923

Reactants:CH_5N_3+$5H_2O$

C	-0.18232	-1.31216	-0.12384
N	-1.31876	-2.03523	-0.37139
N	-0.16440	-0.64679	1.05545
N	0.85425	-1.27579	-0.91375
H	-1.45011	-2.32313	-1.32398
H	-2.16033	-1.71170	0.08757
H	0.56625	0.03819	1.18686
H	-1.05923	-0.42694	1.46695
H	0.72849	-1.86825	-1.72363
O	3.33234	-0.59889	0.02586
H	2.47215	-0.91254	-0.35893
H	3.64492	-1.31232	0.58064
O	-3.07732	-0.11569	0.98929
H	-2.81787	0.62701	0.40538
H	-3.78422	0.20102	1.54817

O	2.05968	1.48643	1.12029
H	2.53728	2.09556	1.68022
H	2.69852	0.80868	0.80819
O	-2.09539	1.83598	-0.61834
H	-1.13607	1.77122	-0.82957
H	-2.51630	2.15394	-1.41520
O	0.52915	1.62769	-1.25605
H	0.71332	0.67861	-1.35689
H	1.07190	1.87407	-0.49333

Reactants:CH_5N_3+6H_2O

C	0.27503	-1.35366	-0.50331
N	1.32306	-0.94273	-1.16744
H	1.32868	-1.31140	-2.10895
N	0.12513	-1.03396	0.79713
N	-0.70270	-2.15300	-1.02900
H	0.76587	-0.37241	1.21161
H	-0.77521	-1.17588	1.22722
H	-1.58795	-2.16292	-0.53751
H	-0.76522	-2.17226	-2.03008
O	2.17728	0.99533	1.75711
H	2.50503	1.22542	2.62451
H	2.89241	0.50959	1.29030
O	-2.78818	-1.52285	0.94863
H	-3.51155	-1.97881	1.37454
H	-3.10233	-0.61725	0.73989
O	-3.48178	1.01536	0.31142
H	-2.74801	1.48096	-0.14363
H	-3.73458	1.59405	1.02958
O	3.71813	-0.45664	0.11656
H	4.25507	0.05908	-0.48432

H	2.90526	-0.69939	-0.39546
O	-1.49520	2.42611	-0.84863
H	-1.62419	2.86149	-1.68922
H	-0.53323	2.22447	-0.78873
O	1.13781	1.88195	-0.74327
H	1.46876	1.90528	0.16403
H	1.24811	0.94589	-1.00333

Reactants:CH_5N_3+7H_2O

C	-0.56928	1.54257	0.16095
N	0.52896	1.63431	0.87031
H	0.42654	2.32295	1.60478
N	-0.60894	0.77382	-0.94174
N	-1.70870	2.24711	0.43004
H	0.14986	0.13741	-1.14083
H	-1.51360	0.54516	-1.32557
H	-2.56307	1.90409	0.00967
H	-1.80353	2.59051	1.36793
O	2.98990	1.80103	-0.45326
H	2.11072	1.79649	-0.01187
H	2.86074	2.24295	-1.29128
O	-0.37872	-2.40857	0.50501
H	0.04707	-2.27756	-0.35606
H	0.20482	-1.93843	1.12034
O	1.48770	-0.76325	1.84129
H	1.16076	0.11914	1.52702
H	1.63099	-0.68647	2.78357
O	1.13074	-1.53657	-1.71211
H	2.00737	-1.38461	-1.27824
H	1.30435	-1.93663	-2.56238
O	-3.53407	0.43238	-0.99484

H	-3.43675	-0.35273	-0.41495
H	-4.26815	0.26560	-1.58245
O	-2.91789	-1.56744	0.69090
H	-1.98007	-1.85920	0.60556
H	-3.41747	-2.35161	0.91091
O	3.31351	-0.95132	-0.32140
H	2.91542	-1.04322	0.55580
H	3.37111	0.01396	-0.44257

Reactants:CH_5N_3+$8H_2O$

C	-0.21579	-0.27409	-1.42370
N	-1.50993	-0.26261	-1.83136
N	0.45941	0.89049	-1.54722
N	0.39111	-1.34891	-0.97772
H	-2.08799	-1.02163	-1.49081
H	-1.95440	0.63938	-1.90866
H	1.38606	0.95867	-1.15538
H	-0.07697	1.74069	-1.62180
H	-0.23300	-2.14612	-1.02126
O	3.07245	-1.53044	-0.69239
H	3.50933	-1.91424	-1.45136
H	2.09497	-1.52812	-0.89954
O	-1.90218	-0.96303	1.91500
H	-0.99123	-1.23934	2.08626
H	-1.83107	-0.02516	1.68609
O	3.15032	1.11216	-0.16440
H	3.95744	1.56812	-0.39552
H	3.29679	0.15559	-0.33115
O	-1.34384	1.85036	1.39608
H	-0.36446	1.75369	1.51462
H	-1.64929	2.32081	2.17189

O	-2.57556	-2.45876	-0.26866
H	-2.40662	-1.95806	0.55606
H	-3.36677	-2.97261	-0.11868
O	-1.87548	2.65839	-1.18742
H	-1.77314	2.48290	-0.23376
H	-2.24505	3.53489	-1.27519
O	1.22327	1.39020	1.89767
H	1.18831	0.42416	2.00975
H	1.91923	1.51109	1.23605
O	0.89479	-1.34744	1.73334
H	1.62905	-1.94040	1.89359
H	0.75925	-1.34403	0.75132

Products: CH_7N_3O+0H_2O

C	-0.00395	-0.00521	-0.00762
N	-1.21342	-0.33392	-0.73319
H	-1.97551	-0.48640	-0.08854
H	-1.45449	0.41258	-1.36858
N	1.20842	-0.49118	-0.63125
H	1.03999	-1.43173	-0.96291
H	1.42860	0.08350	-1.43332
N	0.15350	1.42969	0.11334
H	1.01987	1.64190	0.59133
H	-0.60705	1.80268	0.66521
O	-0.15029	-0.67566	1.22911
H	0.73510	-0.81820	1.56742

Products: CH_7N_3O+1H_2O

C	0.60635	0.00804	0.00139
N	0.44737	-1.14284	-0.86431
H	-0.53674	-1.34324	-1.00076
H	0.86584	-1.94875	-0.41937

N	-0.11680	1.09773	-0.65775
H	0.13154	1.95596	-0.18174
H	0.20569	1.17213	-1.61418
N	2.00230	0.32200	0.20948
H	2.33874	-0.15077	1.03647
H	2.54710	0.02742	-0.58827
O	-2.51553	-0.13085	0.05631
H	-3.32480	0.32763	0.27593
H	-1.91280	0.52302	-0.34958
O	0.08829	-0.15196	1.29478
H	-0.86482	-0.28743	1.21254

