

Supporting information for Dissociation (CID) of Guanine Radical Cation in the Gas Phase: an Experimental and Computational Study

Ping Cheng^a Yanni Li,^b Shuqi Li,^b Mingtao Zhang,^b Zhen Zhou^a

(^a *The School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China;* ^b *College of Chemistry, Nankai University, Tianjin 300071, China;*)

Figure1 is the B3-PMP2/6-311++g(3df,2p) optimized structures of two isoenergetic enantiomers and their transition state for intermediate 26. Table 1-5 show the relative single point energies for 10 guanine radical cation tautomers with their transition states and the single point energies for intermediates and transition states for $[G]^{*+}$ fragmentation to loss of HNCN, $H_2NC\equiv N$ ($HN=C=NH$) and $\bullet N=C=NH$, NH_3 and HCN calculated by B3LYP and MP2 methods with different basis sets. The rest are the optimized structures for all intermediates and transition states with UB3LYP/6-311++G(d,p) method.

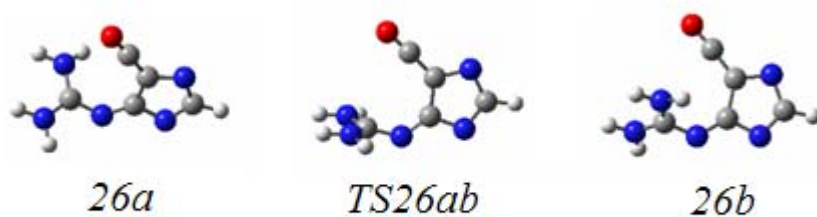


Figure 1 B3-PMP2/6-311++g(3df,2p) optimized structures of two isoenergetic enantiomeres and the transition state for intermediate 26.

Table 1 Relative energies for intermediates and transition states of the guanine radical cations

Radical Cation	Relative Energy ¹						
	B3LYP	B3LYP	MP2	B3-PMP2	B3LYP	MP2	B3-PMP2
	6-31+g(d, p)	6-311++g(2d,p)	6-311++g(2d,p)	6-311++g(2d,p)	6-311++g(3df,2p)	6-311++g(3df,2p)	6-311++g(3df,2p)
04	114	112	113	112	111	114	112
TS0409	288	286	282	284	285	280	282
09	105	101	93	97	101	93	97
TS0109	196	196	184	190	196	184	190
01	0	0	0	0	0	0	0
TS0108	158	160	151	155	161	150	156
08	5	5	1	3	7	1	4
07	13	11	4	8	13	5	9
TS0705	180	177	164	170	179	164	172
05	68	66	63	65	67	65	66
TS0503	325	322	314	318	322	313	318
03	69	66	66	66	66	66	66
TS0310	238	237	231	234	236	229	233
10	65	63	49	56	63	49	56
TS0210	186	186	168	177	186	168	177
02	9	7	7	7	10	7	9
TS0206	176	176	168	172	178	169	173
06	23	21	14	18	23	16	20

¹In units of KJ mol⁻¹ including B3LYP/6-31+g(d, p) ZPVE corrections.

Table 2 Relative energies for intermediates and transition states of loss of HNCO

Radical Cation	Relative Energy ¹						
	B3LYP	B3LYP	MP2	B3-PMP2	B3LYP	MP2	B3-PMP2
	6-31+g(d, p)	6-311++g(2d,p)		6-311++g(3df,2p)			
01	0	0	0	0	0	0	0
07	13	11	4	8	13	5	9
TS0711	188	189	167	178	190	167	178
11	56	57	38	48	58	41	49
TS1112	153	146	146	146	143	148	146
12	151	144	143	143	142	147	145
TS1213	252	247	256	251	246	261	253
13	192	186	188	187	185	193	189
TS1314	332	314	298	306	309	302	306
14	271	253	247	250	246	249	247
15	314	294	317	306	288	321	304

¹In units of KJ mol⁻¹ including B3LYP/6-31+g(d, p) ZPVE corrections.

Table 3 Relative energies for intermediates and transition states of loss of CH₂N₂ and CHN₂

Radical Cation	Relative Energy ¹						
	B3LYP	B3LYP	MP2	B3-PMP2	B3LYP	MP2	B3-PMP2
	6-31+g(d, p)	6-311++g(2d,p)		6-311++g(3df,2p)			
01	0	0	0	0	0	0	0
04	114	112	113	112	111	114	112
TS0416	212	205	198	201	205	205	205
16	209	200	193	196	200	201	201
TS1617	253	236	209	222	235	224	230
17	250	233	205	219	232	220	226
18	313	294	277	286	295	294	294
09	105	101	93	97	101	93	97
TS0919	223	216	210	213	215	217	216
19	223	215	210	212	214	217	216
TS1920	273	256	246	251	255	258	257
20	272	253	242	248	253	255	254
21	313	289	295	292	288	307	298
TS1622	228	219	213	216	220	221	220
22	182	168	171	169	167	175	171
TS2223	262	249	249	249	247	261	254
23	228	212	208	210	210	221	216
24	285	267	270	268	265	284	275

¹In units of KJ mol⁻¹ including B3LYP/6-31+g(d, p) ZPVE corrections.

Table 4 Relative energies for intermediates and transition states of loss of NH₃

Radical Cation	Relative Energy ¹						
	B3LYP	B3LYP	MP2	B3-PMP2	B3LYP	MP2	B3-PMP2
	6-31+g(d, p)	6-311++g(2d,p)		6-311++g(3df,2p)			
01	0	0	0	0	0	0	0
TS0125	298	296	286	291	296	283	290
25	85	85	76	80	85	75	80
TS2526	354	354	340	347	358	344	351
26	236	232	215	224	237	221	229
TS2627	359	350	357	354	351	365	358
27a	177	166	186	176	166	192	179
TS27ab	178	165	185	175	166	192	179
27b	177	166	186	176	166	192	179
TS2728	392	382	398	390	386	408	397
28	300	287	297	292	292	309	300
TS2829	336	315	340	327	315	353	334
29	225	208	214	211	212	233	222
30	336	314	335	325	312	346	329
31	334	318	308	313	324	330	327

¹In units of KJ mol⁻¹ including B3LYP/6-31+g(d, p) ZPVE corrections.**Table 5 Relative energies for intermediates and transition states of loss of HCN**

Radical Cation	Relative Energy ¹						
	B3LYP	B3LYP	MP2	B3-PMP2	B3LYP	MP2	B3-PMP2
	6-31+g(d, p)	6-311++g(2d,p)		6-311++g(3df,2p)			
01	0	0	0	0	0	0	0
TS0132	241	234	225	229	235	236	236
32	206	202	194	198	202	203	203
TS3233	459	454	460	457	452	461	456
33	427	423	394	409	420	391	405
TS3334	482	475	480	478	475	483	479
34	440	431	409	420	428	412	420
35	466	456	448	452	454	453	454

¹In units of KJ mol⁻¹ including B3LYP/6-31+g(d, p) ZPVE corrections.

