

Supplementary Information

Adsorption of nitrogen-containing compounds on hydroxylated α -quartz surfaces

Oksana Tsendra,^{a,b} A. Daniel Boese,^{*c} Olexandr Isayev,^d Leonid Gorb,^{e,f} Andrea Michalkova
Scott,^g Frances C. Hill,^g Mykola M. Ilchenko,^f Victor Lobanov,^b Danuta Leszczynska,^h and
Jerzy Leszczynski^a

^a*Interdisciplinary Nanotoxicity Center, Department of Chemistry and Biochemistry, Jackson State University, 1400 Lynch Street, P. O. Box 17910, Jackson, MS 39217, USA*

^b*Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, 17 General Naumov St., Kyiv, 03164, Ukraine*

^c*Institute of Chemistry, Physical and Theoretical Chemistry, University of Graz, Heinrichstrasse 28/IV, 8010 Graz, Austria*

^d*UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA*

^e*HX5, LLC, Vicksburg, MS 39180, USA*

^f*Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine, 150 Zabolotnogo, Kyiv 03143, Ukraine*

^g*U. S. Army Engineer Research and Development Center (ERDC), Vicksburg, MS 39180, USA*

^h*Department of Civil and Environmental Engineering, Jackson State University, Jackson, MS 39217, USA*

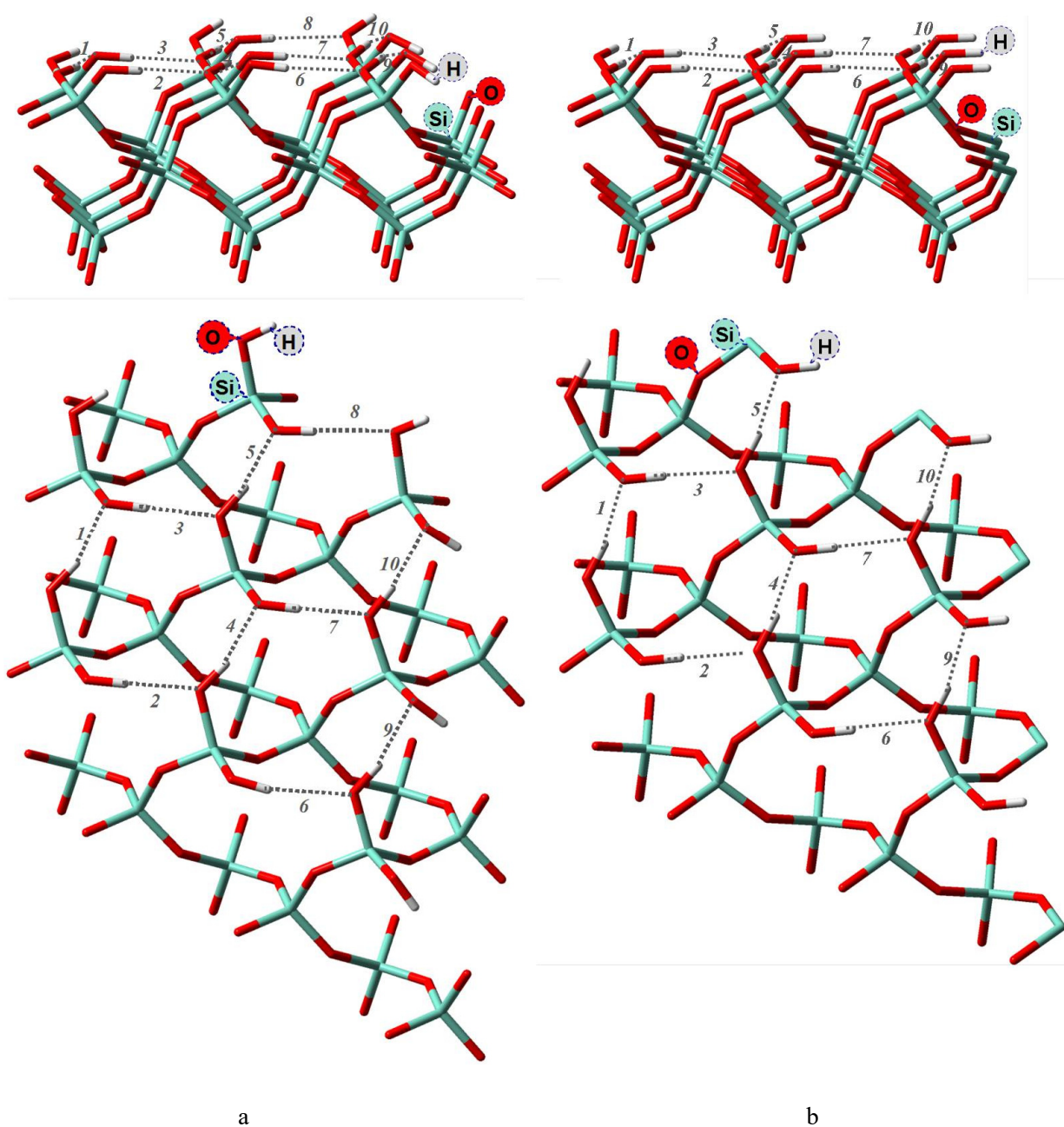


Fig. S1 Optimized structure of (001) α -quartz surface and intra-surface H-bonds (1-10) as obtained at the PBE+D3/6-31G** (a) and the PBE+D2/PBC (b) levels of theory (side and top view). Please note that in (b) some bonds (like 8) are present, but not shown because they go beyond the periodic box limit.

Table S1 Geometrical characteristics of the O-H $\cdots$ O intrasurface hydrogen bonds including H $\cdots$ O, O $\cdots$ O distances (Å), and <O $\cdots$ H-O angles (°), for the isolated model of the (001) surface of α -quartz optimized at the PBE+D3/6-31G** and PBE+D2/PBC levels in comparison with the M06-2x/6-31G** functional

Bond	H $\cdots$ O			O $\cdots$ O			<O $\cdots$ H-O		
	PBE	PBC	M06-2x	PBE	PBC	M06-2x	PBE	PBC	M06-2x
<i>1</i>	1.84	1.80	1.89	2.79	2.78	2.83	162.9	166.5	162.4
<i>2</i>	1.99	2.03	2.02	2.98	3.02	2.98	179.2	174.5	175.0
<i>3</i>	2.00	2.03	2.02	2.99	3.02	2.99	177.3	174.5	176.0
<i>4</i>	1.87	1.80	1.94	2.81	2.78	2.85	159.8	166.5	154.5
<i>5</i>	1.76	1.80	1.83	2.73	2.78	2.76	164.4	166.5	160.7
<i>6</i>	2.28	2.03	2.32	3.23	3.02	3.25	165.7	174.5	159.7
<i>7</i>	1.91	2.03	1.94	2.89	3.02	2.91	179.3	174.5	178.3
<i>8</i>	2.17	-	2.19	3.15	-	3.15	179.1	-	170.7
<i>9</i>	2.02	1.80	2.12	2.93	2.78	2.94	153.1	166.5	142.1
<i>10</i>	1.90	1.80	1.96	2.84	2.78	2.84	159.1	166.5	149.8

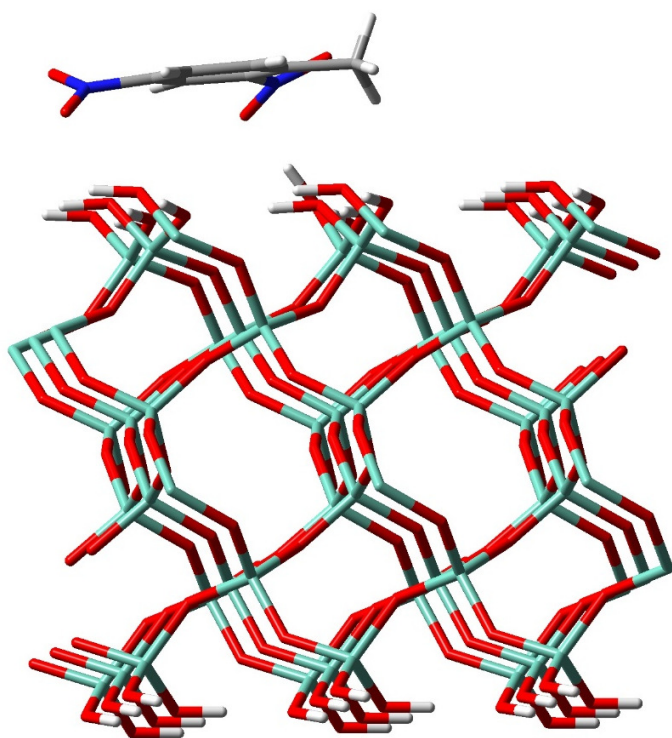


Fig. S2 Full optimized structure of the (001) α -quartz surface with DNT using periodic boundary conditions.

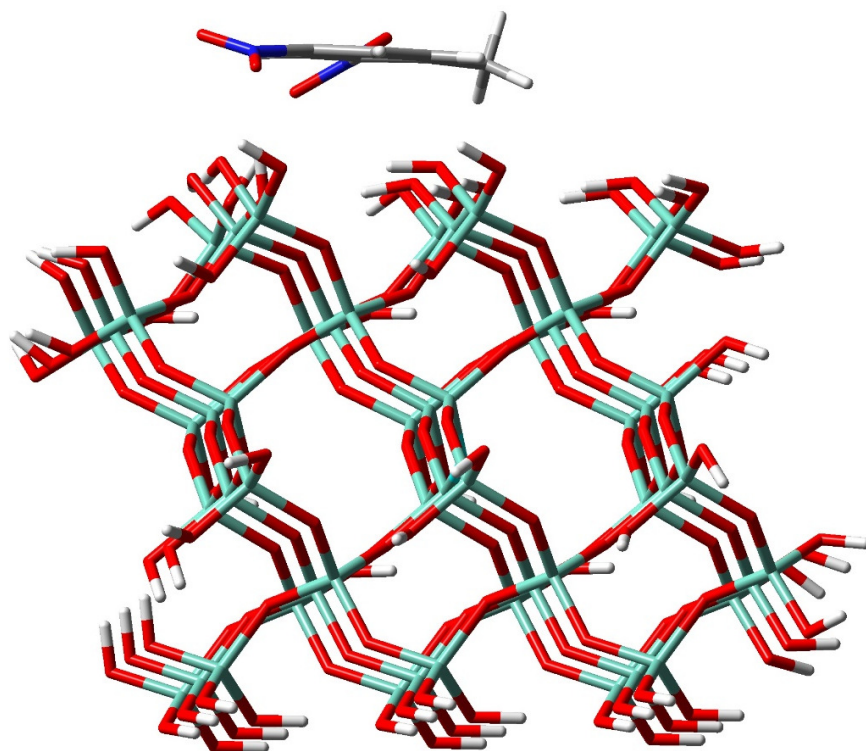


Fig. S3 Full optimized structure of the (001) α -quartz surface with DNT using the cluster approach.