Products: $CH_7N_3O+2H_2O$

C	-1.05107	0.02340	-0.00960
N	-0.80518	-0.36462	1.36371
H	0.19053	-0.43645	1.53715
H	-1.20522	-1.27984	1.52266
N	-0.39121	1.32531	-0.17608
H	-0.66865	1.67433	-1.08590
H	-0.76526	1.96402	0.51614
N	-2.46882	0.11778	-0.28749
H	-2.81203	-0.78138	-0.59474
H	-2.96769	0.39676	0.54557
O	2.38727	1.22644	0.09731
H	2.81172	1.73808	-0.58972
H	1.41419	1.34010	-0.03037
O	-0.55907	-0.85694	-0.97344
H	0.34163	-1.12036	-0.72019
O	1.99876	-1.44718	0.00939
H	2.63595	-2.01928	-0.41465
H	2.37200	-0.54421	0.00458

Products: $CH_6N_3^+ + OH^- + 3H_2O$

C	0.15806	-1.34222	0.16654
N	1.31201	-1.98693	-0.12585
N	0.16179	-0.38399	1.07149
N	-0.98156	-1.72660	-0.40955
H	1.29862	-2.65150	-0.87777
H	2.14650	-1.41273	-0.05531
H	-0.53105	0.43906	0.96723
H	1.08198	-0.11571	1.38675
H	-0.93160	-2.29154	-1.23646
O	-3.10656	0.03834	-0.32076
H	-3.81493	0.00930	0.31993
H	-1.83543	-1.15927	-0.28709
O	0.96739	2.16464	-0.72861
H	0.79788	2.39123	-1.64085
H	0.06313	2.04464	-0.29239
O	-1.27505	1.66791	0.46239
H	-2.49470	0.78693	-0.03053
H	-1.51849	2.33736	1.09922
O	2.85021	0.42493	0.07302
H	3.64907	0.90447	0.28279
H	2.20703	1.08711	-0.27573

Products: $CH_6N_3^+ + OH^- + 4H_2O$

C	-0.13911	-1.21063	-0.64189
N	-1.47219	-1.22886	-0.73032
N	0.58150	-0.68389	-1.63639
N	0.46749	-1.78813	0.39677
H	-1.95111	-1.33729	0.15622
H	-1.86155	-0.50775	-1.32740
H	1.56065	-0.52387	-1.43657

H	0.10693	0.02986	-2.17536
H	-0.09112	-1.82910	1.24177
O	2.90955	-0.32628	0.04535
H	1.44741	-1.55371	0.51397
H	3.83127	-0.30540	0.29408
O	-1.39520	1.40343	-1.75602
H	-1.27391	1.53117	-0.75699
H	-1.88164	2.15468	-2.08754
O	1.56900	1.79275	0.85358
H	1.71405	2.56771	0.31277
H	2.48605	0.50152	0.39294
O	-1.61314	-0.72409	2.03961
H	-2.01069	-0.57979	2.89508
H	-1.38944	0.18205	1.64683
O	-0.98089	1.47261	0.80097
H	0.55852	1.66033	0.86337
H	-1.36286	2.23212	1.23994

Products: $CH_6N_3^+ + OH^- + 5H_2O$

C	0.63027	0.65342	-1.22384
N	-0.65348	0.77943	-1.55615
N	1.25900	1.68254	-0.64491
N	1.30296	-0.45691	-1.53593
H	-1.19293	-0.05855	-1.71799
H	-1.15813	1.51330	-1.06971
H	2.10503	1.44720	-0.14262
H	0.65185	2.36624	-0.20462
H	0.74894	-1.31551	-1.56369
O	2.98750	-0.11125	0.82601
H	2.19854	-0.55850	-1.07873
H	3.73263	-0.27584	1.40021

O	-1.14231	2.59256	0.58270
H	-1.29578	1.71406	1.06458
H	-1.76417	3.22972	0.92635
O	0.64501	-1.20309	1.66710
H	0.61087	-1.69638	2.48576
H	2.19546	-0.50670	1.25217
O	-2.59986	-1.02456	-0.41827
H	-3.50876	-1.26081	-0.24528
H	-2.25043	-0.54525	0.39519
O	-1.44063	0.22654	1.55213
H	-0.19153	-0.59164	1.66585
H	-1.89745	0.20269	2.39208
O	-0.31710	-2.60767	-0.66154
H	-1.23046	-2.28056	-0.63355
H	0.04443	-2.31967	0.19093

Products: $CH_6N_3^+ + OH^- + 6H_2O$

C	0.80099	-0.82163	-1.21399
N	-0.37382	-0.52436	-1.76443
N	1.88788	-0.12897	-1.59528
N	0.91788	-1.83759	-0.36811
H	-1.23751	-0.89486	-1.37861
H	-0.46152	0.40196	-2.15139
H	2.69406	-0.21690	-0.98734
H	1.69610	0.80781	-1.91673
H	0.06538	-2.14442	0.11584
O	1.51718	1.38330	1.34248
H	1.78123	-1.87864	0.15630
H	1.19195	1.79452	0.52649
O	0.18578	2.29037	-1.06526
H	-0.70231	2.06309	-0.61529

H	0.16281	3.22911	-1.24473
O	-0.94723	0.43215	2.16906
H	-1.34239	0.73600	2.98491
H	0.71091	1.04170	1.77043
O	-3.00036	-0.67500	-0.65897
H	-3.86499	-0.61938	-1.05973
H	-2.72364	0.25375	-0.36823
O	-1.97290	1.55297	0.10896
H	-1.41535	0.92362	1.40895
H	-2.57590	2.27049	0.29795
O	-1.44308	-2.13834	1.12852
H	-2.19391	-1.86415	0.58201
H	-1.26509	-1.34643	1.66320
O	3.27312	-0.57298	0.85742
H	2.68576	0.16507	1.14674
H	4.06482	-0.53584	1.39024

Products: $CH_6N_3^+ + OH^- + 7H_2O$

C	-0.86927	-0.14923	-1.44886
N	-1.11370	-1.46216	-1.34901
N	-1.89589	0.71452	-1.46002
N	0.36715	0.29015	-1.60659
H	-0.35009	-2.05651	-1.03297
H	-2.01199	-1.69807	-0.95046
H	-1.67554	1.65474	-1.13108
H	-2.76083	0.34960	-1.08503
H	1.17428	-0.33701	-1.53487
O	-1.06679	2.79188	0.29414
H	0.56507	1.27794	-1.53732
H	-1.14553	2.05370	0.91843
O	-1.47690	0.40496	1.85972