The optimized structures for all intermediates and transition states with UB3ILYP/6-311++G(d,p) method.

04			
7	-1.582537	-0.848993	0.000000
6	-0.607638	-1.692692	0.000000
7	0.784233	-1.305167	0.000000
6	1.048270	0.000167	0.000000
6	0.000000	0.988286	0.000000
6	-1.408808	0.533087	0.000000
7	0.536041	2.218818	0.000000
6	1.849629	2.036964	0.000000
7	2.214077	0.691479	0.000000
7	-0.809416	-3.021500	0.000000
8	-2.339733	1.320774	0.000000
1	2.594067	2.823121	0.000000
1	3.162512	0.332219	0.000000
1	1.522717	-2.003901	0.000000
1	-0.076618	-3.714732	0.000000
1	-1.770310	-3.340233	0.000000
TS0409			
7	-1.583422	0.714868	0.000229
6	-1.686813	-0.626078	-0.000046
7	-0.592821	-1.491575	0.000058
6	0.611969	-0.891184	0.000100
6	0.779151	0.542236	-0.000052
6	-0.402425	1.460066	0.000025
7	2.085349	0.840109	-0.000148
6	2.725384	-0.322291	-0.000068
7	1.861072	-1.413455	0.000080
7	-2.968575	-0.882019	-0.000278
8	-0.328467	2.664411	0.000015
1	3.800462	-0.450900	-0.000063
1	2.136227	-2.389995	0.000287
1	-0.720319	-2.499215	-0.000233
1	-3.426136	-1.788802	0.000397
1	-2.937314	0.461637	0.000155
09			
7	2.133950	0.757877	0.000141

6	2.705591	-0.441272	0.000123
7	1.782973	-1.475719	-0.000129
6	0.559118	-0.881155	-0.000043
6	0.814208	0.525134	-0.000034
6	-0.310210	1.481422	-0.000207
7	-1.546917	0.795971	-0.000084
6	-1.815719	-0.558902	0.000067
7	-0.671974	-1.405344	-0.000032
8	-0.231641	2.683732	0.000046
7	-3.023898	-0.975148	0.000127
1	3.771732	-0.628723	0.000186
1	2.000517	-2.466452	-0.000233
1	-2.376647	1.386183	-0.000021
1	-3.144202	-1.987589	0.000136
1	-0.835128	-2.408102	-0.000029

TS0109

7	-1.560782	0.890008	0.000010
6	-1.777898	-0.444130	0.000139
7	-0.718359	-1.358085	0.000159
6	0.516612	-0.896828	0.000049
6	0.821951	0.507017	-0.000091
6	-0.258672	1.509541	-0.000117
7	2.148605	0.697060	-0.000183
6	2.677102	-0.526614	-0.000106
7	1.727380	-1.526203	0.000036
7	-2.809593	-1.236850	0.000267
8	-0.146628	2.707340	-0.000228
1	3.737438	-0.743369	-0.000147
1	1.899680	-2.525585	0.000113
1	-1.724926	-2.147843	0.000284
1	-3.780081	-0.935387	0.000294
1	-2.344414	1.538036	-0.000002

01

7	-1.466060	-0.873195	0.000000
6	-0.407114	-1.727053	0.000000
7	0.887995	-1.309094	0.000000
6	1.029551	-0.003265	0.000000
6	0.000000	1.004009	0.000000
6	-1.393257	0.564006	0.000000
7	0.522000	2.234813	0.000000
6	1.847611	2.039721	0.000000
7	2.199729	0.717506	0.000000

7	-0.606032	-3.042278	0.000000
8	-2.401298	1.227189	0.000000
1	2.582201	2.834701	0.000000
1	3.139155	0.335195	0.000000
1	0.206634	-3.647288	0.000000
1	-1.523707	-3.467563	0.000000
1	-2.418068	-1.231323	0.000000

TS0108

7	1.534583	0.706517	0.000186
6	1.640425	-0.635633	0.000320
7	0.541882	-1.473312	0.000280
6	-0.607001	-0.847175	0.000180
6	-0.856362	0.578468	0.000028
6	0.339578	1.373009	0.000041
7	-2.165411	0.852234	-0.000177
6	-2.756843	-0.352976	-0.000063
7	-1.874677	-1.392526	-0.000094
7	2.830761	-1.222802	-0.000683
8	0.612439	2.602281	-0.000060
1	-3.828985	-0.502322	-0.000183
1	-2.099668	-2.381654	0.000049
1	2.881746	-2.234211	0.000562
1	3.686335	-0.681989	0.000186
1	1.832318	1.996997	0.000249

08

7	1.487968	-0.919159	0.000000
6	0.385604	-1.715387	0.000000
7	-0.936058	-1.325281	0.000000
6	-1.062787	-0.025231	0.000000
6	0.000000	0.944356	0.000000
6	1.329801	0.387439	0.000000
7	-0.475352	2.196851	0.000000
6	-1.809009	2.045401	0.000000
7	-2.210173	0.741803	0.000000
7	0.593316	-3.028516	0.000000
8	2.357670	1.202121	0.000000
1	-2.513046	2.867606	0.000000
1	-3.163660	0.396774	0.000000
1	-0.195168	-3.664852	0.000000
1	1.539071	-3.392095	0.000000
1	3.191885	0.696253	0.000000

07			
7	-1.499659	-0.925442	0.000000
6	-0.399782	-1.720737	0.000000
7	0.931080	-1.344247	0.000000
6	1.063339	-0.045256	0.000000
6	0.000000	0.915538	0.000000
6	-1.336745	0.377171	0.000000
7	0.464726	2.173652	0.000000
6	1.799598	2.032988	0.000000
7	2.206574	0.731752	0.000000
7	-0.615464	-3.032551	0.000000
8	-2.407004	1.142310	0.000000
1	-2.175594	2.088397	0.000000
1	2.499115	2.858912	0.000000
1	3.163147	0.394793	0.000000
1	0.166821	-3.676841	0.000000
1	-1.566711	-3.384111	0.000000

TS0705

7	-1.520724	1.045393	-0.028164
6	-1.778834	-0.285130	-0.006316
7	-0.900865	-1.416742	-0.024030
6	0.358258	-1.040702	0.051304
6	0.679149	0.294852	0.144046
6	-0.225673	1.383189	0.020001
7	1.977592	0.562912	0.064464
6	2.565458	-0.646404	-0.042376
7	1.625900	-1.641623	-0.040747
7	-3.055762	-0.655555	0.001961
8	0.425469	2.469307	-0.069405
1	1.740753	1.798661	-0.030538
1	3.628156	-0.833152	-0.116051
1	1.836897	-2.632991	-0.113090
1	-3.303464	-1.637406	-0.006159
1	-3.779229	0.054908	0.006745