001 Surface PBE/6-31G**

zpe= 1.4222589 hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.85	21.83	158.77	3202.85	4113.96	3.22608
293.15	0.1000000	22.94	21.88	165.14	3170.08	4143.09	3.32745
298.15	0.1000000	22.98	21.91	168.31	3153.32	4157.92	3.37776
303.15	0.1000000	23.02	21.93	171.48	3136.31	4172.92	3.42780
313.15	0.1000000	23.10	21.98	177.80	3101.53	4203.45	3.52712
323.15	0.1000000	23.18	22.03	184.08	3065.77	4234.63	3.62541
333.15	0.1000000	23.26	22.07	190.34	3029.02	4266.46	3.72267

Table S2 Vibrational frequencies of the 001 surface of α -quartz

1	-592.12	42	-133.68	83	-59.32	124	37.93
2	-583.77	43	-130.63	84	-58.30	125	39.48
3	-573.18	44	-128.31	85	-55.43	126	42.18
4	-569.50	45	-127.37	86	-54.31	127	43.74
5	-566.07	46	-123.74	87	-52.22	128	46.45
6	-560.41	47	-123.01	88	-50.35	129	48.59
7	-538.73	48	-122.34	89	-49.10	130	49.83
8	-521.54	49	-122.07	90	-47.76	131	52.18
9	-506.27	50	-121.02	91	-45.81	132	54.16
10	-503.56	51	-117.66	92	-44.67	133	56.42
11	-495.07	52	-115.48	93	-43.09	134	57.18
12	-488.94	53	-112.93	94	-42.70	135	61.78
13	-484.58	54	-112.20	95	-39.42	136	62.52
14	-470.43	55	-111.16	96	-37.59	137	63.31
15	-467.23	56	-103.72	97	-35.47	138	64.79
16	-459.33	57	-98.28	98	-34.61	139	65.34
17	-446.66	58	-97.46	99	-32.94	140	69.72
18	-434.35	59	-96.67	100	-30.82	141	71.91
19	-423.24	60	-94.97	101	-27.97	142	73.22
20	-419.83	61	-93.61	102	-25.29	143	74.49
21	-417.02	62	-93.52	103	-24.35	144	76.38
22	-409.08	63	-91.43	104	-22.60	145	77.19
23	-402.56	64	-90.50	105	-18.18	146	79.90
24	-399.87	65	-89.29	106	-14.58	147	81.33
25	-395.49	66	-87.48	107	-12.85	148	82.13
26	-392.14	67	-86.10	108	-0.00	149	84.06
27	-391.57	68	-86.02	109	-0.00	150	84.41
28	-388.86	69	-85.14	110	-0.00	151	85.53
29	-387.81	70	-83.53	111	-0.00	152	87.49
30	-386.98	71	-81.53	112	0.00	153	89.46
31	-383.62	72	-80.47	113	0.00	154	91.44
32	-381.68	73	-80.04	114	7.64	155	94.08
33	-378.36	74	-78.69	115	13.29	156	95.75
34	-367.12	75	-75.28	116	18.90	157	96.82
35	-364.11	76	-72.10	117	19.82	158	99.16
36	-354.71	77	-70.28	118	22.27	159	100.93
37	-348.68	78	-69.69	119	24.25	160	101.66
38	-329.38	79	-65.94	120	29.06	161	103.00
39	-324.05	80	-64.73	121	33.96	162	105.34
40	-291.56	81	-63.45	122	35.27	163	105.77
41	-134.92	82	-60.30	123	36.60	164	109.08

165	109.78	223	203.63	281	287.47	339	350.65
166	112.16	224	205.47	282	289.25	340	351.83
167	112.90	225	206.25	283	289.95	341	353.30
168	114.11	226	208.34	284	291.31	342	354.14
169	115.04	227	211.99	285	292.27	343	355.44
170	116.63	228	213.23	286	292.81	344	356.27
171	118.67	229	214.06	287	293.99	345	356.74
172	122.54	230	214.88	288	294.95	346	357.91
173	123.10	231	215.67	289	296.45	347	359.58
174	125.19	232	218.39	290	296.88	348	360.01
175	126.02	233	222.87	291	297.90	349	361.25
176	127.16	234	225.40	292	298.87	350	361.57
177	128.82	235	228.14	293	299.68	351	363.47
178	130.18	236	230.27	294	300.14	352	364.56
179	133.96	237	231.01	295	301.74	353	366.05
180	135.35	238	231.98	296	302.24	354	366.83
181	136.43	239	234.55	297	303.63	355	368.28
182	137.20	240	235.81	298	304.76	356	368.98
183	139.81	241	237.29	299	305.59	357	370.73
184	141.00	242	239.25	300	306.44	358	373.02
185	144.60	243	239.65	301	307.18	359	374.01
186	144.86	244	241.88	302	307.78	360	374.26
187	147.41	245	244.40	303	309.24	361	375.59
188	149.87	246	246.29	304	310.37	362	377.57
189	151.33	247	247.83	305	311.15	363	377.95
190	152.20	248	250.13	306	311.47	364	378.19
191	155.76	249	250.96	307	312.89	365	379.67
192	157.08	250	251.88	308	313.37	366	380.56
193	158.49	251	252.70	309	314.67	367	381.49
194	161.42	252	254.28	310	314.89	368	382.59
195	163.69	253	254.84	311	316.79	369	383.99
196	165.66	254	257.26	312	318.90	370	384.39
197	166.62	255	258.61	313	319.71	371	385.73
198	167.51	256	259.78	314	321.03	372	387.36
199	167.90	257	260.53	315	321.95	373	388.74
200	170.57	258	260.65	316	322.38	374	390.14
201	172.28	259	262.49	317	323.38	375	390.53
202	174.77	260	263.90	318	324.59	376	392.10
203	175.33	261	265.13	319	326.84	377	392.92
204	177.24	262	265.47	320	328.22	378	393.48
205	178.39	263	266.08	321	328.58	379	396.08
206	179.25	264	267.37	322	330.79	380	396.34
207	180.16	265	268.79	323	331.95	381	398.65
208	183.32	266	270.11	324	332.54	382	399.64
209	184.92	267	271.28	325	334.21	383	401.17
210	185.63	268	272.06	326	335.49	384	402.20
211	188.06	269	272.87	327	335.88	385	403.44
212	190.09	270	274.72	328	337.97	386	403.97
213	192.06	271	277.62	329	339.60	387	404.59
214	193.16	272	278.01	330	340.35	388	405.16
215	194.83	273	279.33	331	341.65	389	408.53
216	195.74	274	280.22	332	342.05	390	408.92
217	196.49	275	281.27	333	344.24	391	409.86
218	197.89	276	281.52	334	344.48	392	411.07
219	199.12	277	282.80	335	345.62	393	412.44
220	200.36	278	284.50	336	347.44	394	413.63
221	200.93	279	284.97	337	348.37	395	414.50
222	202.58	280	286.37	338	349.07	396	415.06

397	416.20	455	622.04	513	776.04	571	896.53
398	417.97	456	625.89	514	782.06	572	898.51
399	418.88	457	628.88	515	783.81	573	902.11
400	419.76	458	630.44	516	784.96	574	903.70
401	421.68	459	634.57	517	786.25	575	910.47
402	424.29	460	639.34	518	787.94	576	910.72
403	425.71	461	643.14	519	788.79	577	913.65
404	426.72	462	644.97	520	790.64	578	916.76
405	427.83	463	646.35	521	791.67	579	920.19
406	430.60	464	649.06	522	793.99	580	922.46
407	431.80	465	650.30	523	795.43	581	926.05
408	433.98	466	655.12	524	797.67	582	927.51
409	434.61	467	663.15	525	799.17	583	930.57
410	436.78	468	666.31	526	799.61	584	933.79
411	439.29	469	672.13	527	802.69	585	937.18
412	440.76	470	675.36	528	804.53	586	939.97
413	446.77	471	677.80	529	806.69	587	941.43
414	450.57	472	681.05	530	808.67	588	942.67
415	453.14	473	682.44	531	809.39	589	947.52
416	476.52	474	685.61	532	810.53	590	948.95
417	483.10	475	689.19	533	810.86	591	951.94
418	493.57	476	691.97	534	814.79	592	954.59
419	495.45	477	695.11	535	815.30	593	956.70
420	504.63	478	699.39	536	816.81	594	956.89
421	507.88	479	700.05	537	819.71	595	966.41
422	511.31	480	703.63	538	825.70	596	966.51
423	513.87	481	707.36	539	832.78	597	966.73
424	514.90	482	708.28	540	834.66	598	969.42
425	517.47	483	708.91	541	839.41	599	971.16
426	519.25	484	710.23	542	840.37	600	975.39
427	520.42	485	712.48	543	844.01	601	976.07
428	522.92	486	715.62	544	844.61	602	978.53
429	525.91	487	718.12	545	847.67	603	980.87
430	527.11	488	718.84	546	849.72	604	983.57
431	531.28	489	720.40	547	850.42	605	984.05
432	532.79	490	720.53	548	850.82	606	984.40
433	533.85	491	724.89	549	854.30	607	986.29
434	536.32	492	725.91	550	854.92	608	986.87
435	549.23	493	729.52	551	855.71	609	988.75
436	550.65	494	732.55	552	856.67	610	990.25
437	556.50	495	733.19	553	858.25	611	990.77
438	562.85	496	733.86	554	861.64	612	991.18
439	575.32	497	734.78	555	863.48	613	992.39
440	576.34	498	736.01	556	866.61	614	994.22
441	578.55	499	736.77	557	867.04	615	994.62
442	587.20	500	739.58	558	868.52	616	995.81
443	587.83	501	741.85	559	870.03	617	997.76
444	588.46	502	744.26	560	871.95	618	1000.12
445	593.03	503	746.56	561	872.83	619	1002.61
446	597.78	504	750.82	562	876.29	620	1003.97
447	598.66	505	752.14	563	877.27	621	1004.62
448	600.50	506	756.27	564	878.64	622	1005.12
449	601.05	507	760.07	565	882.67	623	1006.23
450	604.10	508	763.48	566	883.56	624	1008.23
451	607.28	509	764.96	567	885.51	625	1008.87
452	610.32	510	766.89	568	886.77	626	1009.81
453	618.83	511	772.08	569	892.05	627	1010.70
454	619.56	512	773.25	570	894.81	628	1012.97

629	1015.24	672	1088.93	715	1179.10	758	3652.24
630	1016.32	673	1089.97	716	1179.74	759	3664.93
631	1017.61	674	1090.15	717	1183.32	760	3701.36
632	1019.51	675	1091.32	718	1184.86	761	3770.69
633	1020.73	676	1092.37	719	1186.59	762	3859.50
634	1021.87	677	1095.22	720	1189.89	763	3860.82
635	1022.67	678	1110.65	721	1191.85	764	3915.85
636	1023.25	679	1114.33	722	1194.75	765	3921.58
637	1023.97	680	1115.81	723	1194.91	766	3923.51
638	1024.63	681	1117.64	724	1197.93	767	3929.00
639	1026.41	682	1118.55	725	1201.03	768	3929.50
640	1027.67	683	1121.78	726	1203.07	769	3929.57
641	1028.18	684	1124.86	727	1204.43	770	3929.87
642	1028.75	685	1126.63	728	1210.75	771	3930.00
643	1030.98	686	1128.18	729	1216.38	772	3930.36
644	1031.22	687	1131.26	730	3310.38	773	3930.52
645	1033.12	688	1132.93	731	3312.96	774	3931.68
646	1035.99	689	1136.97	732	3322.26	775	3931.88
647	1036.78	690	1140.49	733	3334.23	776	3932.49
648	1044.66	691	1141.94	734	3344.53	777	3933.54
649	1045.25	692	1143.34	735	3357.29	778	3934.21
650	1052.25	693	1143.99	736	3441.66	779	3935.38
651	1055.61	694	1144.17	737	3460.90	780	3937.10
652	1062.33	695	1146.60	738	3463.80	781	3937.59
653	1062.70	696	1148.43	739	3466.80	782	3937.81
654	1069.88	697	1151.22	740	3467.20	783	3937.91
655	1070.99	698	1152.59	741	3468.74	784	3939.67
656	1073.99	699	1153.14	742	3473.85	785	3939.98
657	1075.82	700	1155.02	743	3474.40	786	3942.19
658	1076.16	701	1156.42	744	3477.20	787	3942.66
659	1077.07	702	1157.94	745	3504.93	788	3943.05
660	1077.99	703	1159.66	746	3528.28	789	3943.18
661	1080.29	704	1162.46	747	3529.91	790	3943.40
662	1081.04	705	1163.87	748	3530.43	791	3944.04
663	1081.56	706	1164.68	749	3540.07	792	3944.07
664	1082.00	707	1166.65	750	3542.00	793	3944.74
665	1082.45	708	1167.78	751	3542.77	794	3944.78
666	1083.15	709	1169.01	752	3554.05	795	3945.31
667	1084.55	710	1169.50	753	3560.56	796	3945.67
668	1085.19	711	1172.65	754	3591.39	797	3946.55
669	1086.43	712	1174.81	755	3623.76	798	3946.68
670	1087.68	713	1177.07	756	3628.88	799	3947.07
671	1088.68	714	1178.20	757	3651.29	800	3947.68
						801	3949.24

100 Surface PBE/6-31G**

zpe= 0.9387101 Hartree * 0.986

T	p	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot.	energy	entropy
(K)	(MPa)				(kJ/mol)	(kJ/mol)	(kJ/mol/K)
283.15	0.1000000	22.08	21.04	90.23	2116.12	2683.99	2.01384
293.15	0.1000000	22.16	21.09	93.93	2095.69	2701.05	2.07335
298.15	0.1000000	22.21	21.12	95.77	2085.25	2709.73	2.10285
303.15	0.1000000	22.25	21.14	97.61	2074.66	2718.50	2.13216
313.15	0.1000000	22.33	21.19	101.28	2053.04	2736.32	2.19027
323.15	0.1000000	22.41	21.24	104.93	2030.85	2754.50	2.24767
333.15	0.1000000	22.48	21.29	108.57	2008.09	2773.02	2.30436