H	-0.59851	-0.12613	1.89014
H	-1.65605	0.66878	2.76180
O	2.62385	0.57734	1.05862
H	3.26697	0.69566	1.75570
H	-0.11689	2.93019	0.17854
O	0.91580	-2.80826	0.18094
H	0.88608	-3.67306	0.58523
H	0.81774	-2.11883	0.91598
O	0.71634	-0.88991	1.89602
H	1.86248	0.01100	1.44782
H	0.88226	-1.20324	2.78479
O	2.74336	-1.20185	-1.15224
H	2.33744	-1.97504	-0.73301
H	2.96348	-0.62253	-0.40808
O	-3.39307	-0.92892	0.42807
H	-4.17831	-1.16094	0.91970
H	-2.77386	-0.49667	1.05318
O	1.66361	2.63920	-0.40868
H	2.08114	1.95959	0.16342
H	2.33368	3.28920	-0.61213

2.2 Structure files (xyz format) of reactants and products of the $CH_3O_2^-$-H_2O reaction (*n* = 1-8).

Reactants:$CH_3O_2^-$+Na^++1H_2O

O	-1.48821	0.65293	-0.40969
O	-0.15958	-0.90612	0.63774
C	-1.29337	-0.80036	-0.02895
H	-2.18691	-1.05745	0.56293
H	-1.32009	-1.34542	-0.99012
H	-2.20400	0.72581	-1.04018
O	2.05261	-0.35371	-0.47410

H	2.81291	-0.91878	-0.36403
H	1.24193	-0.84092	-0.11625
Na	0.56162	1.19038	0.37179
Reactants:$CH_3O_2^-$+Na^++2H_2O			
C	-1.61183	-0.00118	-0.58462
H	-2.18933	-0.90126	-0.84927
H	-2.19073	0.89787	-0.84976
O	-0.37615	-0.00042	-1.08048
O	-1.52136	-0.00080	0.90259
H	-2.40150	0.00026	1.27762
O	1.16307	-1.87382	-0.21602
H	0.53847	-1.30998	-0.76197
H	1.77636	-2.29219	-0.81507
O	1.16034	1.87536	-0.21641
H	1.77374	2.29347	-0.81555
H	0.53663	1.31039	-0.76222
Na	0.76546	0.00055	1.08787
Reactants:$CH_3O_2^-$+Na^++3H_2O			
C	-1.09385	-1.50463	0.18137
H	-0.84974	-2.55735	-0.01873
H	-2.16043	-1.42455	0.42204
O	-0.72013	-0.67663	-0.81718
O	-0.43896	-1.15355	1.44799
H	0.43766	-1.54058	1.42294
O	2.15272	1.22099	0.38187
H	2.97283	1.27040	0.86712
H	2.21301	0.43736	-0.21661
O	-1.97788	1.55211	-0.61795
H	-1.66722	0.65229	-0.92407
H	-2.43354	1.97741	-1.33959

O	1.78772	-0.94073	-1.09305
H	0.76800	-0.88009	-1.09626
H	2.06765	-1.08480	-1.99502
Na	-0.11027	1.10548	0.67059

Reactants: $CH_3O_2^- + Na^+ + 4H_2O$

C	-1.73133	-0.81857	-0.57388
H	-2.09918	-1.58467	-1.27201
H	-2.56477	-0.15767	-0.30439
O	-0.65924	-0.15090	-1.05191
O	-1.44024	-1.50889	0.67728
H	-0.73586	-2.13471	0.48697
O	1.26909	-1.80050	-1.04960
H	1.53941	-2.12081	-1.90842
H	0.49733	-1.15263	-1.19094
O	-0.51768	0.42186	2.31318
H	-0.92483	-0.33912	1.84226
H	-1.15648	0.72279	2.95573
O	2.57902	0.02546	0.42123
H	2.27462	-0.72860	-0.13047
H	2.95408	-0.35949	1.21144
O	-0.54669	2.42601	-1.24361
H	-0.75647	1.47160	-1.41840
H	-0.42759	2.85494	-2.08765
Na	0.57396	1.19413	0.42968

Reactants: $CH_3O_2^- + Na^+ + 5H_2O$

C	0.12983	0.81168	-1.74762
H	-0.68914	0.79106	-2.48171
H	1.02769	1.20566	-2.23579
O	0.34343	-0.41203	-1.19460
O	-0.20454	1.82086	-0.77252

H	-1.07717	1.60208	-0.40991
O	2.61977	-1.43217	-0.47944
H	2.93522	-2.25413	-0.84744
H	1.85525	-1.12869	-1.03074
O	-1.76403	-1.56872	-0.65117
H	-0.86105	-1.12731	-0.97323
H	-2.03150	-2.23615	-1.27902
O	-0.93791	-1.11504	1.93665
H	-1.51343	-0.35139	2.03438
H	-1.29784	-1.55505	1.14726
O	-2.62134	0.77737	0.31652
H	-2.55496	-0.08591	-0.14108
H	-3.49540	1.12363	0.14352
O	1.51433	1.84568	1.28472
H	0.93491	2.02670	0.51188
H	2.29655	2.38287	1.17839
Na	1.09947	-0.41737	1.03162

Reactants: $CH_3O_2^- + Na^+ + 6H_2O$

C	-0.19598	-1.48051	1.39359
H	0.45555	-1.52829	2.27340
H	-0.72464	-2.44028	1.29450
O	0.49096	-1.15975	0.26529
O	-1.18673	-0.49333	1.74838
H	-1.89434	-0.53621	1.08855
O	-0.20308	1.98402	1.55962
H	0.17149	2.35544	2.35586
H	-0.55997	1.09626	1.79295
O	-1.58750	1.97598	-0.90851
H	-2.23219	1.25456	-0.86390
H	-1.56628	2.35370	-0.02356

O	2.77777	1.13427	-1.08495
H	3.08131	0.32886	-0.60907
H	3.44000	1.80667	-0.94105
O	-2.90878	-0.48443	-0.54782
H	-3.79313	-0.81167	-0.70312
H	-2.29247	-0.99324	-1.12764
O	-0.86559	-1.54946	-1.82366
H	-0.73150	-2.38741	-2.26135
H	-0.26721	-1.52086	-0.99792
O	3.07919	-1.11156	0.33264
H	2.08398	-1.23061	0.35658
H	3.43724	-1.91195	-0.04751
Na	0.52712	0.97111	-0.57056
Reactants: $CH_3O_2^- + Na^+ + 7H_2O$			
O	-1.66301	0.70735	1.45233
O	0.21245	-0.67702	1.25126
C	-0.67159	-0.10756	2.10921
H	-0.18462	0.58694	2.80447
H	-1.21947	-0.86096	2.69367
H	-2.21719	0.12624	0.91099
O	2.81819	-1.22863	-1.07728
H	2.97612	-0.87603	-0.18181
H	3.40692	-0.73222	-1.64522
O	1.72449	1.75252	-0.70864
H	0.96660	2.29613	-0.45204
H	2.16057	1.49513	0.11398
O	-1.32093	0.63949	-2.05407
H	-1.31985	1.49895	-1.61049
H	-2.06668	0.15649	-1.67461
O	-2.93964	-1.04050	-0.42411