05			
7	-1.613889	-0.868911	0.000000
6	-0.594789	-1.707610	0.000000
7	0.791685	-1.396815	0.000000
6	0.998001	-0.104539	0.000000
6	0.000000	0.881384	0.000000
6	-1.418711	0.483962	0.000000
7	0.633461	2.093073	0.000000

6	1.966064	1.899916	0.000000
7	2.218654	0.587234	0.000000
7	-0.819187	-3.027964	0.000000
8	-2.296476	1.347409	0.000000
1	0.160736	2.994943	0.000000
1	2.710914	2.683666	0.000000
1	3.142870	0.164864	0.000000
1	-0.048729	-3.681073	0.000000
1	-1.772448	-3.366675	0.000000

TS0503

7	-1.546631	0.859760	0.004311
6	-1.735049	-0.437488	-0.004499
7	-0.649442	-1.378438	0.032718
6	0.492693	-0.754315	0.083921
6	0.838486	0.586310	0.062033
6	-0.323186	1.516873	0.015408
7	2.208340	0.527379	-0.021307
6	2.604587	-0.801763	-0.055823
7	1.547298	-1.600261	0.012095
7	-2.955967	-0.977721	-0.045372
8	-0.187921	2.732269	-0.016812
1	2.839831	1.323818	-0.056789
1	3.640767	-1.103861	-0.126145
1	0.386029	-2.409823	-0.062144
1	-3.094211	-1.978034	-0.031170
1	-3.759420	-0.362989	-0.072617

03

7	-1.571767	-0.868748	0.000000
6	-0.572884	-1.702459	0.000000
7	0.799744	-1.305215	0.000000
6	1.081967	0.002195	0.000000
6	0.000000	0.938761	0.000000
6	-1.405854	0.500626	0.000000
7	0.606736	2.138519	0.000000
6	1.979896	1.902332	0.000000
7	2.287016	0.618369	0.000000
7	-0.776565	-3.027760	0.000000
8	-2.316842	1.320067	0.000000
1	1.561582	-1.980679	0.000000
1	0.135615	3.039809	0.000000
1	2.698137	2.712506	0.000000
1	-0.038911	-3.717031	0.000000

1	-1.736584	-3.350025	0.000000
TS0310			
7	1.561649	0.752696	-0.000844
6	1.697272	-0.599130	-0.000198
7	0.642639	-1.486945	-0.000109
6	-0.599273	-0.943681	-0.000030
6	-0.753908	0.479109	-0.000178
6	0.363283	1.451429	-0.000349
7	-2.087107	0.658492	0.000332
6	-2.674227	-0.600153	0.000619
7	-1.786689	-1.581258	0.000152
7	2.992416	-0.793627	0.000719
8	0.209875	2.654399	-0.000457
1	-2.557539	1.560493	0.000362
1	-3.748520	-0.733051	0.000902
1	0.773021	-2.495733	0.000319
1	3.482040	-1.684911	0.001175
1	2.912764	0.547053	-0.000030
10			
7	-1.491366	-0.887592	0.000000
6	-0.475229	-1.832437	0.000000
7	0.833355	-1.329666	0.000000
6	1.074738	-0.003994	0.000000
6	0.000000	0.918186	0.000000
6	-1.404821	0.515400	0.000000
7	0.595398	2.127914	0.000000
6	1.965891	1.904018	0.000000
7	2.277196	0.623326	0.000000
7	-0.792551	-3.079109	0.000000
8	-2.362227	1.256296	0.000000
1	1.615579	-1.981123	0.000000
1	0.118659	3.025788	0.000000
1	2.677977	2.719070	0.000000
1	-0.001194	-3.724083	0.000000
1	-2.430908	-1.281172	0.000000
TS0210			
7	1.566615	-0.881292	0.000000
6	0.526323	-1.752765	0.000000
7	-0.798238	-1.329578	0.000000
6	-1.076364	-0.030994	0.000000
6	0.000000	0.909810	0.000000
6	1.410668	0.539184	0.000000

7	-0.601625	2.116432	0.000000
6	-1.975846	1.880605	0.000000
7	-2.284663	0.606680	0.000000
7	0.391217	-3.049765	0.000000
8	2.357354	1.292461	0.000000
1	-0.136143	3.019548	0.000000
1	-2.687358	2.696430	0.000000
1	-0.933961	-2.624332	0.000000
1	1.150683	-3.725808	0.000000
1	2.526121	-1.217902	0.000000

02

7	1.460558	-0.897498	0.000000
6	0.380826	-1.737665	0.000000
7	-0.906748	-1.313377	0.000000
6	-1.079429	-0.003112	0.000000
6	0.000000	0.945505	0.000000
6	1.384935	0.523129	0.000000
7	-0.580288	2.155649	0.000000
6	-1.966017	1.928514	0.000000
7	-2.284917	0.664769	0.000000
7	0.568167	-3.054519	0.000000
8	2.377622	1.221437	0.000000
1	-0.107296	3.054634	0.000000
1	-2.664764	2.755438	0.000000
1	-0.256227	-3.645327	0.000000
1	1.479355	-3.494107	0.000000
1	2.408666	-1.265527	0.000000

TS0206

7	1.530184	0.736506	0.000111
6	1.657401	-0.608030	0.000124
7	0.582206	-1.467952	0.000128
6	-0.606556	-0.902207	0.000195
6	-0.833554	0.525813	0.000321
6	0.319666	1.357922	0.000035
7	-2.168562	0.683537	0.000047
6	-2.718278	-0.611109	-0.000219
7	-1.825579	-1.556361	-0.000201
7	2.858185	-1.173783	-0.000242
8	0.540126	2.603898	-0.000257
1	-2.683380	1.558823	0.000813
1	-3.791316	-0.755175	-0.000441
1	2.918729	-2.185869	0.000084

1	3.707363	-0.622259	0.000085
1	1.780483	2.045334	-0.000122

06

7	1.480561	-0.944420	0.000000
6	0.361364	-1.726968	0.000000
7	-0.949504	-1.327492	0.000000
6	-1.106789	-0.022691	0.000000
6	0.000000	0.897464	0.000000
6	1.322010	0.357027	0.000000
7	-0.549464	2.124932	0.000000
6	-1.944974	1.932425	0.000000
7	-2.297776	0.681777	0.000000
7	0.556184	-3.043433	0.000000
8	2.346591	1.191406	0.000000
1	-0.062869	3.015555	0.000000
1	-2.618839	2.779755	0.000000
1	-0.245331	-3.665422	0.000000
1	1.496243	-3.422791	0.000000
1	3.188389	0.698564	0.000000