Table S3 Vibrational frequencies of the 100 surface of α -quartz

1	-701.53	57	-162.82	113	0.00	169	191.01
2	-693.37	58	-162.24	114	0.97	170	191.87
3	-689.43	59	-157.16	115	22.22	171	195.50
4	-688.21	60	-154.99	116	23.42	172	197.07
5	-683.17	61	-152.80	117	26.98	173	197.70
6	-680.47	62	-152.15	118	32.31	174	199.02
7	-677.33	63	-148.28	119	39.90	175	202.83
8	-676.39	64	-146.00	120	41.64	176	204.02
9	-672.58	65	-143.81	121	41.74	177	205.29
10	-670.22	66	-141.82	122	47.78	178	208.04
11	-667.98	67	-140.18	123	57.20	179	209.00
12	-663.94	68	-132.44	124	60.71	180	210.56
13	-661.14	69	-131.42	125	64.39	181	213.54
14	-657.94	70	-126.83	126	69.38	182	217.37
15	-657.23	71	-123.67	127	71.75	183	221.76
16	-652.63	72	-123.32	128	72.17	184	224.48
17	-649.52	73	-114.32	129	79.09	185	225.55
18	-648.86	74	-108.62	130	88.11	186	227.80
19	-646.71	75	-105.26	131	98.60	187	229.68
20	-644.54	76	-104.02	132	100.47	188	232.47
21	-642.22	77	-101.46	133	109.84	189	236.21
22	-638.16	78	-99.22	134	113.00	190	236.66
23	-635.30	79	-97.31	135	113.97	191	239.64
24	-631.67	80	-96.12	136	115.84	192	241.62
25	-626.03	81	-92.14	137	117.91	193	243.02
26	-621.46	82	-88.51	138	118.80	194	245.06
27	-604.00	83	-86.96	139	120.75	195	245.39
28	-602.34	84	-85.32	140	121.72	196	247.30
29	-596.53	85	-84.37	141	125.79	197	248.97
30	-596.06	86	-83.30	142	129.45	198	251.69
31	-584.48	87	-79.61	143	134.27	199	252.61
32	-582.83	88	-79.00	144	137.68	200	256.50
33	-565.64	89	-77.41	145	140.19	201	257.91
34	-550.58	90	-75.66	146	141.01	202	259.44
35	-548.89	91	-72.34	147	142.42	203	261.41
36	-536.24	92	-69.52	148	145.13	204	262.52
37	-534.82	93	-68.95	149	147.52	205	264.14
38	-522.30	94	-66.84	150	148.91	206	265.79
39	-521.49	95	-64.64	151	151.96	207	266.73
40	-511.94	96	-63.26	152	153.09	208	269.42
41	-502.77	97	-60.80	153	154.25	209	270.31
42	-398.46	98	-57.73	154	158.24	210	271.84
43	-209.51	99	-56.04	155	159.24	211	272.28
44	-204.66	100	-52.52	156	160.89	212	273.27
45	-197.11	101	-49.26	157	166.31	213	276.37
46	-193.70	102	-46.52	158	167.84	214	277.63
47	-187.18	103	-41.25	159	171.28	215	280.99
48	-186.12	104	-36.83	160	172.30	216	282.81
49	-183.37	105	-36.13	161	173.39	217	286.60
50	-179.89	106	-30.11	162	180.34	218	288.10
51	-178.50	107	-24.85	163	181.84	219	290.32
52	-173.88	108	-0.00	164	183.81	220	294.25
53	-172.21	109	-0.00	165	186.04	221	294.98
54	-167.89	110	-0.00	166	186.90	222	296.10
55	-167.49	111	0.00	167	188.25	223	297.48
56	-165.68	112	0.00	168	189.05	224	300.41

225	300.97	282	480.38	339	699.70	396	899.39
226	303.09	283	482.35	340	703.20	397	902.05
227	304.50	284	492.20	341	709.76	398	906.47
228	305.28	285	493.33	342	713.77	399	907.05
229	307.43	286	495.21	343	714.99	400	908.64
230	310.11	287	500.55	344	730.11	401	908.93
231	311.83	288	504.85	345	737.35	402	910.40
232	314.72	289	509.72	346	741.42	403	915.12
233	315.64	290	519.87	347	745.01	404	917.86
234	319.86	291	523.69	348	753.37	405	918.28
235	320.89	292	526.86	349	760.80	406	920.27
236	321.80	293	527.18	350	765.59	407	922.46
237	324.10	294	530.62	351	768.17	408	930.04
238	325.74	295	531.10	352	776.19	409	935.88
239	328.79	296	535.93	353	777.46	410	938.91
240	330.80	297	540.31	354	783.85	411	940.98
241	332.25	298	543.14	355	787.58	412	942.01
242	334.94	299	543.72	356	791.29	413	944.10
243	336.34	300	546.24	357	810.23	414	949.06
244	337.34	301	549.15	358	817.18	415	952.90
245	340.05	302	552.14	359	823.06	416	959.37
246	342.66	303	552.57	360	823.68	417	961.89
247	342.98	304	558.72	361	824.09	418	979.39
248	344.09	305	561.96	362	828.90	419	1017.93
249	347.72	306	565.90	363	830.44	420	1025.03
250	348.05	307	568.36	364	833.76	421	1031.02
251	349.92	308	573.51	365	835.26	422	1038.82
252	352.59	309	576.26	366	836.25	423	1048.54
253	353.13	310	578.01	367	836.66	424	1059.08
254	355.61	311	579.57	368	838.91	425	1062.20
255	358.80	312	579.95	369	840.80	426	1071.30
256	360.19	313	581.45	370	841.80	427	1261.55
257	361.85	314	586.51	371	842.97	428	1273.87
258	362.33	315	588.52	372	844.81	429	1300.83
259	365.09	316	594.67	373	845.84	430	1337.47
260	366.83	317	594.95	374	847.56	431	1338.61
261	368.90	318	595.30	375	849.81	432	1341.67
262	370.85	319	596.49	376	854.48	433	1353.87
263	371.41	320	600.52	377	855.90	434	1354.69
264	375.05	321	602.89	378	859.01	435	1360.04
265	377.46	322	608.85	379	860.58	436	1363.41
266	379.40	323	611.99	380	861.53	437	1367.84
267	382.36	324	615.87	381	865.06	438	1369.88
268	383.42	325	619.25	382	868.37	439	1371.42
269	384.82	326	619.85	383	869.12	440	1373.33
270	388.57	327	623.10	384	871.66	441	1376.59
271	389.68	328	630.54	385	873.15	442	1377.94
272	390.70	329	635.84	386	876.43	443	1380.19
273	398.07	330	644.22	387	879.19	444	1381.44
274	399.26	331	646.31	388	881.71	445	1382.82
275	408.60	332	660.59	389	882.42	446	1384.42
276	411.54	333	663.70	390	884.12	447	1386.27
277	449.56	334	675.68	391	889.54	448	1388.48
278	458.96	335	678.77	392	891.48	449	1391.79
279	469.54	336	681.70	393	894.66	450	1394.75
280	469.68	337	687.31	394	896.12	451	1395.48
281	474.65	338	692.35	395	897.84	452	1396.76

453	1402.16	468	3678.40	483	4118.31	498	4150.29
454	1405.33	469	3698.03	484	4119.96	499	4152.26
455	1408.47	470	3763.17	485	4123.16	500	4155.89
456	1410.14	471	3775.63	486	4124.08	501	4156.31
457	1418.50	472	3862.36	487	4124.26	502	4156.89
458	1420.17	473	4100.61	488	4125.35	503	4158.66
459	1460.37	474	4105.26	489	4127.67	504	4160.15
460	3240.28	475	4109.18	490	4131.20	505	4161.39
461	3323.64	476	4110.78	491	4134.22	506	4161.50
462	3401.62	477	4112.58	492	4135.44	507	4162.90
463	3410.39	478	4113.96	493	4139.26	508	4165.31
464	3624.64	479	4115.59	494	4140.04	509	4166.09
465	3637.02	480	4116.07	495	4141.19	510	4168.61
466	3657.25	481	4117.12	496	4142.51	511	4169.39
467	3658.77	482	4118.08	497	4143.20	512	4170.00
						513	4170.46

TNT PBE/6-31G**

zpe= 0.1315676 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	18.61	14.89	10.39	237.26	374.19	0.49189
293.15	0.1000000	18.70	14.95	10.78	232.30	376.25	0.49935
298.15	0.1000000	18.74	14.97	10.98	229.80	377.31	0.50306
303.15	0.1000000	18.78	15.00	11.18	227.27	378.37	0.50675
313.15	0.1000000	18.86	15.04	11.58	222.17	380.55	0.51407
323.15	0.1000000	18.94	15.09	11.97	216.99	382.77	0.52134
333.15	0.1000000	19.02	15.14	12.36	211.74	385.05	0.52854

Table S4 Vibrational frequencies of TNT

1	-0.00	17	313.63	33	780.21	49	1369.89
2	-0.00	18	320.30	34	806.41	50	1397.33
3	-0.00	19	342.89	35	885.29	51	1431.89
4	0.00	20	356.46	36	908.97	52	1434.86
5	0.00	21	380.47	37	912.19	53	1451.79
6	0.00	22	450.04	38	917.93	54	1571.22
7	49.70	23	464.42	39	1006.83	55	1583.69
8	54.45	24	519.05	40	1009.14	56	1590.06
9	55.47	25	528.37	41	1061.96	57	1620.84
10	92.22	26	635.83	42	1143.85	58	1621.39
11	116.35	27	641.95	43	1166.07	59	3018.01
12	145.01	28	687.68	44	1197.25	60	3091.65
13	165.12	29	710.12	45	1330.77	61	3124.88
14	179.29	30	719.57	46	1332.47	62	3185.44
15	192.27	31	752.92	47	1345.28	63	3185.83
16	284.28	32	755.40	48	1354.86		

DNT PBE/6-31G**

zpe= 0.1297692 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	18.28	14.18	7.41	242.08	362.86	0.43489
293.15	0.1000000	18.37	14.23	7.71	237.70	364.55	0.44106
298.15	0.1000000	18.41	14.26	7.86	235.48	365.42	0.44413
303.15	0.1000000	18.45	14.28	8.01	233.25	366.30	0.44719
313.15	0.1000000	18.53	14.33	8.31	228.75	368.09	0.45328
323.15	0.1000000	18.61	14.38	8.60	224.19	369.93	0.45933
333.15	0.1000000	18.69	14.42	8.90	219.57	371.82	0.46534

Table S5 Vibrational frequencies of DNT

1	-0.00	15	341.60	29	823.93	43	1375.34
2	0.00	16	345.20	30	903.54	44	1401.74
3	0.00	17	384.19	31	918.55	45	1433.29
4	0.00	18	429.95	32	953.48	46	1449.84
5	0.00	19	483.43	33	990.10	47	1468.25
6	0.00	20	512.91	34	1017.14	48	1566.69
7	39.04	21	559.24	35	1045.24	49	1578.20
8	56.16	22	629.92	36	1114.32	50	1618.16
9	101.53	23	659.14	37	1134.02	51	1619.26
10	151.49	24	694.57	38	1198.59	52	3000.90
11	164.62	25	721.33	39	1243.43	53	3075.87
12	220.22	26	755.78	40	1328.88	54	3090.26
13	282.95	27	778.45	41	1341.82	55	3133.69
14	285.51	28	817.92	42	1359.22	56	3173.96
						57	3189.25

DNAN PBE/6-31G**

zpe= 0.1343476 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	18.41	14.47	8.56	250.24	377.43	0.45753
293.15	0.1000000	18.49	14.52	8.90	245.63	379.27	0.46419
298.15	0.1000000	18.54	14.54	9.07	243.30	380.21	0.46750
303.15	0.1000000	18.58	14.57	9.24	240.95	381.16	0.47080
313.15	0.1000000	18.66	14.62	9.58	236.21	383.09	0.47736
323.15	0.1000000	18.74	14.66	9.91	231.41	385.08	0.48387
333.15	0.1000000	18.81	14.71	10.25	226.54	387.12	0.49033