H	-3.79780	-1.46092	-0.43555
H	-2.25806	-1.74714	-0.41195
O	-0.68190	-2.42686	-0.29245
H	-0.37025	-3.32352	-0.19012
H	-0.30820	-1.85698	0.47050
O	2.63935	0.04514	1.34874
H	1.67448	-0.26311	1.43382
H	3.07825	-0.11728	2.18121
O	-0.86832	2.68457	-0.13802
H	-1.15238	2.01374	0.52899
H	-1.25769	3.51958	0.11634
Na	0.59576	-0.31437	-1.10633

Reactants: $CH_3O_2^- + Na^+ + 8H_2O$

C	-0.01616	-1.98821	-0.75553
H	0.65491	-2.75828	-1.16067
H	-1.03968	-2.20131	-1.08308
O	0.38330	-0.73211	-1.10623
O	-0.06453	-2.16924	0.67298
H	0.84174	-2.19938	1.00066
O	-1.04494	1.39060	2.10679
H	-1.64935	0.61144	1.98938
H	-1.19612	1.73945	2.98305
O	-1.44508	0.69973	-2.06651
H	-0.68703	0.08914	-1.73809
H	-1.38565	0.73653	-3.02004
O	2.87703	-0.41356	-1.34190
H	3.28530	-0.78850	-2.11971
H	1.87201	-0.58051	-1.39125
O	2.56773	-1.18313	1.22885
H	3.30399	-1.15966	1.83774

H	2.92745	-1.00339	0.33664
O	-2.35352	-0.82087	1.59017
H	-2.87083	-0.73973	0.76764
H	-1.63042	-1.43308	1.38186
O	-3.59548	-0.47630	-0.85822
H	-4.37347	0.07762	-0.90077
H	-2.90110	-0.01657	-1.37068
O	-0.38027	2.67127	-0.40179
H	-0.85639	2.54236	0.42617
H	-0.83990	2.12360	-1.05963
O	2.33534	2.01131	0.05505
H	2.70167	1.45063	-0.64020
H	1.58426	2.48121	-0.33376
Na	0.73808	0.46691	0.87222
Products: CH_4O_2+OH^-+0H_2O+Na^+			
C	1.50796	0.10134	-0.00001
H	2.28559	-0.65916	0.00034
H	1.95883	1.09861	-0.00047
O	0.73459	-0.07488	-1.16239
H	0.02943	0.61620	-1.08844
O	0.73453	-0.07384	1.16247
H	0.02931	0.61713	1.08781
O	-1.28508	1.07212	-0.00043
H	-1.79822	1.87332	-0.00069
Na	-1.18409	-1.04922	0.00040
Products: CH_4O_2+OH^-+1H_2O+Na^+			
O	-1.47358	-0.07167	1.06402
O	-1.08229	-0.18179	-1.22308
C	-2.05101	-0.00564	-0.21894
H	-2.76867	-0.81840	-0.30131

H	-2.55634	0.95563	-0.35092
H	-0.82171	0.66830	1.06819
H	-0.46702	0.57793	-1.10168
O	2.69452	-0.16291	-0.10924
H	2.05997	0.61797	-0.06684
H	3.27327	-0.02862	-0.85584
Na	0.62896	-1.02634	0.31879
O	0.60323	1.30511	0.15907
H	0.73303	2.24082	0.28923

Products: CH_4O_2+OH^-+2H_2O+Na^+

C	-2.01101	-0.63741	0.28474
H	-2.82185	-1.26149	-0.08469
H	-2.21610	-0.32502	1.31258
O	-0.83342	-1.37597	0.21996
H	-0.17271	-1.01234	0.88105
O	-1.97446	0.49890	-0.56254
H	-1.51944	1.21699	-0.09843
O	2.45787	-0.58136	-0.58723
H	2.88685	-1.43365	-0.62019
H	2.09427	-0.47835	0.34381
O	0.22779	1.90332	0.27932
H	0.64061	2.74376	0.46301
H	0.59827	1.20843	0.94031
O	1.01899	-0.12680	1.49837
H	1.24998	-0.19331	2.42126
Na	0.37746	0.07407	-1.27728

Products: CH_4O_2+OH^-+3H_2O+Na^+

C	-1.36914	-1.49220	-0.67812
H	-2.15860	-1.56380	-1.42360
H	-1.08511	-2.49186	-0.33624

O	-0.27731	-0.84449	-1.24052
H	0.56544	-1.18126	-0.80809
O	-1.93470	-0.77220	0.40597
H	-1.26642	-0.72815	1.11325
O	-1.95077	1.89375	-0.12329
H	-2.20604	0.96713	0.05804
H	-2.57507	2.45314	0.33354
O	2.53788	1.11603	-0.50321
H	3.05959	1.19605	-1.29856
H	2.48564	0.13727	-0.28943
O	0.34248	-0.19144	1.82251
H	0.64374	-0.11921	2.72526
H	1.03441	-0.74475	1.29251
O	1.82719	-1.27213	0.14721
H	2.34509	-2.06713	0.24124
Na	0.27399	1.24178	-0.14625

Products: CH_4O_2+OH^-+4H_2O+Na^+

C	-1.90784	-1.32682	-0.80095
H	-1.81425	-2.37944	-0.51702
H	-2.63525	-1.22214	-1.60353
O	-2.44175	-0.59418	0.29071
H	-1.81537	-0.66332	1.03227
O	-0.68212	-0.83522	-1.23002
H	0.04623	-1.33840	-0.74808
O	-0.16799	-0.34138	1.83746
H	0.42248	-1.02992	1.34637
H	0.09543	-0.32273	2.75471
O	2.15714	1.91123	-0.25591
H	2.68401	1.07430	-0.28981
H	2.69126	2.55251	0.20714