TS0711

7	1.570578	0.646092	0.000138
6	1.625533	-0.760094	0.000100
7	0.582216	-1.614867	-0.000090
6	-0.558884	-0.948507	-0.000148
6	-0.740255	0.474438	-0.000157
6	0.430233	1.304202	-0.000058
7	-2.045017	0.810003	-0.000079
6	-2.687427	-0.358207	0.000074
7	-1.844170	-1.436542	0.000100
7	2.926638	-0.951247	-0.000047
8	0.424247	2.614812	0.000068
1	-0.483242	2.969936	-0.000222
1	-3.764099	-0.466977	0.000248
1	-2.110038	-2.415536	0.000277
1	3.356188	-1.875060	-0.000059
1	2.860302	0.424082	0.000188

11

7	-1.536037	0.735813	0.000012
6	-1.743775	-0.672696	0.000033
7	-0.682514	-1.526024	0.000029
6	0.499318	-0.939440	0.000005

6	0.772795	0.455900	-0.000017
6	-0.336400	1.326864	-0.000012
7	2.103793	0.715433	-0.000038
6	2.663434	-0.487316	-0.000031
7	1.749777	-1.510786	-0.000005
7	-2.999635	-1.021168	0.000055
8	-0.301193	2.635405	-0.000029
1	0.613655	2.973754	-0.000046
1	3.730164	-0.668969	-0.000043
1	1.951188	-2.505131	0.000005
1	-3.083546	-2.041469	0.000069
1	-2.381848	1.305824	0.000016

TS1112

7	-0.885604	1.795687	-0.000146
6	-2.321110	-0.569164	0.000019
7	-1.282026	-1.296120	-0.000017
6	0.005880	-1.014202	-0.000029
6	0.824917	0.187974	0.000013
6	0.379365	1.576406	-0.000024
7	2.128292	-0.141535	0.000028
6	2.179122	-1.471807	0.000017
7	0.934687	-2.030063	-0.000035
7	-3.400344	-0.126204	0.000068
8	1.317767	2.527337	0.000081
1	2.213569	2.143322	0.000145
1	3.086211	-2.061770	0.000008
1	0.707606	-3.018901	-0.000068
1	-4.326515	0.253933	0.000232
1	-1.097089	2.797123	-0.000237

12

7	0.983808	1.719747	-0.000008
6	2.264245	-0.616261	0.000101
7	1.219347	-1.326055	0.000256
6	-0.060532	-1.021017	0.000008
6	-0.819988	0.215002	0.000024
6	-0.292485	1.575564	0.000025
7	-2.136408	-0.051729	-0.000234
6	-2.248058	-1.379741	0.000122
7	-1.030750	-1.996149	-0.000079
7	3.411629	-0.319814	-0.000315
8	-1.168820	2.581907	0.000051
1	-2.087593	2.256718	0.000044

1	-3.181551	-1.926958	0.000050
1	-0.851418	-2.994913	-0.000124
1	4.025395	0.479505	0.000590
1	1.253254	2.707106	0.000009

TS1213

7	0.529425	2.233216	-0.065724
6	2.443618	-0.403468	-0.018713
7	1.499687	-1.231464	-0.087381
6	0.184152	-1.006615	-0.033076
6	-0.648047	0.126510	-0.000836
6	-0.642114	1.583531	-0.011162
7	-1.951819	-0.290620	0.040462
6	-1.981093	-1.609568	0.030344
7	-0.704430	-2.075329	-0.016149
7	3.453237	0.186793	0.155585
8	-1.828672	2.052236	0.024258
1	-2.439575	0.834775	0.049195
1	-2.859656	-2.238897	0.054048
1	-0.423472	-3.051001	-0.029796
1	4.073149	0.890176	-0.212045
1	0.357126	3.246548	-0.042351

13

7	0.941128	1.947356	-0.115784
6	2.333032	-0.659291	-0.018590
7	1.276396	-1.311107	-0.147612
6	-0.015532	-0.950075	-0.050467
6	-0.743112	0.237959	0.010483
6	-0.402695	1.667036	-0.003910
7	-2.081283	-0.128978	0.072152
6	-2.206001	-1.448412	0.046697
7	-0.970693	-1.965769	-0.029529
7	3.432219	-0.264731	0.229536
8	-1.305398	2.513631	0.016737
1	-3.128818	-2.008303	0.080333
1	-0.739957	-2.953790	-0.063215
1	4.109162	0.314344	-0.244843
1	1.057144	2.962172	0.014153
1	-2.832865	0.555828	0.113050

TS1314

7	0.351997	2.307962	-0.025535
---	----------	----------	-----------

6	2.477569	-0.287235	-0.054965
7	1.618325	-1.175745	0.040816
6	0.261331	-1.055179	0.023104
6	-0.645560	-0.020531	0.061096
6	-0.887193	2.087316	0.033493
7	-1.902435	-0.581556	0.015896
6	-1.812390	-1.914901	-0.022942
7	-0.508806	-2.219645	-0.013927
7	3.384164	0.502166	0.045512
8	-2.044264	2.248672	-0.091499
1	-2.764005	-0.041457	0.013172
1	-2.633950	-2.614814	-0.048429
1	-0.118982	-3.156934	-0.037122
1	3.973730	0.885946	-0.683469
1	0.932062	2.248795	0.809788

14

7	-5.385696	-1.090579	0.228218
6	-4.350237	-0.558620	-0.043591
8	-3.284725	-0.045961	-0.162909
1	-6.235204	-1.343317	-0.247138
6	3.654644	-0.885342	0.042761
7	3.060312	0.206576	0.052556
6	1.719325	0.425386	0.025363
6	0.575766	-0.330670	-0.034864
7	-0.518297	0.486824	-0.053541
6	-0.098479	1.757163	0.004452
7	1.241173	1.739433	0.054576
7	4.336208	-1.860009	-0.133631
1	-0.728515	2.633373	0.014458
1	1.844539	2.554696	0.099198
1	4.758858	-2.497333	0.528714
1	-1.503880	0.197050	-0.093931

15

6	-2.197246	-0.089030	0.051507
7	-1.112251	-0.721584	0.080082
6	0.120349	-0.196735	0.008042
6	0.610002	1.124849	-0.068659
7	1.974551	0.987847	0.059377
6	2.345513	-0.303535	0.002777
7	1.227437	-1.041428	-0.042433
7	-3.290395	0.338902	-0.122189
1	3.354862	-0.680489	-0.086791

1	1.190069	-2.056654	-0.058472
1	-4.041643	0.815868	0.351636
1	2.629607	1.761823	0.007769