Table S6 Vibrational frequencies of DNAN

1	-0.00	10	119.76	19	397.61	28	750.36
2	0.00	11	155.83	20	453.74	29	780.25
3	0.00	12	159.96	21	509.48	30	810.61
4	0.00	13	195.51	22	522.70	31	815.74
5	0.00	14	240.50	23	603.28	32	907.96
6	0.00	15	297.48	24	628.65	33	916.34
7	44.64	16	311.79	25	665.66	34	943.06
8	58.03	17	333.67	26	695.51	35	1021.52
9	78.09	18	362.57	27	731.92	36	1053.60

37	1124.69	43	1325.52	49	1461.25	55	2965.19
38	1130.16	44	1343.32	50	1488.68	56	3041.66
39	1130.99	45	1378.55	51	1561.80	57	3111.99
40	1170.67	46	1417.90	52	1579.92	58	3164.27
41	1231.28	47	1433.87	53	1611.80	59	3175.72
42	1291.07	48	1456.13	54	1623.92	60	3185.62

NTO PBE/6-31G**

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	17.78	12.83	3.12	88.33	185.13	0.35018
293.15	0.1000000	17.86	12.88	3.27	84.81	186.19	0.35416
298.15	0.1000000	17.91	12.90	3.35	83.03	186.74	0.35614
303.15	0.1000000	17.95	12.93	3.43	81.25	187.29	0.35811
313.15	0.1000000	18.03	12.98	3.59	77.65	188.41	0.36202
323.15	0.1000000	18.11	13.02	3.75	74.01	189.56	0.36589
333.15	0.1000000	18.18	13.07	3.91	70.33	190.73	0.36973

Table S7 Vibrational frequencies of NTO

1	-0.00	9	196.63	17	701.75	25	1237.54
2	0.00	10	294.78	18	725.08	26	1330.27
3	0.00	11	393.89	19	725.62	27	1350.54
4	0.00	12	446.04	20	800.84	28	1435.37
5	0.00	13	477.27	21	956.77	29	1562.98
6	0.00	14	535.22	22	980.67	30	1596.92
7	88.95	15	556.02	23	1072.59	31	1844.39
8	136.83	16	634.51	24	1160.46	32	3591.37
						33	3604.63

001 Surface - TNT PBE/6-31G**

zpe= 1.5543606 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.94	21.98	177.39	3500.45	4492.08	3.51045
293.15	0.1000000	23.02	22.03	184.29	3464.79	4523.42	3.61954
298.15	0.1000000	23.07	22.06	187.73	3446.56	4539.39	3.67367
303.15	0.1000000	23.11	22.09	191.17	3428.06	4555.54	3.72753
313.15	0.1000000	23.19	22.13	198.01	3390.25	4588.39	3.83441
323.15	0.1000000	23.27	22.18	204.83	3351.37	4621.96	3.94020
333.15	0.1000000	23.34	22.23	211.61	3311.44	4656.23	4.04489

Table S8 Vibrational frequencies of TNT on the 001 surface

1	-590.15	9	-510.40	17	-451.39	25	-398.43
2	-584.81	10	-502.00	18	-430.44	26	-397.92
3	-572.62	11	-491.12	19	-424.85	27	-393.11
4	-570.45	12	-490.30	20	-420.50	28	-391.64
5	-567.28	13	-485.23	21	-418.93	29	-387.25
6	-560.70	14	-473.59	22	-416.33	30	-385.51
7	-535.80	15	-468.76	23	-402.11	31	-384.83
8	-518.02	16	-464.55	24	-399.76	32	-379.51

33	-379.12	91	-46.11	149	72.30	207	163.98
34	-365.73	92	-44.30	150	73.62	208	167.27
35	-363.71	93	-43.94	151	75.89	209	167.45
36	-351.13	94	-42.37	152	76.55	210	168.48
37	-344.57	95	-40.43	153	78.05	211	171.25
38	-331.32	96	-39.32	154	80.73	212	171.93
39	-327.59	97	-36.59	155	81.97	213	173.04
40	-291.62	98	-34.60	156	83.30	214	175.48
41	-142.86	99	-32.51	157	84.76	215	175.81
42	-133.02	100	-30.50	158	86.28	216	177.01
43	-131.23	101	-28.99	159	86.34	217	178.85
44	-128.98	102	-25.78	160	89.16	218	180.11
45	-127.99	103	-24.36	161	89.58	219	180.38
46	-124.20	104	-23.57	162	91.33	220	181.40
47	-123.58	105	-18.59	163	91.97	221	183.31
48	-121.79	106	-16.75	164	95.83	222	185.47
49	-120.79	107	-12.48	165	96.90	223	186.16
50	-120.55	108	-4.06	166	98.86	224	189.17
51	-115.24	109	-0.00	167	99.68	225	190.02
52	-113.92	110	-0.00	168	101.79	226	192.01
53	-112.85	111	-0.00	169	102.97	227	192.08
54	-111.06	112	0.00	170	103.48	228	193.72
55	-109.78	113	0.00	171	105.97	229	195.20
56	-103.11	114	0.00	172	106.96	230	196.87
57	-102.09	115	2.91	173	109.34	231	197.15
58	-97.18	116	13.57	174	111.56	232	199.32
59	-96.18	117	17.44	175	113.20	233	200.22
60	-94.83	118	19.08	176	113.89	234	200.98
61	-94.01	119	20.98	177	114.15	235	201.55
62	-93.51	120	23.49	178	115.53	236	203.29
63	-91.38	121	24.01	179	118.05	237	205.72
64	-89.93	122	27.67	180	119.23	238	205.76
65	-88.74	123	29.45	181	120.83	239	207.24
66	-88.23	124	32.86	182	123.70	240	208.67
67	-86.81	125	33.77	183	124.90	241	210.48
68	-86.37	126	36.66	184	126.08	242	213.47
69	-85.92	127	37.24	185	127.31	243	213.93
70	-85.46	128	38.64	186	128.99	244	214.50
71	-82.51	129	40.31	187	130.48	245	215.81
72	-80.69	130	41.51	188	132.16	246	217.00
73	-79.75	131	43.18	189	134.21	247	218.61
74	-78.04	132	46.15	190	136.72	248	222.35
75	-76.31	133	46.95	191	137.69	249	225.41
76	-72.91	134	48.71	192	138.26	250	225.67
77	-70.80	135	50.98	193	140.23	251	228.97
78	-67.70	136	52.61	194	142.24	252	229.37
79	-65.86	137	53.23	195	144.31	253	231.29
80	-63.90	138	54.71	196	145.68	254	233.53
81	-63.17	139	56.26	197	146.81	255	234.73
82	-60.32	140	58.05	198	147.72	256	236.56
83	-59.14	141	61.18	199	149.44	257	237.54
84	-57.88	142	62.82	200	150.52	258	238.14
85	-55.42	143	64.19	201	152.93	259	240.83
86	-54.51	144	66.33	202	154.22	260	242.70
87	-52.56	145	67.93	203	157.67	261	245.57
88	-50.91	146	69.14	204	158.40	262	246.80
89	-49.41	147	70.21	205	160.96	263	248.88
90	-47.88	148	72.16	206	162.00	264	249.54

265	251.53	323	311.97	381	375.54	439	469.65
266	252.67	324	312.46	382	376.25	440	476.86
267	253.70	325	313.12	383	377.18	441	485.23
268	254.19	326	314.67	384	377.90	442	493.76
269	257.79	327	315.51	385	378.60	443	495.53
270	258.43	328	316.71	386	379.36	444	504.75
271	259.98	329	317.93	387	380.31	445	505.93
272	260.31	330	318.77	388	381.34	446	508.74
273	261.06	331	319.16	389	382.16	447	511.12
274	261.99	332	320.86	390	383.42	448	516.07
275	263.80	333	321.93	391	383.98	449	517.78
276	264.70	334	322.29	392	385.12	450	519.64
277	265.38	335	323.68	393	386.57	451	520.91
278	265.93	336	324.64	394	387.25	452	522.29
279	267.27	337	325.93	395	387.90	453	524.36
280	268.63	338	328.14	396	390.47	454	526.17
281	270.64	339	329.17	397	391.43	455	529.90
282	271.87	340	329.80	398	392.33	456	532.48
283	273.23	341	331.38	399	393.10	457	535.30
284	273.42	342	332.43	400	394.14	458	547.89
285	275.04	343	333.91	401	396.26	459	548.50
286	276.04	344	334.93	402	397.66	460	550.06
287	276.62	345	336.00	403	399.20	461	556.59
288	278.88	346	337.58	404	401.33	462	562.55
289	280.14	347	338.45	405	401.62	463	574.57
290	280.85	348	340.34	406	403.09	464	576.20
291	281.26	349	341.58	407	403.33	465	579.31
292	282.65	350	342.12	408	404.68	466	584.93
293	284.02	351	343.68	409	405.55	467	587.37
294	284.44	352	344.76	410	407.22	468	590.10
295	285.98	353	345.05	411	407.88	469	591.79
296	286.35	354	346.92	412	409.12	470	597.76
297	286.83	355	347.36	413	410.43	471	599.77
298	288.53	356	347.40	414	412.30	472	600.85
299	289.95	357	348.46	415	413.88	473	605.44
300	291.14	358	350.31	416	414.44	474	609.67
301	291.68	359	351.87	417	415.27	475	610.46
302	292.83	360	352.79	418	416.32	476	613.82
303	294.06	361	353.28	419	417.41	477	619.05
304	294.48	362	355.43	420	418.07	478	620.14
305	296.25	363	355.94	421	419.27	479	623.15
306	296.60	364	356.85	422	419.75	480	624.59
307	297.35	365	357.76	423	423.35	481	626.00
308	298.49	366	358.76	424	424.26	482	630.88
309	299.32	367	359.26	425	426.13	483	634.91
310	300.71	368	360.02	426	426.64	484	636.86
311	301.51	369	360.70	427	427.89	485	639.82
312	302.03	370	361.25	428	430.25	486	642.76
313	302.92	371	362.66	429	432.21	487	644.38
314	304.60	372	363.69	430	433.55	488	645.44
315	305.03	373	364.94	431	436.39	489	646.86
316	305.85	374	366.70	432	437.71	490	649.90
317	306.34	375	367.20	433	439.01	491	654.90
318	307.52	376	368.87	434	442.56	492	662.12
319	308.30	377	369.44	435	446.37	493	663.55
320	309.31	378	372.16	436	447.32	494	671.04
321	310.64	379	373.39	437	453.21	495	672.55
322	311.43	380	374.14	438	463.85	496	674.88