O	3.28324	-0.48048	-0.30055
H	2.49817	-1.06803	-0.06569
H	3.59555	-0.78555	-1.15107
O	-2.11294	2.06437	-0.14723
H	-2.71625	2.70578	0.22088
H	-2.49946	1.17962	0.00020
O	1.13907	-1.79348	0.28485
H	1.24509	-2.73001	0.43776
Na	0.02293	1.14012	-0.05935
Products: CH_4O_2+OH^-+5H_2O+Na^+			
C	0.49733	-1.85987	-1.27584
H	-0.12995	-2.27594	-2.06120
H	1.32631	-2.54010	-1.05918
O	0.99867	-0.63415	-1.76115
H	1.80030	-0.41186	-1.25769
O	-0.29742	-1.68645	-0.14316
H	0.30178	-1.51838	0.64922
O	-2.79979	-0.78342	0.84503
H	-2.13032	-1.37668	0.47591
H	-2.29375	-0.25670	1.48200
O	2.82423	0.18969	0.14762
H	2.27627	-0.27274	0.89781
H	3.75325	0.05846	0.32557
O	1.32433	2.39643	-0.34601
H	2.02581	1.75024	-0.13184
H	1.67339	2.94751	-1.04415
O	-0.70921	0.78652	1.89498
H	-0.55375	1.55019	2.44718
H	0.07770	0.16370	2.00958
O	-2.70593	1.06287	-1.11828

H	-2.98416	0.38403	-0.46747
H	-3.26846	0.96928	-1.88369
O	1.22787	-0.86913	1.74142
H	1.50379	-1.41694	2.47281
Na	-0.47857	0.88240	-0.48030
Products: CH_4O_2+OH^-+6H_2O+Na^+			
C	1.64347	0.45820	-1.66838
H	1.58815	1.33666	-2.30829
H	2.14467	-0.35901	-2.19563
O	2.41294	0.83586	-0.54800
H	2.51742	0.05405	0.02853
O	0.34940	0.07041	-1.32009
H	0.38745	-0.92242	-1.08920
O	-2.78109	1.85654	0.15725
H	-2.91731	1.09843	-0.44782
H	-3.26398	2.59850	-0.19948
O	2.23192	-1.42038	1.00748
H	1.63982	-1.94631	0.36844
H	2.89079	-2.01401	1.36260
O	1.08195	2.85915	0.63911
H	1.51309	3.36773	1.32257
H	1.74980	2.24887	0.26875
O	-2.52154	-0.37299	-1.31301
H	-1.65634	-0.24376	-1.71759
H	-2.39661	-1.11148	-0.68937
O	-0.21294	-0.45624	2.10262
H	-0.80852	-1.16240	1.80737
H	0.67706	-0.80570	1.94759
O	-1.72567	-2.26130	0.56379
H	-2.13573	-3.09581	0.78382

H	-0.85212	-2.45649	0.08370
O	0.52381	-2.35641	-0.60390
H	0.70882	-3.00382	-1.28093
Na	-0.59250	1.23916	0.58939
Products: CH_4O_2+OH^-+7H_2O+Na^+			
C	2.67005	-0.69667	1.08925
H	2.89735	-1.53505	1.74503
H	3.53856	-0.03483	1.01923
O	2.40719	-1.24688	-0.18258
H	2.39916	-0.51721	-0.83330
O	1.59412	-0.00098	1.62816
H	1.54455	0.92127	1.20142
O	-3.57983	-0.82685	-0.47579
H	-3.45335	-0.06277	0.12900
H	-4.13746	-0.51977	-1.18792
O	2.14181	0.98061	-1.70639
H	1.96369	1.60294	-0.91037
H	2.74367	1.41642	-2.30632
O	0.33028	-2.89068	-0.73963
H	0.59960	-3.52737	-1.39851
H	1.13233	-2.37647	-0.50948
O	-2.72043	1.04811	1.25372
H	-2.09781	0.45964	1.70180
H	-2.16211	1.72137	0.82604
O	-0.62494	0.51225	-1.86800
H	-0.87762	1.33685	-1.42059
H	0.32670	0.61788	-2.01886
O	-0.97564	2.68062	-0.15473
H	-1.12626	3.59735	-0.37756
H	0.00189	2.58897	0.11168

O	1.47866	2.21895	0.38014
H	1.99812	2.92127	0.76672
Na	-1.29398	-1.25341	-0.56914
O	-0.83541	-1.00874	1.74269
H	0.09624	-0.67475	1.76647
H	-0.90009	-1.69955	2.39974

2.3 Structure files (xyz format) of reactants and products of the reaction guanidine-CO_2 (*n*=1-8)

Reactants:CH_5N_3+CO_2+1H_2O

C	2.12011	-0.01394	0.02407
N	1.87400	1.22217	-0.21524
N	1.16850	-0.81555	0.60473
N	3.30299	-0.67454	-0.26091
H	2.68492	1.72444	-0.55053
H	1.14229	-1.76618	0.27661
H	0.25437	-0.38636	0.65359
H	4.07769	-0.08191	-0.50296
H	3.55244	-1.40595	0.38402
O	-0.85156	1.45509	0.14302
H	0.10508	1.59036	-0.03855
H	-1.12818	2.18778	0.69055
C	-2.75973	-0.50871	-0.14148
O	-3.60422	0.26996	-0.02282
O	-1.95288	-1.33139	-0.25875

Reactants:CH_5N_3+CO_2+2H_2O

C	1.89873	-0.00707	0.00261
N	1.23680	-1.14727	0.03741
H	0.16793	-1.14697	0.02979
H	1.73657	-2.00829	-0.08074
N	1.24888	1.13676	0.03720

H	0.17325	1.15135	0.02352
H	1.76266	1.99663	-0.00625
N	3.25998	-0.01891	-0.09773
H	3.74756	0.82876	0.12952
H	3.73538	-0.85821	0.18099
C	-1.90974	0.03673	-0.00284
O	-1.34571	1.14577	-0.00193
O	-3.26712	0.06995	-0.02007
H	-3.55118	-0.84687	-0.01857
O	-1.37789	-1.10178	0.01012

Reactants: $CH_5N_3+CO_2+3H_2O$

C	-1.19713	-1.46884	0.15155
N	-2.46588	-1.55062	-0.07338
N	-0.71911	-0.55677	1.05246
N	-0.24780	-2.29520	-0.39617
H	-2.70275	-2.33274	-0.66866
H	0.14961	-0.08924	0.82473
H	-1.42674	0.08617	1.36835
H	-0.48062	-2.71454	-1.27764
H	0.71575	-2.02026	-0.30528
O	1.13229	1.54122	0.07333
H	0.26547	1.90395	-0.19740
H	1.57124	2.24889	0.54379
O	-3.46569	0.93885	0.08255
H	-4.14814	1.03782	0.74339
H	-3.24395	-0.03152	0.02332
O	-1.35192	2.52827	-0.54530
H	-2.12936	1.99181	-0.28725
H	-1.52179	2.80952	-1.44313
C	3.33407	-0.13971	-0.05558