HNCO

6	0.043771	0.026788	-0.000102
7	-1.164690	-0.123701	0.000031
8	1.218277	0.011924	0.000041
1	-1.856014	0.609783	0.000065

TS0416

7	-1.568558	0.865858	0.231805
6	-2.177771	-0.133920	0.055361
7	-0.461125	-1.675519	0.013238
6	0.641340	-0.982535	0.012602
6	0.800635	0.469958	0.005883
6	-0.254085	1.482108	0.014019
7	2.103007	0.812845	-0.020033
6	2.775930	-0.331572	-0.021002
7	1.963294	-1.427272	-0.001932
7	-3.193761	-0.921303	-0.109553
8	-0.153882	2.667024	-0.099008
1	3.855424	-0.409172	-0.034956
1	2.269155	-2.392649	-0.004558
1	-0.323422	-2.687544	-0.005758
1	-3.095949	-1.918599	0.033050
1	-4.090450	-0.534722	-0.391563

16

7	2.068565	0.910388	-0.034663
6	2.832631	-0.173858	-0.042728
7	2.114500	-1.328310	-0.008859
6	0.751564	-1.001660	0.023447
6	0.796086	0.460820	0.013967
6	-0.299543	1.419539	0.028317
7	-0.276105	-1.799267	0.032530
8	-0.285852	2.600577	-0.133981
1	3.914618	-0.160086	-0.071191
1	2.497926	-2.265515	-0.014233
1	-0.002191	-2.784015	0.016573
7	-1.600255	0.754107	0.338971
6	-2.378881	-0.074688	0.061404
7	-3.310463	-0.936601	-0.157486
1	-4.203660	-0.657455	-0.553680

1	-3.104713	-1.920687	-0.005511
TS1617			
7	-1.777836	-0.029367	-0.311750
6	-2.910691	-0.309314	-0.371872
7	0.480362	-1.633058	1.135287
6	1.228360	-0.873388	0.414618
6	1.032807	0.531554	0.083097
6	-0.020027	1.378127	0.438121
7	2.057870	1.043140	-0.646873
6	2.892408	0.020382	-0.811727
7	2.465168	-1.118662	-0.219173
7	-4.176287	-0.662664	-0.478126
8	-0.616292	2.283726	0.789238
1	3.822697	0.085873	-1.361857
1	2.959602	-2.003807	-0.213570
1	0.846399	-2.581551	1.250046
1	-4.557544	-1.370513	0.134985
1	-4.822892	-0.079691	-0.992490
17			
7	1.408804	-0.092141	-1.509177
6	2.185602	-1.103921	-1.132156
7	2.331608	-1.203183	0.211529
6	1.599177	-0.169771	0.827280
6	1.039418	0.494736	-0.344014
6	0.176653	1.577893	-0.291170
7	1.433510	0.165712	2.057363
8	-0.435895	2.532990	-0.241575
1	2.662780	-1.784887	-1.825887
1	2.885696	-1.900077	0.697313
1	1.913667	-0.434757	2.731715
7	-1.889056	-0.127066	-0.020154
6	-2.990053	-0.515678	0.020080
7	-4.219295	-1.007599	0.083731
1	-4.807223	-0.745503	0.864363
1	-4.691535	-1.248316	-0.778059
18			
7	-0.208311	2.064625	-0.000151
6	-0.551545	0.827320	-0.000008
6	0.348540	-0.326969	0.000092
6	1.726591	-0.242008	0.000041
7	-0.318471	-1.510501	-0.000194

6	-1.603934	-1.160933	-0.000048
7	-1.801187	0.178207	0.000199
8	2.860382	-0.151448	0.000058
1	-2.418338	-1.875537	-0.000083
1	-2.704459	0.642686	0.000350
1	-0.982391	2.733652	-0.000173

H₂NCN

7	-1.121978	0.000003	-0.076569
6	0.219626	-0.000017	0.000177
7	1.386084	0.000007	0.011803
1	-1.583231	0.848752	0.226150
1	-1.583265	-0.848724	0.226156

TS0919

7	-1.755659	0.753641	-0.280256
6	-2.274637	-0.376145	0.076856
7	-0.280720	-1.712159	-0.430194
6	0.749842	-0.967194	-0.175153
6	0.734779	0.467100	0.041504
6	-0.397155	1.368738	-0.076625
7	1.976230	0.938143	0.286382
6	2.772299	-0.122539	0.235150
7	2.104193	-1.279747	-0.043017
7	-3.035344	-1.147141	0.554746
8	-0.385153	2.567050	-0.087283
1	3.842389	-0.093982	0.395804
1	2.517641	-2.200387	-0.126468
1	-0.077671	-2.703555	-0.567681
1	-3.348945	-2.090637	0.364840
1	-2.423871	1.463240	-0.592251

19

7	1.896196	0.987663	0.359628
6	2.746627	-0.028804	0.308041
7	2.152499	-1.202611	-0.042915
6	0.785703	-0.959762	-0.226814
6	0.688912	0.467598	0.042838
6	-0.451538	1.352141	-0.106504
7	-1.812627	0.707667	-0.337749
6	-2.309065	-0.386051	0.116122
7	-0.173542	-1.766236	-0.560414
8	-0.466671	2.548003	-0.125570
7	-2.916789	-1.220500	0.690797

1	3.805108	0.047636	0.521751
1	2.615546	-2.097947	-0.140604
1	-2.470449	1.376618	-0.745333
1	0.133997	-2.724902	-0.735301
1	-3.134833	-2.198036	0.536522

TS1920

7	1.921402	0.728333	-0.663576
6	2.612753	-0.284770	-0.468357
7	0.185248	-1.365266	1.166193
6	-0.775892	-0.856424	0.478223
6	-0.945934	0.537738	0.090857
6	-0.101537	1.611532	0.373242
7	-2.095251	0.751068	-0.601691
6	-2.662476	-0.449450	-0.678056
7	-1.943547	-1.423349	-0.069060
7	3.126249	-1.374517	-0.335248
8	0.309769	2.626597	0.692300
1	-3.606867	-0.637773	-1.173419
1	-2.206299	-2.400827	-0.005684
1	0.092148	-2.369372	1.336980
1	2.290823	1.426690	-1.306642
1	3.831851	-1.597124	0.358597

20

6	2.541110	-0.341216	-0.577273
7	1.902820	0.658960	-0.928187
7	2.967539	-1.422958	-0.216096
1	3.747139	-1.525516	0.425368
1	2.205584	1.151363	-1.765877
7	0.095632	-1.118501	1.505983
6	-0.779537	-0.757784	0.636220
6	-0.977085	0.584282	0.096890
6	-0.222756	1.698143	0.426730
7	-1.994475	0.644236	-0.802009
6	-2.454652	-0.601801	-0.857050
7	-1.788947	-1.461642	-0.047292
8	0.290921	2.656822	0.759785
1	-3.283653	-0.908227	-1.483014
1	-1.988413	-2.450774	0.057550
1	0.071501	-2.111820	1.747799