497	678.30	555	793.72	613	910.03	671	1017.59
498	681.57	556	795.51	614	910.50	672	1018.26
499	682.23	557	797.49	615	913.52	673	1020.38
500	685.55	558	799.38	616	914.54	674	1021.26
501	688.27	559	799.88	617	914.95	675	1021.77
502	689.69	560	802.82	618	920.58	676	1022.70
503	691.58	561	804.09	619	924.28	677	1024.06
504	695.24	562	804.86	620	924.94	678	1024.81
505	697.28	563	806.91	621	930.59	679	1026.31
506	699.33	564	808.58	622	934.06	680	1028.58
507	700.86	565	809.77	623	934.57	681	1029.27
508	703.57	566	811.04	624	938.19	682	1030.05
509	705.39	567	811.54	625	938.79	683	1030.47
510	707.89	568	814.27	626	940.15	684	1031.14
511	708.64	569	815.50	627	942.60	685	1033.11
512	709.65	570	819.18	628	943.56	686	1033.83
513	711.20	571	820.10	629	946.94	687	1038.16
514	711.82	572	825.34	630	950.54	688	1039.45
515	715.67	573	831.46	631	955.25	689	1043.05
516	718.26	574	834.45	632	956.50	690	1050.03
517	718.42	575	837.20	633	965.96	691	1061.72
518	719.60	576	837.89	634	966.50	692	1066.92
519	720.51	577	840.89	635	968.40	693	1069.64
520	724.25	578	842.31	636	970.24	694	1070.49
521	725.03	579	844.35	637	972.18	695	1073.11
522	726.42	580	845.85	638	972.85	696	1075.03
523	729.60	581	851.18	639	975.07	697	1075.56
524	732.67	582	851.81	640	975.42	698	1075.99
525	733.78	583	854.10	641	976.34	699	1077.03
526	734.51	584	854.37	642	979.97	700	1078.03
527	735.50	585	855.69	643	982.15	701	1079.86
528	736.25	586	855.96	644	983.95	702	1080.31
529	738.09	587	856.37	645	984.62	703	1081.00
530	741.40	588	859.70	646	988.75	704	1082.00
531	742.48	589	861.17	647	989.46	705	1082.40
532	743.11	590	862.27	648	989.64	706	1083.48
533	743.97	591	864.31	649	990.32	707	1084.19
534	750.25	592	867.42	650	992.29	708	1085.38
535	750.52	593	868.59	651	992.77	709	1085.75
536	752.52	594	869.41	652	993.68	710	1087.13
537	754.90	595	871.80	653	994.60	711	1088.25
538	759.04	596	872.33	654	997.28	712	1089.40
539	760.52	597	872.84	655	998.50	713	1089.52
540	763.85	598	876.23	656	999.97	714	1090.06
541	764.69	599	879.79	657	1000.27	715	1091.10
542	767.15	600	880.61	658	1001.59	716	1091.36
543	771.94	601	883.55	659	1003.64	717	1092.19
544	773.72	602	886.11	660	1005.56	718	1095.12
545	776.26	603	887.19	661	1005.89	719	1111.07
546	780.23	604	887.51	662	1008.27	720	1114.56
547	782.06	605	889.80	663	1008.42	721	1118.01
548	783.52	606	891.96	664	1008.59	722	1118.65
549	784.64	607	892.86	665	1010.28	723	1120.36
550	785.35	608	898.09	666	1010.71	724	1121.26
551	788.19	609	899.51	667	1013.72	725	1125.15
552	789.16	610	901.95	668	1016.08	726	1126.61
553	790.24	611	903.81	669	1016.22	727	1128.77
554	791.60	612	907.04	670	1016.78	728	1132.41

729	1134.16	763	1189.07	797	3343.00	831	3929.42
730	1137.12	764	1192.08	798	3356.45	832	3929.53
731	1139.77	765	1194.48	799	3365.40	833	3929.86
732	1141.08	766	1195.52	800	3395.21	834	3929.96
733	1142.39	767	1197.15	801	3442.13	835	3930.45
734	1143.85	768	1198.70	802	3460.21	836	3930.65
735	1143.90	769	1201.07	803	3464.53	837	3931.76
736	1146.71	770	1202.85	804	3465.46	838	3932.16
737	1147.96	771	1204.82	805	3466.73	839	3932.65
738	1150.79	772	1210.95	806	3471.50	840	3933.87
739	1151.28	773	1216.92	807	3472.29	841	3935.11
740	1152.15	774	1330.43	808	3472.86	842	3936.09
741	1152.91	775	1335.01	809	3475.55	843	3936.42
742	1154.36	776	1347.88	810	3489.46	844	3936.68
743	1156.45	777	1352.04	811	3528.08	845	3937.58
744	1157.80	778	1370.83	812	3533.35	846	3938.45
745	1159.58	779	1402.15	813	3539.92	847	3940.27
746	1161.91	780	1428.81	814	3542.33	848	3940.45
747	1162.53	781	1432.71	815	3543.16	849	3942.19
748	1165.14	782	1457.91	816	3554.04	850	3942.72
749	1166.54	783	1563.21	817	3641.35	851	3942.99
750	1167.66	784	1579.57	818	3644.94	852	3943.21
751	1168.58	785	1589.28	819	3645.45	853	3943.77
752	1169.78	786	1613.28	820	3649.13	854	3944.10
753	1172.80	787	1618.77	821	3667.72	855	3944.22
754	1174.57	788	3012.01	822	3716.54	856	3944.49
755	1174.72	789	3081.09	823	3725.14	857	3945.05
756	1176.39	790	3140.99	824	3768.06	858	3945.65
757	1177.83	791	3178.63	825	3858.06	859	3945.91
758	1178.92	792	3194.47	826	3861.11	860	3946.47
759	1179.74	793	3310.65	827	3916.18	861	3947.12
760	1183.20	794	3314.87	828	3922.04	862	3947.41
761	1184.42	795	3321.16	829	3923.32	863	3947.63
762	1186.27	796	3334.35	830	3929.38	864	3949.13

001 Surface - DNT PBE/6-31G**

zpe= 1.5527106 Hartree

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.92	21.95	172.78	3507.14	4481.09	3.44801
293.15	0.1000000	23.01	22.00	179.59	3472.12	4512.06	3.55578
298.15	0.1000000	23.05	22.03	182.98	3454.20	4527.83	3.60927
303.15	0.1000000	23.09	22.05	186.36	3436.02	4543.78	3.66248
313.15	0.1000000	23.17	22.10	193.11	3398.87	4576.25	3.76810
323.15	0.1000000	23.25	22.15	199.83	3360.66	4609.42	3.87264
333.15	0.1000000	23.33	22.19	206.51	3321.42	4643.29	3.97610

Table S9 Vibrational frequencies of DNT on the 001 surface

1	-592.31	6	-560.36	11	-495.26	16	-459.42
2	-583.41	7	-535.43	12	-488.90	17	-446.88
3	-573.06	8	-514.83	13	-483.67	18	-437.59
4	-569.36	9	-506.30	14	-470.26	19	-426.56
5	-566.27	10	-502.33	15	-467.27	20	-424.52

21	-418.89	79	-65.70	137	56.22	195	147.12
22	-416.38	80	-64.69	138	57.27	196	148.87
23	-402.74	81	-63.16	139	58.56	197	149.88
24	-401.93	82	-60.21	140	61.14	198	152.25
25	-395.71	83	-59.16	141	63.29	199	153.69
26	-392.25	84	-57.67	142	63.98	200	156.20
27	-391.69	85	-55.27	143	64.29	201	158.08
28	-388.84	86	-53.90	144	65.50	202	159.63
29	-387.02	87	-51.96	145	66.20	203	160.85
30	-384.67	88	-50.48	146	70.60	204	162.00
31	-383.67	89	-48.79	147	72.23	205	163.90
32	-381.36	90	-47.61	148	72.57	206	166.19
33	-378.28	91	-45.82	149	74.01	207	166.95
34	-367.65	92	-44.29	150	76.49	208	167.21
35	-364.12	93	-41.64	151	77.24	209	167.67
36	-354.78	94	-41.35	152	78.27	210	169.80
37	-349.00	95	-38.62	153	81.04	211	171.77
38	-329.27	96	-37.45	154	81.13	212	173.57
39	-324.27	97	-35.78	155	82.07	213	174.57
40	-291.76	98	-34.58	156	83.07	214	176.25
41	-134.88	99	-32.30	157	85.01	215	177.91
42	-133.69	100	-30.67	158	85.44	216	178.28
43	-130.63	101	-27.80	159	88.58	217	179.91
44	-128.10	102	-24.24	160	89.81	218	180.45
45	-127.39	103	-23.84	161	90.98	219	183.95
46	-123.73	104	-22.80	162	92.19	220	184.75
47	-123.00	105	-17.56	163	95.96	221	185.61
48	-122.20	106	-15.41	164	96.58	222	188.57
49	-122.03	107	-12.35	165	99.93	223	190.34
50	-120.82	108	-9.10	166	101.28	224	191.98
51	-117.06	109	-0.00	167	103.04	225	192.99
52	-114.25	110	-0.00	168	103.48	226	194.77
53	-112.94	111	-0.00	169	104.79	227	195.72
54	-112.17	112	-0.00	170	106.58	228	196.30
55	-111.17	113	0.00	171	107.74	229	197.86
56	-103.69	114	0.00	172	109.63	230	199.36
57	-98.33	115	12.15	173	111.79	231	200.33
58	-97.45	116	12.51	174	112.88	232	201.90
59	-96.67	117	14.30	175	114.05	233	202.75
60	-95.25	118	19.38	176	115.53	234	203.65
61	-93.58	119	21.95	177	116.68	235	205.37
62	-93.53	120	24.11	178	118.48	236	206.24
63	-91.32	121	25.24	179	119.51	237	208.26
64	-90.35	122	26.43	180	123.22	238	208.60
65	-87.96	123	33.66	181	123.91	239	209.73
66	-87.26	124	35.04	182	124.93	240	213.53
67	-85.93	125	35.78	183	125.74	241	214.12
68	-85.62	126	37.17	184	127.74	242	214.94
69	-85.27	127	38.39	185	129.71	243	215.92
70	-83.37	128	39.27	186	130.97	244	217.49
71	-81.26	129	40.86	187	134.30	245	222.85
72	-79.99	130	43.09	188	134.92	246	225.27
73	-79.25	131	43.72	189	136.23	247	228.01
74	-78.47	132	46.68	190	138.24	248	230.08
75	-74.26	133	48.36	191	139.98	249	230.67
76	-71.24	134	51.60	192	140.66	250	231.89
77	-70.37	135	52.55	193	144.12	251	234.93
78	-69.64	136	55.09	194	144.94	252	235.10

253	236.27	311	304.10	369	365.99	427	434.01
254	238.04	312	304.73	370	367.04	428	436.56
255	239.25	313	306.40	371	368.24	429	439.07
256	240.79	314	307.06	372	368.81	430	440.42
257	243.62	315	307.66	373	370.60	431	446.51
258	245.78	316	308.21	374	373.22	432	446.82
259	247.98	317	309.91	375	374.10	433	453.08
260	249.57	318	310.50	376	374.27	434	476.26
261	250.78	319	311.17	377	375.64	435	476.67
262	252.22	320	312.06	378	377.62	436	482.73
263	253.08	321	312.46	379	378.26	437	484.81
264	253.97	322	313.44	380	379.43	438	493.86
265	255.07	323	314.40	381	379.47	439	495.68
266	256.99	324	314.73	382	380.55	440	505.66
267	258.48	325	316.69	383	381.47	441	509.69
268	259.78	326	319.24	384	382.58	442	512.16
269	260.66	327	320.06	385	383.93	443	513.78
270	260.75	328	321.00	386	384.48	444	516.79
271	262.48	329	321.65	387	385.11	445	517.66
272	264.41	330	322.28	388	386.12	446	518.56
273	264.82	331	323.73	389	387.49	447	519.20
274	265.34	332	324.71	390	389.34	448	522.03
275	266.24	333	326.85	391	390.71	449	523.60
276	267.08	334	328.58	392	390.90	450	526.79
277	268.84	335	329.40	393	392.41	451	529.84
278	269.97	336	331.20	394	393.42	452	532.86
279	270.63	337	331.98	395	394.36	453	535.18
280	272.14	338	332.99	396	396.00	454	538.46
281	273.12	339	334.50	397	397.36	455	550.11
282	274.48	340	335.18	398	398.68	456	551.73
283	275.82	341	335.82	399	400.57	457	556.71
284	277.49	342	337.08	400	402.18	458	562.72
285	278.26	343	337.67	401	402.32	459	571.04
286	279.05	344	339.40	402	403.30	460	575.43
287	279.46	345	340.81	403	404.07	461	575.80
288	281.11	346	340.98	404	404.79	462	580.26
289	281.76	347	342.03	405	405.80	463	586.68
290	282.69	348	344.32	406	408.54	464	588.19
291	284.03	349	344.60	407	408.73	465	593.66
292	284.32	350	345.44	408	410.01	466	596.00
293	284.95	351	347.28	409	411.41	467	597.88
294	285.56	352	348.22	410	413.29	468	599.56
295	287.30	353	348.72	411	413.93	469	602.77
296	288.74	354	349.59	412	415.00	470	606.28
297	289.87	355	350.61	413	415.96	471	607.24
298	291.20	356	351.39	414	416.69	472	612.24
299	292.31	357	352.87	415	417.67	473	619.66
300	292.90	358	353.75	416	418.95	474	620.02
301	293.89	359	355.53	417	419.64	475	623.10
302	294.77	360	355.87	418	421.91	476	625.50
303	296.38	361	356.49	419	424.10	477	628.98
304	296.51	362	357.91	420	425.50	478	633.67
305	298.01	363	359.59	421	426.29	479	638.08
306	298.83	364	360.30	422	426.79	480	638.94
307	299.03	365	361.41	423	428.23	481	642.11
308	300.25	366	361.71	424	430.53	482	644.32
309	301.48	367	363.54	425	432.10	483	645.60
310	302.26	368	364.86	426	433.10	484	646.31