O	3.97464	0.75889	0.28223
O	2.73058	-1.06977	-0.39036

Reactants:CH_5N_3+CO_2+4H_2O

C	-0.00728	-0.93463	0.56750
N	-0.72672	-0.22294	1.37481
N	0.17352	-0.52417	-0.72384
N	0.54681	-2.15201	0.86292
H	-0.82802	-0.66012	2.28056
H	0.97442	-0.90887	-1.20323
H	0.03212	0.45942	-0.88296
H	0.58390	-2.39278	1.83628
H	1.36271	-2.41567	0.32670
O	1.37549	2.44861	-0.62292
H	1.65025	3.32637	-0.88292
H	0.56902	2.55385	-0.06519
O	2.88564	-1.74436	-0.89122
H	3.13980	-0.88658	-0.49455
H	3.60162	-2.01107	-1.46462
O	3.29207	0.69665	0.25216
H	2.61497	1.33693	-0.04591
H	3.25568	0.71141	1.20771
O	-0.85205	2.42835	0.84805
H	-0.87582	1.46873	1.11648
H	-1.65899	2.56134	0.35008
C	-3.07442	-0.35952	-0.57135
O	-2.94075	0.75899	-0.84297
O	-3.24624	-1.47377	-0.32468

Reactants:CH_5N_3+CO_2+5H_2O

C	-1.50959	1.33785	-0.26708
N	-2.43605	0.65309	0.34511

N	-0.62642	0.71457	-1.07963
N	-1.37146	2.69674	-0.18801
H	-3.07037	1.25719	0.85051
H	0.24818	1.18363	-1.25626
H	-0.59397	-0.29322	-1.05023
H	-1.83102	3.13803	0.58746
H	-0.45132	3.06259	-0.39557
O	1.56525	2.68958	-0.42210
H	1.69471	2.04365	0.29866
H	2.35861	2.65883	-0.95440
O	-0.42605	-0.83697	1.86194
H	-0.29717	-1.55169	1.22172
H	-1.20226	-0.36181	1.51590
O	-3.12335	-1.87852	-0.46478
H	-3.63813	-2.28829	0.22934
H	-2.97445	-0.94043	-0.17625
O	-0.49428	-2.34134	-0.52783
H	-0.18436	-3.18218	-0.86006
H	-1.47741	-2.35647	-0.56230
O	1.72390	0.74698	1.51190
H	2.15107	0.84463	2.36144
H	0.92396	0.19328	1.67153
C	2.46934	-1.21601	-0.49379
O	2.37562	-0.38853	-1.29792
O	2.58177	-2.06490	0.28147

Reactants:$CH_5N_3+CO_2+6H_2O$

C	-0.15356	2.08312	-0.37786
N	1.08322	2.25389	0.01700
N	-0.49957	0.99002	-1.07920
N	-1.15881	2.98380	-0.15138

H	1.20817	3.15121	0.46606
H	-1.47721	0.75356	-1.12639
H	0.16446	0.22868	-1.16968
H	-0.99299	3.64863	0.58211
H	-2.09847	2.60788	-0.17382
O	-1.74866	-0.62441	1.65415
H	-0.80567	-0.36278	1.76482
H	-2.04424	-0.89381	2.52261
O	0.81427	0.14159	2.00575
H	0.99205	0.89562	1.41660
H	1.52027	-0.48940	1.80485
O	-3.30829	0.95835	0.03442
H	-3.90279	0.38469	-0.44705
H	-2.82218	0.38183	0.65563
O	1.36797	-1.26556	-1.47067
H	1.64064	-1.74661	-0.68322
H	2.09004	-0.63628	-1.60027
O	3.18592	0.79760	-0.80223
H	2.42868	1.39746	-0.52421
H	3.84070	1.34328	-1.23394
O	3.02444	-1.28895	0.95318
H	3.33168	-0.53560	0.41650
H	3.78355	-1.63765	1.41736
C	-1.29565	-2.45982	-0.55344
O	-2.03216	-1.83997	-1.19631
O	-0.57039	-3.10671	0.07107

Reactants:CH_5N_3+CO_2+7H_2O

C	1.23802	-0.73276	-1.38458
N	2.17357	0.18897	-1.38839
N	1.23465	-1.70521	-0.45656

N	0.25862	-0.79616	-2.33412
H	2.11648	0.73843	-2.23676
H	0.37205	-2.20721	-0.30223
H	1.87415	-1.63119	0.32108
H	-0.01308	0.09907	-2.70604
H	-0.52567	-1.39693	-2.11382
O	0.54536	0.56308	2.27849
H	1.26563	-0.08218	2.30240
H	0.92176	1.31066	1.79431
O	-0.64434	2.16644	-1.33580
H	0.11270	2.46235	-0.80278
H	-1.26217	2.89699	-1.35501
O	2.85932	-1.12362	2.00586
H	3.55059	-0.65696	1.49073
H	3.29785	-1.59625	2.71115
O	-1.55693	0.18166	0.52662
H	-1.30623	0.84489	-0.13384
H	-0.86192	0.22706	1.21235
O	4.38380	0.17605	0.19562
H	5.13858	-0.24758	-0.21080
H	3.64793	0.14189	-0.47234
O	1.60263	2.29600	0.28780
H	1.90543	1.50661	-0.22653
H	2.37620	2.84342	0.42104
O	-1.64165	-2.24082	-0.61025
H	-1.71192	-1.38121	-0.13778
H	-2.41786	-2.74653	-0.37599
C	-4.34310	0.15206	0.53066
O	-4.38650	1.26939	0.23785
O	-4.35140	-0.96996	0.81355

Reactants: $CH_5N_3+CO_2+8H_2O$

C	-1.76257	1.19621	0.45231
N	-1.94039	1.32444	-0.83981
N	-2.10111	0.03598	1.06331
N	-1.30255	2.18812	1.25688
H	-1.71213	2.26578	-1.13484
H	-1.72214	-0.15471	1.97763
H	-2.30768	-0.74955	0.47225
H	-0.72987	2.88351	0.79526
H	-0.99550	1.91302	2.17892
O	-0.70344	-2.85547	1.09243
H	-1.14500	-2.74770	0.21885
H	-0.60066	-3.79567	1.22974
O	-3.81695	-0.52236	-1.72511
H	-3.24905	0.24283	-1.47088
H	-4.67552	-0.36201	-1.33673
O	-0.32620	-0.28714	-2.31281
H	-0.96589	0.31182	-1.83302
H	-0.39243	-0.06911	-3.24227
O	1.61168	0.73662	-0.57054
H	1.33685	0.25318	0.22343
H	1.08312	0.34912	-1.28733
O	-0.34945	0.41754	3.47452
H	-0.32560	0.13328	4.38634
H	0.33608	-0.08329	2.99925
O	0.62194	3.32173	-0.61532
H	1.32315	3.96338	-0.71219
H	1.05099	2.44404	-0.59692
O	1.14739	-0.97882	1.66354
H	0.54072	-1.71384	1.42591