HNCNH

6	0.000000	0.025001	0.000083
---	----------	----------	----------

7	-1.219550	-0.082321	0.100276
7	1.219543	-0.082014	-0.100554
1	1.822826	0.499442	0.471004
1	-1.822776	0.500894	-0.469553

TS1621

7	1.887277	1.002613	-0.050420
6	2.722687	-0.028733	-0.039240
7	2.071810	-1.222469	0.017211
6	0.699521	-0.981806	0.038287
6	0.646245	0.488879	0.002023
6	-0.487031	1.450961	0.029828
7	-0.230989	-1.905898	0.067144
8	-0.433026	2.609695	-0.234946
1	3.801902	0.049501	-0.069024
1	2.510689	-2.135814	0.021173
1	0.137301	-2.855914	0.116219
7	-1.732869	0.830747	0.520080
6	-2.367169	-0.073776	0.076814
7	-2.711477	-1.245394	-0.253939
1	-3.544625	-1.477578	-0.786856
1	-1.712838	-1.808093	-0.148749

21

7	1.856640	1.088530	0.110577
6	2.775402	0.131105	0.110919
7	2.219235	-1.121512	0.008358
6	0.860492	-0.964877	-0.057510
6	0.663250	0.487836	0.018909
6	-0.586169	1.332855	-0.026878
7	-1.736154	0.762647	0.534675
6	-2.428818	-0.196116	0.226336
7	0.018392	-1.980801	-0.184399
8	-0.536146	2.460695	-0.439226
7	-3.118102	-1.150366	-0.080708
1	3.844185	0.286412	0.185113
1	2.732335	-1.995739	-0.028223
1	0.352799	-2.937690	-0.227624
1	-0.992475	-1.864692	-0.248025
1	-4.032700	-1.108166	-0.517602

TS2122

7	-1.800964	1.315728	0.424993
6	-2.798702	0.515908	0.634249

7	-2.510065	-0.801153	0.275543
6	-1.234345	-0.851237	-0.194950
6	-0.789575	0.512851	-0.096070
6	0.398748	1.147230	-0.442174
7	1.708152	-0.450704	-0.237520
6	2.811859	-0.398162	0.252771
7	-0.651350	-1.946929	-0.672676
8	1.011366	2.082811	-0.727884
7	3.911590	-0.520882	0.837150
1	-3.764294	0.797188	1.032556
1	-3.150564	-1.583336	0.339359
1	-1.103042	-2.850452	-0.631960
1	0.339382	-1.910476	-0.885692
1	4.658146	0.152630	0.653422

22

7	-2.703664	0.991178	0.000036
6	-3.365304	-0.114428	0.000047
7	-2.536849	-1.246727	0.000014
6	-1.241358	-0.839922	-0.000019
6	-1.351588	0.595385	-0.000006
6	-0.361368	1.520944	-0.000027
7	-0.180144	-1.635172	-0.000055
8	0.455385	2.324915	-0.000043
1	-4.443213	-0.206002	0.000078
1	-2.854665	-2.208701	0.000017
1	-0.278967	-2.641209	-0.000048
1	0.769270	-1.249268	-0.000084
7	2.459585	-0.348299	-0.000001
6	3.653990	-0.270687	0.000025
7	4.921673	-0.357028	0.000009
1	5.434053	0.530438	0.000240

23

7	1.367393	0.828659	0.000000
6	1.973961	-0.308182	0.000000
7	1.087502	-1.397888	0.000000
6	0.000000	0.501062	0.000000
6	-0.180968	-0.924612	0.000000
6	-0.957462	1.462711	0.000000
8	-1.773710	2.266183	0.000000
7	-1.281355	-1.677739	0.000000
1	3.045832	-0.455099	0.000000
1	1.357341	-2.375233	0.000000

1	-1.236500	-2.688072	0.000000
1	-2.204959	-1.268164	0.000000
HNCN raical			
7	1.306971	0.015892	0.000019
6	0.108227	0.014077	-0.000042
7	-1.161586	-0.135882	0.000014
1	-1.667053	0.755468	0.000020
TS0124			
7	1.440452	0.801395	-0.018610
6	1.669498	-0.543830	0.002426
7	0.598796	-1.380337	-0.084754
6	-0.560834	-0.748060	-0.157849
6	-0.959664	0.603559	-0.084565
6	0.158075	1.549909	-0.029265
7	-2.283423	0.607546	0.078667
6	-2.635258	-0.735840	0.105479
7	-1.584431	-1.590761	-0.034590
7	2.896129	-1.043066	0.097196
8	0.191328	2.747931	0.014569
1	-3.660827	-1.056433	0.230417
1	3.717398	-0.459335	0.188365
1	-0.358886	-2.371218	0.095515
1	2.237714	1.432371	0.009195
1	3.030412	-2.046699	0.077245
24			
7	-1.472971	0.872668	-0.000327
6	-1.721947	-0.491892	0.000273
7	-0.671777	-1.416344	0.001173
6	0.631709	-0.958541	0.000573
6	0.943189	0.534048	-0.000227
6	-0.168673	1.482862	-0.000527
7	2.256257	0.697787	-0.000727
6	2.774508	-0.648400	-0.000227
7	1.824064	-1.652347	0.000673
7	-3.010117	-0.954826	0.000173
8	-0.124620	2.706402	-0.000827
1	3.861242	-0.841212	-0.000527
1	-3.782814	-0.322035	-0.000227
1	-2.250129	1.512909	-0.000827
1	-3.212721	-1.932324	0.000273
1	-0.849534	-2.405578	0.001973

TS2425

7	-1.557065	0.663452	0.369733
6	-1.634501	-0.758867	0.048173
7	-0.530653	-1.540205	0.121172
6	0.697313	-0.909785	0.096148
6	0.845329	0.549327	-0.022341
6	-0.286662	1.469489	-0.000243
7	2.130985	0.816414	-0.134444
6	2.718619	-0.436252	-0.073069
7	1.874125	-1.498392	0.053398
7	-2.848972	-0.884724	-0.348051
8	-0.370148	2.647679	-0.139872
1	3.793544	-0.557866	-0.120566
1	-2.758274	0.472685	-0.169303
1	-0.577121	-2.544704	-0.042358
1	-1.720445	0.818886	1.374218
1	-3.296051	-1.749724	-0.647679