485	649.91	543	786.67	601	898.45	659	1009.62
486	651.32	544	787.79	602	900.18	660	1010.86
487	655.14	545	788.21	603	902.08	661	1012.93
488	659.02	546	790.30	604	903.71	662	1015.06
489	663.41	547	790.93	605	906.25	663	1016.34
490	665.86	548	791.94	606	909.26	664	1017.73
491	670.82	549	794.07	607	910.55	665	1019.35
492	673.80	550	795.45	608	913.59	666	1020.76
493	676.67	551	797.59	609	914.53	667	1021.56
494	678.57	552	798.90	610	920.18	668	1021.87
495	681.51	553	799.70	611	921.73	669	1022.70
496	682.72	554	802.47	612	925.25	670	1023.16
497	688.94	555	803.69	613	927.48	671	1023.96
498	691.79	556	806.67	614	930.51	672	1024.57
499	692.19	557	808.56	615	933.74	673	1026.37
500	695.18	558	808.67	616	937.48	674	1027.80
501	695.58	559	809.85	617	939.80	675	1028.07
502	699.44	560	810.82	618	940.13	676	1028.52
503	700.08	561	814.28	619	941.41	677	1031.24
504	703.58	562	814.90	620	947.42	678	1032.23
505	707.32	563	815.30	621	951.89	679	1032.91
506	708.50	564	816.80	622	954.35	680	1036.80
507	708.99	565	819.47	623	954.63	681	1042.75
508	710.43	566	823.66	624	956.02	682	1045.34
509	712.81	567	825.67	625	956.58	683	1052.22
510	715.84	568	832.16	626	961.75	684	1054.63
511	718.41	569	834.64	627	966.44	685	1056.38
512	718.90	570	839.95	628	966.70	686	1059.95
513	720.17	571	840.35	629	968.89	687	1062.31
514	720.56	572	844.15	630	969.47	688	1063.44
515	725.29	573	844.51	631	975.33	689	1069.86
516	725.93	574	847.31	632	975.99	690	1073.97
517	727.47	575	847.70	633	977.71	691	1075.82
518	729.69	576	850.22	634	978.64	692	1076.07
519	733.04	577	851.04	635	980.81	693	1077.03
520	733.94	578	853.49	636	981.41	694	1077.98
521	735.13	579	854.18	637	983.93	695	1080.27
522	735.31	580	856.19	638	984.36	696	1081.05
523	736.09	581	856.74	639	986.00	697	1081.57
524	736.74	582	858.43	640	987.46	698	1081.86
525	740.14	583	863.56	641	988.80	699	1082.31
526	742.13	584	864.43	642	989.54	700	1083.01
527	744.54	585	866.40	643	990.74	701	1084.07
528	746.81	586	867.02	644	990.94	702	1084.89
529	750.88	587	868.42	645	992.38	703	1086.39
530	752.21	588	870.30	646	993.39	704	1087.00
531	755.64	589	872.02	647	994.38	705	1087.68
532	756.32	590	872.95	648	995.43	706	1088.69
533	760.29	591	877.03	649	998.12	707	1089.15
534	763.69	592	877.82	650	1002.03	708	1089.95
535	764.92	593	878.85	651	1002.47	709	1090.21
536	767.18	594	883.23	652	1003.70	710	1091.49
537	772.35	595	883.56	653	1003.96	711	1092.30
538	773.24	596	885.50	654	1004.64	712	1095.22
539	776.50	597	886.74	655	1005.18	713	1111.68
540	781.85	598	891.68	656	1006.28	714	1115.45
541	782.32	599	892.09	657	1007.33	715	1115.63
542	784.64	600	895.80	658	1008.46	716	1117.65

717	1118.58	752	1179.07	787	3310.32	823	3923.62
718	1120.33	753	1179.59	788	3312.88	824	3929.07
719	1121.63	754	1183.29	789	3322.17	825	3929.57
720	1124.84	755	1184.86	790	3334.06	826	3929.62
721	1126.55	756	1186.60	791	3344.51	827	3929.91
722	1128.02	757	1189.80	792	3345.79	828	3930.03
723	1131.43	758	1191.80	793	3357.25	829	3930.36
724	1132.56	759	1194.63	794	3425.92	830	3930.59
725	1134.98	760	1194.80	795	3461.23	831	3931.64
726	1140.06	761	1197.98	796	3464.08	832	3931.93
727	1141.20	762	1200.94	797	3466.50	833	3932.59
728	1143.13	763	1203.04	798	3466.98	834	3933.71
729	1143.54	764	1204.26	799	3467.25	835	3934.25
730	1144.10	765	1204.87	800	3469.06	836	3935.41
731	1145.09	766	1210.69	801	3473.94	837	3937.15
732	1146.58	767	1216.29	802	3474.69	838	3937.60
733	1148.16	768	1247.76	803	3483.51	839	3937.62
734	1151.14	769	1333.00	804	3515.35	840	3937.97
735	1152.41	770	1346.90	805	3529.87	841	3939.55
736	1152.98	771	1360.80	806	3530.44	842	3940.72
737	1154.92	772	1372.21	807	3541.96	843	3942.22
738	1156.38	773	1407.25	808	3542.75	844	3942.87
739	1157.89	774	1442.62	809	3549.89	845	3943.20
740	1159.60	775	1463.44	810	3554.05	846	3943.23
741	1162.46	776	1470.11	811	3566.87	847	3943.43
742	1163.60	777	1550.84	812	3626.95	848	3944.08
743	1164.52	778	1568.79	813	3628.34	849	3944.15
744	1166.61	779	1606.05	814	3642.14	850	3944.61
745	1167.85	780	1613.18	815	3652.40	851	3944.79
746	1169.10	781	2994.35	816	3656.85	852	3945.19
747	1169.63	782	3069.95	817	3702.74	853	3945.73
748	1172.66	783	3104.46	818	3770.14	854	3946.60
749	1174.68	784	3152.68	819	3859.47	855	3946.67
750	1177.04	785	3170.80	820	3860.84	856	3947.09
751	1178.15	786	3194.18	821	3915.87	857	3947.65
				822	3921.59	858	3949.03

001 Surface - DNAN parallel PBE/6-31G**

zpe= 1.5539276 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.93	21.96	175.92	3502.87	4492.91	3.50486
293.15	0.1000000	23.01	22.01	182.86	3467.27	4524.39	3.61439
298.15	0.1000000	23.06	22.03	186.31	3449.06	4540.42	3.66874
303.15	0.1000000	23.10	22.06	189.76	3430.58	4556.63	3.72281
313.15	0.1000000	23.18	22.11	196.63	3392.81	4589.61	3.83010
323.15	0.1000000	23.26	22.15	203.48	3353.98	4623.30	3.93627
333.15	0.1000000	23.33	22.20	210.28	3314.09	4657.69	4.04131

Table S10 Vibrational frequencies of DNAN with the 001 surface

1	-620.80	5	-560.26	9	-515.20	13	-486.23
2	-594.97	6	-560.24	10	-514.35	14	-479.46
3	-590.27	7	-545.94	11	-504.67	15	-475.05
4	-569.85	8	-518.09	12	-496.42	16	-470.42

17	-470.31	75	-64.75	133	51.43	191	141.94
18	-466.55	76	-62.12	134	54.99	192	143.29
19	-440.78	77	-60.48	135	55.36	193	144.79
20	-438.69	78	-59.53	136	56.33	194	147.98
21	-428.59	79	-57.04	137	59.26	195	148.22
22	-425.38	80	-54.91	138	61.05	196	150.57
23	-424.12	81	-53.14	139	62.42	197	150.95
24	-422.10	82	-52.03	140	64.37	198	153.66
25	-400.95	83	-49.46	141	64.61	199	154.76
26	-400.94	84	-48.66	142	66.45	200	157.48
27	-396.87	85	-47.19	143	67.57	201	159.97
28	-392.92	86	-46.86	144	70.21	202	161.09
29	-386.35	87	-45.86	145	71.05	203	161.83
30	-381.19	88	-43.59	146	73.87	204	164.34
31	-377.49	89	-40.69	147	75.01	205	165.85
32	-376.76	90	-40.00	148	75.31	206	167.61
33	-372.23	91	-38.62	149	76.09	207	169.78
34	-363.96	92	-37.18	150	78.53	208	170.47
35	-362.07	93	-35.91	151	79.15	209	171.79
36	-355.16	94	-33.08	152	82.55	210	174.21
37	-313.92	95	-30.76	153	83.74	211	174.91
38	-311.15	96	-28.58	154	85.19	212	176.27
39	-287.79	97	-27.43	155	86.95	213	177.26
40	-277.21	98	-26.18	156	87.25	214	178.14
41	-143.54	99	-24.66	157	87.94	215	178.58
42	-132.97	100	-22.70	158	89.72	216	180.40
43	-132.95	101	-20.87	159	91.43	217	181.97
44	-129.89	102	-18.65	160	92.91	218	184.21
45	-127.98	103	-14.33	161	94.57	219	184.85
46	-123.10	104	-10.04	162	96.59	220	187.04
47	-122.74	105	-5.35	163	98.16	221	187.59
48	-118.96	106	-0.00	164	99.78	222	190.15
49	-115.17	107	-0.00	165	101.70	223	190.27
50	-111.62	108	0.00	166	102.42	224	192.28
51	-109.18	109	0.00	167	105.06	225	193.26
52	-105.17	110	0.00	168	105.82	226	194.59
53	-101.06	111	0.00	169	107.15	227	195.23
54	-98.82	112	12.99	170	109.50	228	196.36
55	-96.44	113	15.92	171	109.76	229	197.26
56	-95.74	114	19.87	172	111.12	230	199.14
57	-94.74	115	21.52	173	113.29	231	199.71
58	-91.90	116	22.27	174	115.53	232	202.40
59	-89.26	117	23.18	175	116.73	233	203.36
60	-88.32	118	26.34	176	117.59	234	203.56
61	-86.39	119	28.08	177	119.55	235	204.11
62	-86.04	120	30.24	178	120.99	236	206.54
63	-85.63	121	32.22	179	122.42	237	207.54
64	-84.50	122	33.99	180	123.86	238	210.37
65	-83.07	123	35.93	181	126.08	239	211.97
66	-82.37	124	39.69	182	126.45	240	213.10
67	-79.79	125	40.10	183	126.99	241	214.80
68	-77.20	126	40.71	184	127.81	242	215.57
69	-75.09	127	43.06	185	133.24	243	217.95
70	-72.03	128	43.78	186	134.32	244	218.77
71	-70.01	129	44.78	187	135.74	245	221.44
72	-67.43	130	46.82	188	137.01	246	223.82
73	-66.56	131	48.25	189	137.72	247	226.97
74	-65.66	132	48.50	190	141.37	248	228.05