H	2.04263	-1.31681	1.60421
O	-1.83025	-2.41161	-1.28973
H	-2.68454	-1.96938	-1.43156
H	-1.20429	-1.84192	-1.76523
C	4.17044	-0.50465	-0.61655
O	4.45816	-0.01060	-1.61751
O	3.93185	-1.02805	0.39079

Products: $CH_6N_3^+$+HCO_3^-+0H_2O

C	1.89873	-0.00707	0.00261
N	1.23680	-1.14727	0.03741
H	0.16793	-1.14697	0.02979
H	1.73657	-2.00829	-0.08074
N	1.24888	1.13676	0.03720
H	0.17325	1.15135	0.02352
H	1.76266	1.99663	-0.00625
N	3.25998	-0.01891	-0.09773
H	3.74756	0.82876	0.12952
H	3.73538	-0.85821	0.18099
C	-1.90974	0.03673	-0.00284
O	-1.34571	1.14577	-0.00193
O	-3.26712	0.06995	-0.02007
H	-3.55118	-0.84687	-0.01857
O	-1.37789	-1.10178	0.01012

Products: $CH_6N_3^+$+HCO_3^-+1H_2O

C	-1.98308	-0.37841	0.05162
N	-1.27185	0.68029	0.37802
H	-0.22787	0.59471	0.43017
H	-1.62086	1.60959	0.21478
N	-1.40095	-1.56081	-0.03803
H	-0.34438	-1.62157	-0.03713

H	-1.94567	-2.36631	-0.28078
N	-3.31286	-0.24706	-0.19757
H	-3.87426	-1.07732	-0.24119
H	-3.77515	0.56556	0.16775
O	0.30073	3.03498	-0.30506
H	0.76067	3.81848	-0.00910
H	0.92320	2.30323	-0.16951
C	1.86815	-0.54921	0.05198
O	1.38983	0.56589	0.34412
O	3.21554	-0.58261	-0.10730
H	3.43246	-1.49259	-0.32275
O	1.25153	-1.62763	-0.10311

Products: $CH_6N_3^+ + HCO_3^- + 2H_2O$

C	1.23714	-1.24834	0.10413
N	0.93662	-0.41479	1.09218
H	-0.02098	-0.02403	1.08352
H	1.66956	0.21867	1.37298
N	0.28084	-1.96706	-0.46098
H	-0.72162	-1.72260	-0.26962
H	0.49294	-2.48971	-1.29002
N	2.53189	-1.39560	-0.25505
H	2.72626	-1.93217	-1.08060
H	3.10950	-0.57379	-0.12077
O	3.01781	1.43387	0.20076
H	2.19519	1.79005	-0.19482
H	3.57418	2.18100	0.41221
O	0.57230	2.10407	-0.82641
H	0.27201	2.95379	-1.14454
H	-0.20278	1.69629	-0.38311
C	-2.32102	0.08322	0.12951

O	-1.40746	0.84903	0.51677
O	-3.52832	0.67528	-0.05977
H	-4.12250	-0.02398	-0.34242
O	-2.24358	-1.14235	-0.09108

Products: $CH_6N_3^+ + HCO_3^- + 3H_2O$

C	-0.90715	-1.71356	-0.01527
N	-0.74146	-0.66872	-0.80473
H	-1.57012	-0.16754	-1.08705
H	0.18518	-0.20284	-0.83330
N	-2.15782	-2.17420	0.20865
H	-2.91184	-1.52138	0.02703
H	-2.29539	-2.83677	0.94834
N	0.14594	-2.32700	0.50427
H	0.01287	-3.10523	1.12074
H	1.10711	-1.93767	0.36614
O	-3.50489	0.28898	-0.51024
H	-4.20951	0.62340	-1.06241
H	-3.12753	1.06192	-0.03386
O	-2.28678	2.34995	0.70201
H	-1.34477	2.50496	0.46513
H	-2.33195	2.45032	1.65162
O	0.31248	2.79347	0.17613
H	0.59703	3.54968	-0.33405
H	0.89743	2.04908	-0.09111
C	2.58551	-0.02537	-0.12799
O	1.62882	0.62496	-0.61228
O	3.73961	0.67519	0.02011
H	4.37365	0.06077	0.39728
O	2.58839	-1.22076	0.22023

Products: $CH_6N_3^+ + HCO_3^- + 4H_2O$

C	-0.83465	0.29006	-1.36821
N	0.40147	0.42727	-1.85123
H	0.90018	1.27194	-1.59791
H	0.93602	-0.41765	-1.99463
N	-1.49962	1.35825	-0.93125
H	-0.95532	2.18745	-0.72972
H	-2.33464	1.18128	-0.38665
N	-1.43051	-0.90228	-1.39661
H	-2.28071	-0.99907	-0.85564
H	-0.82762	-1.70858	-1.50404
O	-3.33046	-0.21278	0.63892
H	-2.63624	-0.35685	1.33043
H	-4.18157	-0.28025	1.06721
O	0.88629	2.82972	-0.30101
H	1.03919	2.20541	0.44720
H	1.49396	3.55843	-0.19254
O	-1.28088	-0.54167	2.28079
H	-0.62033	0.15565	2.09902
H	-0.75784	-1.32109	2.06226
O	1.04086	-2.40291	-1.35503
H	1.16845	-2.16697	-0.40450
H	1.41965	-3.26923	-1.49152
C	1.56334	-0.17433	1.01422
O	0.93189	0.81930	1.42292
O	2.75449	0.11169	0.40497
H	3.15688	-0.73013	0.18023
O	1.22387	-1.37678	1.07698

Products: $CH_6N_3^+ + HCO_3^- + 5H_2O$

C	0.20429	-1.64695	0.64750
N	-1.12527	-1.73597	0.64864

H	-1.58980	-1.83893	-0.24007
H	-1.62086	-1.19859	1.34682
N	0.90194	-2.11758	-0.38428
H	0.39924	-2.16283	-1.26613
H	1.88317	-1.86857	-0.40835
N	0.83246	-1.15972	1.71961
H	1.81921	-0.95534	1.62318
H	0.27891	-0.63612	2.38220
O	-0.87050	-1.21539	-2.45261
H	-0.51383	-0.36888	-2.12839
H	-1.82082	-1.09639	-2.34187
O	2.84491	1.39696	-1.01766
H	1.88231	1.28670	-1.18182
H	2.89857	2.22784	-0.54462
O	-3.16992	-0.35807	-1.01676
H	-4.00386	0.02588	-1.28171
H	-2.63088	0.37446	-0.64958
O	3.37554	-0.79521	0.40390
H	3.27608	0.04419	-0.10607
H	4.30380	-1.02152	0.39731
O	-1.53133	0.39283	2.59930
H	-1.63780	0.93945	1.79186
H	-2.19139	0.67904	3.22807
C	-0.41232	1.68298	-0.28243
O	0.16413	1.03407	-1.16603
O	0.32780	2.68106	0.28632
H	-0.24115	3.12099	0.92158
O	-1.57896	1.52941	0.16095