25

7	1.546701	0.793380	0.319474
6	1.804283	-0.639588	0.002515
7	0.655113	-1.423502	0.101682
6	-0.596705	-0.906849	0.068375
6	-0.916126	0.514232	-0.012477
6	0.068305	1.547099	-0.020995
7	-2.233371	0.643758	-0.098702
6	-2.672416	-0.672892	-0.047436
7	-1.723872	-1.621815	0.047421
7	2.987867	-0.936145	-0.285169
8	0.136328	2.716841	-0.146537
1	-3.728923	-0.908251	-0.081884
1	2.277470	1.341478	-0.153092
1	3.170895	-1.915060	-0.509454
1	0.751252	-2.436420	0.055085
1	1.687563	0.941796	1.328812

TS2526

7	2.107578	1.005965	0.519581
6	2.042885	-0.263523	0.072253
7	0.898593	-1.078749	0.087207
6	-0.392674	-0.818452	0.069507
6	-1.183443	0.438325	0.026496
6	-0.828407	1.741646	-0.158918

7	-2.507596	0.119306	-0.002688
6	-2.492319	-1.251353	0.041905
7	-1.301351	-1.834533	0.067084
7	2.903656	-1.072030	-0.474090
8	-0.546700	2.842034	-0.306836
1	-3.419752	-1.810949	0.053162
1	1.533035	1.265954	1.312465
1	1.796559	-1.874782	-0.414787
1	3.006818	1.473005	0.493017
1	3.874532	-0.849067	-0.676284

26a

7	2.070616	0.169792	1.195187
6	1.845909	-0.542206	0.074531
7	0.713090	-1.249779	-0.078753
6	-0.514023	-0.817715	-0.017786
6	-1.113458	0.556319	-0.051143
6	-0.515706	1.770909	-0.167749
7	-2.468267	0.451692	-0.010939
6	-2.661711	-0.910989	0.047473
7	-1.583585	-1.674700	0.036774
7	2.770247	-0.615138	-0.882788
8	0.021955	2.780324	-0.267718
1	-3.665945	-1.314277	0.098645
1	2.987881	0.546058	1.402660
1	3.699167	-0.229094	-0.779624
1	1.461852	0.026648	1.990559
1	2.580638	-1.182898	-1.698824

TS26ab

7	2.426713	-0.287508	1.163802
6	1.836884	-0.580996	0.000006
7	0.671559	-1.255862	0.000000
6	-0.543929	-0.801209	-0.000003
6	-1.110570	0.586890	-0.000008
6	-0.471503	1.783888	-0.000014
7	-2.468882	0.512616	-0.000003
6	-2.694058	-0.846569	0.000005
7	-1.635364	-1.635826	0.000003
7	2.426758	-0.287564	-1.163781
8	0.111196	2.774296	-0.000018
1	-3.708467	-1.227052	0.000011
1	3.379489	0.049924	1.216372
1	3.379530	0.049881	-1.216328

1	2.006681	-0.620015	2.022069
1	2.006768	-0.620121	-2.022050

26b

7	-2.770771	-0.616293	-0.881840
6	-1.845804	-0.542182	0.074724
7	-0.713211	-1.250276	-0.078509
6	0.513885	-0.817915	-0.017612
6	1.113221	0.556182	-0.051360
6	0.515573	1.770772	-0.168670
7	2.468034	0.451648	-0.011379
6	2.661592	-0.910985	0.047599
7	1.583510	-1.674762	0.037260
7	-2.069507	0.171559	1.194520
8	-0.021854	2.780382	-0.267858
1	3.665859	-1.314173	0.098880
1	-3.699256	-0.229103	-0.779087
1	-2.986675	0.548028	1.402129
1	-2.581569	-1.184828	-1.697438
1	-1.460708	0.028643	1.989923

TS2627

7	2.276519	0.378555	1.065386
6	1.836543	-0.411959	0.125873
7	0.752094	-1.116984	-0.124023
6	-0.515096	-0.810475	-0.031039
6	-1.237005	0.499263	-0.045925
6	-0.751021	1.764189	-0.165302
7	-2.573374	0.270894	0.022236
6	-2.639551	-1.104029	0.074530
7	-1.492665	-1.763042	0.033910
7	3.073927	-0.576909	-0.662874
8	-0.300222	2.813832	-0.268936
1	-3.600208	-1.600048	0.143042
1	3.395374	0.220601	0.333726
1	3.432788	-1.536006	-0.662387
1	1.728722	0.671045	1.871824
1	3.026376	-0.235787	-1.625984

27

7	3.084659	-0.720351	-0.530715
6	1.832216	-0.235695	0.194387
7	0.836257	-1.115783	-0.034064
6	-0.443697	-0.834458	-0.040722

6	-1.212252	0.446379	-0.142137
6	-0.789747	1.737034	-0.205403
7	-2.542099	0.175480	-0.042088
6	-2.560448	-1.191291	0.093699
7	-1.389836	-1.809224	0.118222
7	2.072561	0.767497	0.932546
8	-0.410979	2.818904	-0.265954
1	-3.503404	-1.717286	0.182489
1	3.857347	-0.080768	-0.309528
1	3.317330	-1.669963	-0.213697
1	1.285166	1.065213	1.508672
1	2.944157	-0.763580	-1.546557

TS2728

7	2.476197	-1.885079	-0.553534
6	1.348136	-1.572912	-0.316187
7	0.135559	-1.556189	-0.060863
6	-0.927628	-0.797691	0.040585
6	-1.095243	0.671098	-0.109136
6	-0.181102	1.637930	-0.429866
7	-2.391699	0.987844	0.087948
6	-2.965169	-0.243311	0.351162
7	-2.156135	-1.292951	0.330463
7	3.170483	0.954003	0.921691
8	0.593567	2.430893	-0.704040
1	-4.025362	-0.318613	0.560506
1	3.631774	1.663868	0.353367
1	2.686668	1.464827	1.659408
1	3.323495	-1.337603	-0.642261
1	3.920092	0.456303	1.402016

28

7	-2.351836	-0.366841	0.000428
6	-1.255191	-0.789834	-0.000179
7	-0.113298	-1.403743	0.000009
6	1.073064	-0.839399	0.000026
6	1.509137	0.584687	-0.000012
6	0.763595	1.720164	-0.000046
7	2.868514	0.635238	-0.000080
6	3.212421	-0.694321	-0.000031
7	2.221109	-1.574772	0.000017
8	0.107216	2.662232	0.000063
1	4.255140	-0.987215	-0.000079
1	-3.948417	-0.195369	-0.000366

7	-5.031021	-0.110907	-0.000157
1	-5.307372	0.870796	-0.079520
1	-5.409388	-0.494791	0.869456
1	-5.420126	-0.631885	-0.790071