249	229.11	307	299.73	365	359.06	423	426.68
250	231.24	308	300.10	366	359.72	424	429.02
251	232.54	309	301.00	367	360.83	425	429.56
252	234.71	310	302.11	368	361.37	426	431.67
253	236.72	311	302.83	369	363.29	427	433.39
254	237.67	312	303.36	370	364.52	428	436.45
255	238.43	313	303.60	371	365.44	429	439.67
256	239.99	314	305.85	372	368.16	430	439.90
257	240.84	315	306.62	373	368.70	431	445.80
258	242.18	316	306.93	374	369.41	432	450.37
259	244.85	317	307.75	375	370.55	433	453.82
260	246.87	318	308.01	376	371.30	434	457.26
261	249.33	319	308.43	377	373.61	435	470.79
262	250.02	320	310.18	378	374.37	436	478.86
263	252.05	321	311.63	379	375.39	437	485.74
264	252.74	322	311.79	380	376.54	438	491.80
265	254.51	323	312.16	381	376.79	439	495.64
266	255.51	324	312.81	382	377.52	440	497.62
267	256.09	325	315.32	383	378.81	441	497.98
268	257.07	326	317.00	384	379.79	442	500.18
269	258.17	327	318.05	385	380.51	443	501.61
270	260.28	328	318.59	386	381.86	444	503.56
271	260.98	329	319.94	387	383.88	445	505.71
272	262.47	330	320.67	388	384.18	446	508.72
273	263.31	331	322.67	389	384.30	447	511.18
274	263.84	332	322.90	390	385.97	448	515.64
275	264.91	333	324.33	391	387.20	449	517.73
276	266.19	334	326.18	392	389.58	450	519.66
277	267.91	335	327.51	393	390.50	451	522.28
278	268.20	336	329.84	394	391.44	452	523.06
279	268.86	337	330.27	395	392.38	453	524.07
280	271.21	338	331.59	396	393.01	454	524.96
281	272.96	339	332.04	397	394.60	455	532.94
282	274.49	340	333.38	398	395.57	456	534.86
283	275.95	341	333.81	399	396.60	457	537.51
284	276.14	342	334.36	400	397.76	458	538.47
285	278.07	343	335.55	401	398.52	459	540.16
286	278.95	344	337.06	402	400.02	460	549.39
287	280.04	345	339.01	403	401.66	461	551.93
288	280.44	346	340.11	404	402.40	462	556.81
289	280.88	347	340.75	405	403.57	463	564.19
290	282.10	348	342.40	406	404.18	464	568.91
291	282.95	349	343.42	407	405.34	465	575.22
292	283.64	350	343.69	408	406.88	466	575.98
293	285.58	351	344.57	409	407.67	467	581.34
294	285.99	352	345.10	410	408.08	468	586.17
295	287.47	353	346.18	411	408.89	469	586.65
296	289.56	354	347.07	412	410.54	470	591.42
297	290.18	355	348.13	413	412.66	471	594.25
298	290.83	356	349.49	414	414.25	472	597.52
299	291.19	357	349.98	415	415.83	473	598.40
300	293.40	358	352.13	416	416.86	474	601.38
301	293.83	359	352.84	417	417.47	475	604.90
302	295.38	360	354.65	418	419.19	476	605.80
303	296.21	361	355.64	419	419.45	477	611.91
304	296.79	362	356.41	420	421.55	478	613.76
305	298.04	363	357.29	421	423.99	479	615.65
306	299.40	364	358.45	422	424.58	480	619.75

481	620.89	539	765.23	597	874.74	655	998.14
482	623.49	540	766.23	598	876.42	656	1002.42
483	626.29	541	768.59	599	878.61	657	1003.09
484	629.46	542	769.04	600	883.86	658	1003.93
485	633.31	543	774.72	601	885.34	659	1004.24
486	638.46	544	776.41	602	887.53	660	1005.16
487	642.22	545	777.78	603	888.45	661	1005.78
488	643.62	546	781.97	604	889.58	662	1006.69
489	647.02	547	783.89	605	892.19	663	1007.56
490	653.49	548	785.66	606	893.39	664	1007.71
491	654.06	549	786.81	607	895.52	665	1009.43
492	658.50	550	791.11	608	898.49	666	1009.53
493	661.59	551	791.39	609	901.72	667	1011.21
494	665.90	552	793.57	610	903.18	668	1015.21
495	669.32	553	795.19	611	905.07	669	1016.53
496	670.00	554	795.55	612	910.91	670	1017.06
497	673.02	555	797.34	613	912.54	671	1018.64
498	677.60	556	798.88	614	915.91	672	1019.68
499	678.93	557	800.18	615	917.60	673	1020.82
500	680.24	558	802.73	616	921.77	674	1022.18
501	681.39	559	803.69	617	922.57	675	1022.28
502	683.05	560	805.98	618	923.24	676	1024.55
503	686.97	561	806.55	619	924.22	677	1024.74
504	691.73	562	807.32	620	930.56	678	1026.20
505	694.54	563	810.03	621	931.42	679	1029.49
506	697.66	564	810.35	622	934.59	680	1029.97
507	698.88	565	810.73	623	936.39	681	1030.34
508	699.45	566	811.45	624	937.10	682	1031.59
509	701.31	567	812.43	625	937.81	683	1032.20
510	704.03	568	813.68	626	941.65	684	1034.97
511	705.43	569	815.62	627	945.12	685	1043.77
512	707.39	570	816.45	628	947.45	686	1057.09
513	711.17	571	817.07	629	949.76	687	1061.25
514	711.52	572	820.61	630	950.46	688	1067.91
515	712.75	573	825.83	631	957.00	689	1069.63
516	713.73	574	830.33	632	957.68	690	1071.27
517	715.18	575	834.62	633	965.74	691	1072.40
518	717.59	576	839.35	634	966.60	692	1075.43
519	718.74	577	842.20	635	967.23	693	1075.58
520	719.57	578	843.11	636	968.73	694	1077.41
521	724.97	579	845.74	637	971.02	695	1078.94
522	733.39	580	849.28	638	972.74	696	1080.19
523	734.68	581	850.07	639	975.49	697	1080.68
524	734.88	582	852.84	640	977.46	698	1081.03
525	735.79	583	854.55	641	979.66	699	1081.55
526	736.13	584	855.52	642	981.88	700	1081.68
527	737.27	585	856.79	643	983.14	701	1082.67
528	738.74	586	857.17	644	983.97	702	1082.71
529	739.43	587	862.24	645	986.09	703	1084.65
530	741.02	588	863.45	646	988.03	704	1084.97
531	741.60	589	864.84	647	988.27	705	1086.33
532	743.03	590	865.20	648	989.62	706	1087.20
533	744.37	591	867.43	649	990.91	707	1088.74
534	744.80	592	868.55	650	992.01	708	1089.77
535	750.88	593	868.73	651	994.19	709	1090.04
536	753.48	594	870.96	652	994.58	710	1091.15
537	755.65	595	872.60	653	995.57	711	1092.34
538	762.07	596	873.18	654	996.60	712	1093.90

713	1094.41	750	1171.94	787	3165.48	824	3914.51
714	1104.86	751	1172.12	788	3179.56	825	3921.84
715	1111.65	752	1173.19	789	3185.94	826	3923.47
716	1114.67	753	1175.50	790	3312.38	827	3928.53
717	1116.64	754	1178.06	791	3319.95	828	3929.32
718	1119.15	755	1179.65	792	3324.61	829	3929.38
719	1121.46	756	1181.81	793	3335.47	830	3929.86
720	1122.24	757	1183.34	794	3341.88	831	3930.31
721	1124.35	758	1184.53	795	3349.10	832	3930.60
722	1126.13	759	1186.47	796	3382.46	833	3930.78
723	1127.93	760	1190.56	797	3419.38	834	3932.21
724	1129.98	761	1192.89	798	3447.89	835	3933.01
725	1131.29	762	1194.51	799	3460.97	836	3933.92
726	1133.09	763	1194.85	800	3462.95	837	3934.75
727	1134.37	764	1197.24	801	3467.44	838	3935.82
728	1135.47	765	1200.50	802	3469.55	839	3935.99
729	1137.20	766	1201.45	803	3470.92	840	3936.12
730	1139.56	767	1207.27	804	3480.84	841	3936.45
731	1140.74	768	1209.56	805	3488.04	842	3940.07
732	1142.87	769	1214.38	806	3501.26	843	3940.52
733	1144.27	770	1234.84	807	3525.58	844	3940.62
734	1144.57	771	1307.55	808	3528.08	845	3941.16
735	1148.45	772	1321.05	809	3530.67	846	3942.29
736	1150.65	773	1341.96	810	3534.68	847	3942.92
737	1151.44	774	1377.80	811	3537.65	848	3943.33
738	1152.89	775	1430.16	812	3542.80	849	3943.65
739	1155.45	776	1441.73	813	3543.84	850	3944.13
740	1156.37	777	1446.24	814	3546.46	851	3944.43
741	1157.23	778	1455.98	815	3624.61	852	3944.82
742	1158.20	779	1495.76	816	3625.54	853	3944.95
743	1161.54	780	1528.68	817	3630.90	854	3945.83
744	1163.28	781	1576.57	818	3651.85	855	3946.02
745	1165.42	782	1594.10	819	3657.42	856	3946.55
746	1166.03	783	1624.55	820	3688.18	857	3946.80
747	1167.95	784	2972.90	821	3761.66	858	3947.17
748	1168.44	785	3068.20	822	3854.43	859	3947.34
749	1170.63	786	3137.62	823	3865.19	860	3948.78
						861	3949.69

001 Surface - NTO PBE/6-31G**

zpe= 1.4883385 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.90	21.92	169.39	3348.58	4305.02	3.38619
293.15	0.1000000	22.99	21.97	176.06	3314.19	4335.35	3.49173
298.15	0.1000000	23.03	22.00	179.38	3296.60	4350.79	3.54410
303.15	0.1000000	23.07	22.02	182.69	3278.75	4366.41	3.59620
313.15	0.1000000	23.15	22.07	189.30	3242.27	4398.19	3.69961
323.15	0.1000000	23.23	22.12	195.88	3204.76	4430.67	3.80195
333.15	0.1000000	23.31	22.17	202.43	3166.23	4463.81	3.90321

Table S11 Vibrational frequencies of NTO on the 001 surface

1	-591.56	57	-98.45	113	0.00	169	108.90
2	-582.44	58	-97.69	114	6.65	170	110.80
3	-574.75	59	-96.83	115	11.00	171	112.38
4	-573.75	60	-95.70	116	15.81	172	113.33
5	-567.12	61	-93.51	117	19.79	173	114.77
6	-555.35	62	-93.08	118	20.75	174	115.03
7	-532.67	63	-91.95	119	24.33	175	116.94
8	-515.03	64	-90.11	120	26.53	176	118.23
9	-512.28	65	-89.03	121	28.75	177	119.23
10	-497.38	66	-87.67	122	30.58	178	122.61
11	-495.82	67	-86.53	123	34.52	179	124.15
12	-492.91	68	-85.62	124	35.20	180	125.06
13	-474.64	69	-84.89	125	37.01	181	126.71
14	-473.99	70	-83.80	126	38.67	182	127.74
15	-467.84	71	-81.56	127	41.89	183	130.19
16	-467.24	72	-79.43	128	42.62	184	131.44
17	-445.27	73	-79.06	129	44.12	185	134.13
18	-425.91	74	-76.87	130	45.46	186	136.88
19	-422.21	75	-73.45	131	46.69	187	137.61
20	-419.23	76	-71.40	132	49.22	188	139.47
21	-412.29	77	-69.04	133	51.55	189	141.17
22	-403.36	78	-68.15	134	53.34	190	141.97
23	-401.71	79	-65.55	135	55.10	191	144.55
24	-396.61	80	-63.91	136	56.73	192	145.39
25	-393.10	81	-63.13	137	59.99	193	147.85
26	-390.48	82	-60.26	138	62.12	194	150.04
27	-388.73	83	-58.35	139	62.59	195	150.68
28	-387.38	84	-57.33	140	64.91	196	151.73
29	-380.43	85	-55.08	141	67.21	197	154.69
30	-375.59	86	-53.53	142	68.15	198	156.84
31	-375.26	87	-51.80	143	70.47	199	159.82
32	-370.64	88	-50.19	144	71.53	200	161.16
33	-361.27	89	-49.04	145	72.91	201	162.58
34	-358.84	90	-47.15	146	74.01	202	164.24
35	-356.95	91	-46.47	147	75.75	203	167.10
36	-347.32	92	-44.44	148	77.14	204	168.24
37	-338.02	93	-43.45	149	79.44	205	170.52
38	-332.06	94	-42.65	150	79.89	206	170.99
39	-316.54	95	-40.80	151	82.07	207	172.08
40	-277.86	96	-37.76	152	83.41	208	172.99
41	-138.20	97	-34.83	153	83.79	209	174.51
42	-134.47	98	-33.29	154	85.13	210	176.30
43	-133.45	99	-31.07	155	86.45	211	178.33
44	-127.67	100	-30.49	156	88.94	212	179.07
45	-126.86	101	-25.95	157	89.48	213	179.79
46	-123.96	102	-24.62	158	91.77	214	180.19
47	-122.24	103	-23.08	159	94.01	215	183.16
48	-121.57	104	-18.40	160	95.87	216	184.86
49	-121.35	105	-15.20	161	97.03	217	185.92
50	-120.63	106	-12.97	162	97.65	218	187.05
51	-115.43	107	-4.69	163	99.76	219	190.42
52	-113.83	108	-0.00	164	100.51	220	191.00
53	-113.34	109	-0.00	165	102.26	221	192.97
54	-111.15	110	-0.00	166	103.00	222	193.59
55	-108.96	111	-0.00	167	103.56	223	194.67
56	-102.78	112	0.00	168	104.88	224	196.15