Products: $CH_6N_3^+ + HCO_3^- + 6H_2O$

C	0.35086	-0.71994	-1.55841

N	1.59420	-0.24409	-1.49204
H	2.29125	-0.85744	-1.08988
H	1.75208	0.75314	-1.40945
N	0.14118	-2.02698	-1.36692
H	0.88697	-2.55556	-0.93234
H	-0.81596	-2.32786	-1.25086
N	-0.66621	0.06798	-1.87886
H	-1.59307	-0.33180	-1.83030
H	-0.56481	1.08604	-1.88973
O	-3.17001	-0.49197	1.21265
H	-2.24381	-0.53878	1.58028
H	-3.76955	-0.70102	1.92751
O	2.64312	-2.50433	-0.01123
H	2.43315	-2.08791	0.86169
H	3.37580	-3.10169	0.12596
O	-2.80014	-1.79450	-1.14721
H	-3.06352	-1.40861	-0.28759
H	-3.59244	-2.14003	-1.55488
O	-0.54889	2.87962	-1.52463
H	-0.88462	2.77382	-0.62536
H	0.38984	3.06871	-1.38855
O	1.92146	-1.21161	2.18807
H	1.95384	-0.26561	1.97248
H	0.96313	-1.31052	2.28331
O	2.04025	2.53596	-0.58656
H	2.80895	3.05210	-0.35052
H	1.64147	2.20036	0.25050
C	-0.29082	0.87934	1.48848
O	0.88348	1.27762	1.43128
O	-1.24051	1.77602	1.06508

H	-2.10545	1.34905	1.11552
O	-0.69222	-0.24070	1.88212

Products: $CH_6N_3^+ + HCO_3^- + 7H_2O$

C	1.46080	-0.44831	-1.21439
N	2.65437	0.14225	-1.35110
H	3.45604	-0.34035	-0.97252
H	2.66287	1.15482	-1.39026
N	1.38308	-1.70290	-0.80149
H	2.22283	-2.13516	-0.44557
H	0.48745	-2.19632	-0.72489
N	0.35873	0.22509	-1.54926
H	-0.53635	-0.08337	-1.17944
H	0.46373	1.21565	-1.71586
O	4.02222	-1.71074	0.42968
H	4.72853	-2.23138	0.80740
H	3.60373	-1.20911	1.15812
O	0.22830	2.85281	1.02717
H	-0.64992	2.95468	0.61357
H	0.17699	1.98815	1.45811
O	1.76447	2.83950	-1.17369
H	1.25581	2.90809	-0.33208
H	1.79833	3.71683	-1.55041
O	-2.12088	2.66806	-0.37335
H	-2.20445	1.69852	-0.25694
H	-2.98820	3.02384	-0.18541
O	-0.11666	0.13600	1.92538
H	-0.79084	-0.04723	1.23061
H	-0.54795	-0.04259	2.76103
O	-0.93860	-3.21169	-0.51254
H	-1.22960	-3.78149	-1.22264

H	-1.75007	-2.75563	-0.18881
O	2.62086	-0.15632	2.15383
H	2.86034	0.77026	2.14100
H	1.65823	-0.17470	2.00617
C	-3.05095	-0.69500	0.10994
O	-1.98874	-0.01261	0.02321
O	-4.18671	0.05505	0.07961
H	-4.91820	-0.56441	0.13993
O	-3.15822	-1.91761	0.21926

2.4 Structure files (xyz format) of transition states of the guanidine-H_2O reaction (*n*=1-3)

TS1

C	-0.44578	-0.00911	0.16287
N	0.19998	-0.44562	1.26968
H	0.14079	-1.44848	1.36710
H	1.19177	-0.17698	1.05946
N	-1.09820	-0.87525	-0.64076
H	-0.54047	-1.67632	-0.89062
H	-1.59363	-0.47422	-1.41894
N	-0.73376	1.30594	0.06940
H	-0.71081	1.67564	-0.86644
H	-0.19627	1.86371	0.71333
O	1.68978	0.00361	-0.57546
H	2.28883	0.36697	-1.22567

TS2

C	0.49825	-0.43385	0.12704
N	-0.14338	0.41120	1.01782
H	0.32499	0.38588	1.91375
H	0.10576	1.32938	0.54003
N	1.69406	-0.98035	0.46049

H	2.34830	-0.25444	0.72134
H	2.08481	-1.60556	-0.22600
N	-0.23171	-0.97067	-0.84637
H	0.23237	-1.30615	-1.67039
H	-1.18266	-0.63034	-0.94227
O	1.29601	1.51420	-0.56519
H	1.39879	1.95062	-1.40923
O	-2.79038	0.17142	-0.07037
H	-3.46824	-0.33509	0.37482
H	-2.11150	0.36267	0.59650

TS3_1 (CH_7N_3O)

C	1.05324	-0.40574	-0.23103
N	0.17966	-1.06606	0.62792
H	0.67276	-1.75517	1.17772
H	-0.16886	-0.33963	1.26177
N	2.37023	-0.70975	-0.14750
H	2.72407	-0.72063	0.79475
H	2.98005	-0.23573	-0.79212
N	0.56330	0.09243	-1.36860
H	1.17525	0.73099	-1.85066
H	-0.38219	0.49220	-1.25136
O	0.69604	1.29792	1.09818
H	1.19761	2.09872	1.24320
O	-2.73487	-1.11353	0.17085
H	-3.12152	-1.42911	-0.64498
H	-1.79801	-1.34776	0.12865
O	-1.51574	1.57733	-0.36590
H	-0.77912	1.64372	0.30093
H	-2.17530	0.98680	0.01063

TS3_2 ($CH_6N_3^+$)

C	0.04372	-1.15577	0.12620
N	1.22880	-1.53915	-0.38043
N	0.01190	-0.46139	1.25765
N	-1.10992	-1.53296	-0.43428
H	1.22253	-1.88877	-1.32194
H	1.98601	-0.89002	-0.18214
H	-0.85450	0.07113	1.37498
H	0.85947	0.05642	1.45587
H	-1.06477	-1.88151	-1.37484
O	2.16424	1.06204	0.18975
H	1.30896	1.41743	-0.22533
H	2.73434	1.80820	0.35971
O	-2.16255	0.84605	0.26205
H	-2.84271	1.48661	0.45116
H	-1.87682	-0.87319	-0.24376
O	-0.14389	1.69436	-0.74521
H	-0.26041	2.19827	-1.54704
H	-1.25242	1.34501	-0.25711