29

7	1.135830	-0.754615	0.000671
6	0.246011	0.224758	0.000335
6	-1.215866	0.051288	0.000313
6	-1.930060	-1.122786	0.000742
7	-1.810568	1.258803	0.000111
6	-0.724863	2.120833	-0.000350
7	0.479674	1.562404	-0.000203
8	-2.492614	-2.113517	-0.000826
1	-0.879881	3.193114	-0.000780
6	2.401710	-0.585529	0.000542
7	3.565748	-0.623584	-0.001250
1	4.564411	-0.517424	0.002592

NH₃

7	-0.000017	-0.000009	0.101715
1	0.732304	-0.586863	-0.237323
1	0.142200	0.927575	-0.237317
1	-0.874386	-0.340651	-0.237368

30

7	-3.127535	-0.680334	-0.000746
6	-1.996195	-0.998734	-0.000546
7	-0.801960	-1.503289	-0.000346
6	0.326452	-0.830761	-0.000046
6	0.627835	0.627714	0.000254
6	-0.220180	1.688702	0.000054
7	1.976609	0.804798	0.000654
6	2.443137	-0.486892	0.000654
7	1.538186	-1.455911	0.000254
8	-0.961493	2.565521	-0.000246
1	3.508541	-0.681189	0.001054

NH₄⁺

7	-0.000003	0.000019	0.000011
1	-0.040102	0.414488	0.936837
1	0.791991	-0.649037	-0.052978
1	-0.871007	-0.507731	-0.186676

1	0.119136	0.742148	-0.697264
TS0131			
7	-1.411844	0.970250	0.000143
6	-1.780499	-0.369837	0.000185
7	-0.922947	-1.370004	0.000100
6	0.409972	-1.093488	-0.000039
6	0.849352	0.299237	-0.000088
6	-0.090191	1.420999	0.000006
7	2.196863	0.477573	-0.000229
6	3.152324	-0.206344	-0.000325
7	1.382592	-1.968671	-0.000138
7	-3.093512	-0.636533	0.000321
8	0.223529	2.595095	-0.000029
1	4.152283	-0.609681	-0.000432
1	1.054666	-2.936975	-0.000102
1	-3.377828	-1.606777	0.000351
1	-3.808401	0.075297	0.000388
1	-2.112766	1.705663	0.000213
31			
7	-2.220656	0.031595	-0.000007
6	-3.371834	-0.015076	-0.000025
1	-4.447453	-0.044146	-0.000070
7	1.189767	-1.151457	0.000028
6	1.856201	0.050834	0.000050
7	1.229402	1.223235	0.000051
6	-0.120668	1.235008	0.000017
6	-0.870608	0.021909	0.000042
6	-0.211199	-1.285056	0.000046
7	-0.830736	2.381129	-0.000030
7	3.193333	0.039192	-0.000128
8	-0.763317	-2.366361	-0.000024
1	3.744671	-0.806368	0.000288
1	3.673132	0.929610	-0.000035
1	1.694190	-2.033915	-0.000166
1	-0.177122	3.174127	-0.000005
TS3132			
7	-1.119642	1.038913	0.179530
6	-1.854944	-0.088487	-0.202286
7	-1.321484	-1.284956	-0.237551
6	0.000471	-1.372557	-0.052855
6	0.951619	-0.213824	0.058620

6	0.276563	1.105646	0.285225
7	2.201259	-0.152129	-0.441676
6	3.311291	-0.138591	-0.778745
7	0.722265	-1.613852	1.048960
7	-3.155139	0.095260	-0.471753
8	0.868245	2.150433	0.444879
1	4.355708	-0.137879	-1.034863
1	0.196810	-1.621855	1.943824
1	-3.710249	-0.714267	-0.714443
1	-3.613797	0.991820	-0.414055
1	-1.575245	1.942941	0.258181

32

7	2.255258	-0.212953	-0.311391
6	3.329144	-0.171793	-0.712146
1	4.337955	-0.139819	-1.090028
7	-1.102396	1.027105	0.167629
6	-1.869585	-0.091604	-0.188378
7	-1.350674	-1.280256	-0.324320
6	-0.029558	-1.454252	-0.137511
6	0.944795	-0.279059	0.163792
6	0.288468	1.073705	0.227287
7	0.685945	-1.411271	1.059585
7	-3.184058	0.117837	-0.373810
8	0.910620	2.114497	0.271262
1	-3.632267	1.009362	-0.229277
1	-3.759469	-0.676400	-0.618220
1	-1.533436	1.946760	0.189804
1	0.194145	-1.201098	1.935519

TS3233

7	2.120664	0.050232	-1.027182
6	3.172617	-0.477372	-0.987369
1	4.115309	-0.984010	-0.886291
7	-1.200795	0.969413	-0.157877
6	-1.817312	-0.261811	-0.209697
7	-1.205995	-1.375729	0.265605
6	0.068796	-1.144171	0.394185
6	0.920596	-0.051458	0.218689
6	0.135729	1.220416	0.313690
7	1.173362	-1.177127	1.185723
7	-3.070342	-0.354833	-0.642384
8	0.505084	2.326418	0.606679
1	-3.612207	0.438332	-0.956195

1	-3.512792	-1.265834	-0.628562
1	-1.742048	1.811977	-0.334710
1	1.110236	-1.109138	2.208136
33			
7	1.706873	1.446460	-0.158937
6	2.616650	2.160281	-0.150709
1	3.461742	2.821712	-0.143398
7	-0.867103	-0.089154	1.077403
6	-1.503762	0.447288	-0.010654
7	-1.175159	0.143025	-1.320567
6	-0.293001	-0.796366	-1.255202
6	0.332862	-1.529245	-0.279381
6	0.280038	-0.990730	1.079605
7	0.860421	-1.456122	-1.605859
7	-2.470967	1.335195	0.159493
8	0.902962	-1.210346	2.080875
1	-2.780527	1.659299	1.065913
1	-2.910074	1.720948	-0.668514
1	-1.086436	0.272784	2.001481
1	1.116427	-2.195187	-2.265173
34			
7	-0.464998	1.058869	-0.075739
6	-1.333718	-0.001998	0.000960
7	-0.895109	-1.301338	0.144726
6	0.361996	-1.312236	-0.143281
6	1.345598	-0.380607	-0.420540
6	0.993472	1.000601	-0.039158
7	1.653082	-1.693095	0.077128
7	-2.639260	0.204165	0.023150
8	1.652910	1.975671	0.184435
1	-3.062473	1.122019	-0.025132
1	-3.248351	-0.602549	0.105832
1	-0.831444	2.007273	-0.036948
1	2.138887	-2.046871	0.908036
HCN			
7	0.000128	-0.657883	0.000000
6	0.000128	0.503353	0.000000
1	-0.001659	1.585066	0.000000