225	197.68	283	280.79	341	341.39	399	407.24
226	198.46	284	281.50	342	343.14	400	408.43
227	199.32	285	282.60	343	343.82	401	408.86
228	201.25	286	283.12	344	345.43	402	409.87
229	201.65	287	284.28	345	345.97	403	411.59
230	202.10	288	284.57	346	346.41	404	412.10
231	204.08	289	286.63	347	347.59	405	414.48
232	206.09	290	287.31	348	348.50	406	416.34
233	208.66	291	288.52	349	349.97	407	417.26
234	210.27	292	290.64	350	352.27	408	417.87
235	212.14	293	291.62	351	352.67	409	418.57
236	212.70	294	292.23	352	354.58	410	419.67
237	214.24	295	293.40	353	355.31	411	420.96
238	215.22	296	293.59	354	355.58	412	422.57
239	216.81	297	295.33	355	357.05	413	425.50
240	217.93	298	296.58	356	359.15	414	425.76
241	219.31	299	297.29	357	359.91	415	427.87
242	223.50	300	297.76	358	360.62	416	428.18
243	226.26	301	298.76	359	360.89	417	431.57
244	228.12	302	300.14	360	362.33	418	433.04
245	229.37	303	300.48	361	364.47	419	434.29
246	231.02	304	302.10	362	364.77	420	437.28
247	232.08	305	302.52	363	366.21	421	439.31
248	235.51	306	303.23	364	366.60	422	439.82
249	237.13	307	303.59	365	368.36	423	446.98
250	238.34	308	305.03	366	369.88	424	453.53
251	239.11	309	307.28	367	371.19	425	458.80
252	241.12	310	307.62	368	372.48	426	467.47
253	242.42	311	308.60	369	373.12	427	468.09
254	245.14	312	309.09	370	374.69	428	480.70
255	246.02	313	310.62	371	375.08	429	486.01
256	246.96	314	311.38	372	376.55	430	491.53
257	249.24	315	312.00	373	377.90	431	491.92
258	251.17	316	312.79	374	379.09	432	494.18
259	252.45	317	313.37	375	380.30	433	497.70
260	253.48	318	313.64	376	380.81	434	506.16
261	253.91	319	316.13	377	382.79	435	508.60
262	256.35	320	316.88	378	383.26	436	512.46
263	257.43	321	317.80	379	384.03	437	515.97
264	257.92	322	319.92	380	384.44	438	517.21
265	260.03	323	320.50	381	385.21	439	519.74
266	260.42	324	322.05	382	386.26	440	521.78
267	261.05	325	322.87	383	387.85	441	523.39
268	263.07	326	323.43	384	389.71	442	527.20
269	264.40	327	324.39	385	390.40	443	529.03
270	265.51	328	324.71	386	392.23	444	530.35
271	267.05	329	326.91	387	392.50	445	534.66
272	268.73	330	328.81	388	395.09	446	538.34
273	269.88	331	329.19	389	396.35	447	545.45
274	270.31	332	331.66	390	398.09	448	549.56
275	271.81	333	332.46	391	398.45	449	554.99
276	272.70	334	333.12	392	398.76	450	559.80
277	272.95	335	335.05	393	400.69	451	566.52
278	274.51	336	335.18	394	400.94	452	571.48
279	274.62	337	336.34	395	401.99	453	572.79
280	276.57	338	337.99	396	403.11	454	575.39
281	278.76	339	339.58	397	403.84	455	581.06
282	279.80	340	340.34	398	405.86	456	582.71

457	587.63	515	737.71	573	859.30	631	991.91
458	591.53	516	738.87	574	859.90	632	992.78
459	599.13	517	741.02	575	862.89	633	995.34
460	599.58	518	742.81	576	866.11	634	995.83
461	605.82	519	744.39	577	867.38	635	997.26
462	606.50	520	746.47	578	868.82	636	998.07
463	607.62	521	750.98	579	869.06	637	998.75
464	612.58	522	753.55	580	871.15	638	1002.37
465	618.85	523	759.09	581	872.48	639	1003.88
466	619.96	524	761.82	582	873.70	640	1005.27
467	623.63	525	764.16	583	878.29	641	1006.12
468	625.59	526	765.51	584	881.30	642	1007.60
469	630.20	527	767.97	585	882.03	643	1008.05
470	634.63	528	769.79	586	883.76	644	1009.21
471	638.65	529	773.57	587	884.81	645	1009.29
472	641.78	530	775.31	588	887.95	646	1010.85
473	642.71	531	778.15	589	891.65	647	1012.08
474	644.77	532	780.29	590	894.49	648	1014.25
475	646.21	533	784.14	591	898.56	649	1015.69
476	647.05	534	786.40	592	902.36	650	1016.19
477	651.37	535	787.35	593	905.53	651	1017.22
478	656.81	536	788.85	594	910.07	652	1019.19
479	662.58	537	789.54	595	912.30	653	1019.51
480	667.35	538	791.35	596	915.23	654	1020.53
481	671.33	539	791.80	597	919.68	655	1021.63
482	674.51	540	795.63	598	922.89	656	1023.21
483	678.11	541	795.85	599	923.89	657	1023.92
484	680.45	542	797.39	600	930.19	658	1024.55
485	681.77	543	799.61	601	932.13	659	1024.57
486	684.40	544	800.78	602	935.18	660	1026.53
487	685.77	545	803.05	603	935.91	661	1026.73
488	689.78	546	804.77	604	936.75	662	1027.46
489	691.60	547	807.24	605	939.26	663	1029.30
490	696.19	548	809.26	606	939.40	664	1030.28
491	698.58	549	809.99	607	940.95	665	1031.13
492	699.86	550	810.45	608	944.87	666	1032.45
493	703.90	551	811.24	609	947.44	667	1038.07
494	703.96	552	813.16	610	948.07	668	1039.46
495	704.52	553	816.04	611	950.09	669	1041.20
496	706.06	554	816.57	612	956.16	670	1046.63
497	708.72	555	817.84	613	960.49	671	1049.21
498	709.42	556	820.74	614	962.03	672	1054.09
499	710.94	557	826.01	615	964.10	673	1056.49
500	713.48	558	833.63	616	965.64	674	1062.40
501	715.48	559	834.78	617	970.21	675	1069.64
502	717.31	560	838.81	618	972.26	676	1073.56
503	718.43	561	839.42	619	975.69	677	1074.77
504	719.17	562	840.70	620	976.46	678	1075.85
505	720.86	563	842.99	621	979.02	679	1075.97
506	726.25	564	847.11	622	980.81	680	1077.41
507	728.90	565	848.22	623	982.00	681	1078.37
508	729.29	566	850.47	624	982.36	682	1079.84
509	731.28	567	851.28	625	984.21	683	1080.89
510	733.37	568	853.06	626	986.95	684	1081.13
511	734.77	569	854.48	627	987.28	685	1081.91
512	735.56	570	854.59	628	988.69	686	1082.98
513	736.57	571	856.83	629	989.30	687	1083.65
514	737.53	572	857.95	630	991.00	688	1086.57

689	1087.27	726	1159.52	762	3229.75	798	3921.71
690	1087.67	727	1161.52	763	3264.12	799	3922.49
691	1088.75	728	1163.04	764	3309.69	800	3928.75
692	1089.23	729	1165.16	765	3314.45	801	3929.47
693	1090.08	730	1166.12	766	3320.69	802	3929.72
694	1090.45	731	1168.12	767	3334.48	803	3929.82
695	1092.20	732	1169.64	768	3344.31	804	3929.87
696	1092.44	733	1170.21	769	3356.02	805	3930.12
697	1095.10	734	1173.13	770	3363.61	806	3930.34
698	1101.79	735	1175.13	771	3446.45	807	3931.56
699	1106.41	736	1177.25	772	3459.76	808	3931.79
700	1110.75	737	1178.27	773	3459.83	809	3932.30
701	1115.36	738	1179.77	774	3461.69	810	3933.88
702	1116.83	739	1180.13	775	3465.60	811	3933.89
703	1118.05	740	1183.14	776	3468.71	812	3934.96
704	1118.16	741	1184.44	777	3469.67	813	3935.45
705	1118.47	742	1186.85	778	3475.48	814	3936.68
706	1121.75	743	1190.78	779	3476.52	815	3938.63
707	1124.27	744	1191.92	780	3480.85	816	3939.50
708	1126.08	745	1194.82	781	3526.80	817	3940.28
709	1128.21	746	1195.76	782	3533.15	818	3942.07
710	1130.73	747	1198.65	783	3538.51	819	3942.11
711	1133.47	748	1200.86	784	3543.75	820	3942.89
712	1136.37	749	1202.80	785	3559.40	821	3942.99
713	1140.79	750	1204.25	786	3578.11	822	3943.12
714	1142.68	751	1211.20	787	3579.27	823	3943.97
715	1143.40	752	1216.66	788	3598.99	824	3944.05
716	1144.31	753	1254.12	789	3608.17	825	3944.83
717	1145.22	754	1280.49	790	3622.68	826	3945.04
718	1146.83	755	1342.91	791	3651.80	827	3945.30
719	1148.88	756	1355.56	792	3677.80	828	3945.45
720	1151.35	757	1471.60	793	3691.46	829	3946.11
721	1151.63	758	1560.26	794	3769.77	830	3946.62
722	1154.13	759	1598.71	795	3858.67	831	3946.91
723	1155.97	760	1770.13	796	3861.84	832	3947.22
724	1157.06	761	3021.54	797	3914.63	833	3948.04
725	1157.97					834	3949.55

100 Surface - TNT PBE/6-31G**

zpe= 1.0718637 Hartree * 0.986

T	p	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot.	energy	entropy
(K)	(MPa)				(kJ/mol)	(kJ/mol)	(kJ/mol/K)
283.15	0.1000000	22.22	21.17	104.40	2426.83	3063.79	2.25788
293.15	0.1000000	22.31	21.22	108.63	2403.91	3083.05	2.32500
298.15	0.1000000	22.35	21.24	110.73	2392.20	3092.84	2.35827
303.15	0.1000000	22.39	21.27	112.83	2380.33	3102.74	2.39134
313.15	0.1000000	22.47	21.32	117.01	2356.09	3122.87	2.45692
323.15	0.1000000	22.55	21.36	121.18	2331.19	3143.40	2.52172
333.15	0.1000000	22.63	21.41	125.32	2305.65	3164.33	2.58576

Table S12 Vibrational frequencies of TNT on the 001 surface

1	-705.46	57	-162.32	113	0.00	169	164.98
2	-691.04	58	-162.09	114	0.00	170	168.29
3	-690.62	59	-157.03	115	14.35	171	170.33
4	-689.14	60	-153.48	116	16.16	172	172.46
5	-680.18	61	-152.58	117	20.15	173	174.09
6	-679.48	62	-151.31	118	25.67	174	180.23
7	-679.16	63	-146.08	119	28.87	175	181.15
8	-676.57	64	-145.10	120	31.07	176	184.17
9	-674.38	65	-143.88	121	34.03	177	185.36
10	-668.90	66	-140.31	122	36.88	178	186.21
11	-667.60	67	-139.81	123	39.84	179	186.87
12	-665.07	68	-133.45	124	44.68	180	188.29
13	-662.90	69	-132.18	125	50.25	181	189.87
14	-662.54	70	-124.62	126	51.07	182	190.40
15	-654.70	71	-123.13	127	55.42	183	193.86
16	-652.48	72	-121.02	128	58.59	184	195.43
17	-647.61	73	-114.92	129	60.65	185	196.55
18	-647.48	74	-109.23	130	61.64	186	198.46
19	-645.22	75	-104.56	131	64.46	187	200.10
20	-643.96	76	-102.65	132	67.27	188	200.29
21	-643.53	77	-101.46	133	68.06	189	202.09
22	-641.51	78	-99.49	134	69.46	190	203.78
23	-633.55	79	-96.46	135	73.10	191	207.23
24	-631.67	80	-94.57	136	79.04	192	209.31
25	-629.37	81	-90.89	137	92.35	193	210.78
26	-620.84	82	-88.31	138	96.25	194	211.43
27	-605.70	83	-85.56	139	99.62	195	212.21
28	-597.85	84	-85.28	140	102.58	196	214.93
29	-596.59	85	-83.92	141	109.55	197	217.47
30	-592.35	86	-81.05	142	110.40	198	222.42
31	-582.22	87	-80.47	143	111.45	199	224.93
32	-581.82	88	-77.00	144	113.22	200	226.43
33	-568.36	89	-74.61	145	114.54	201	228.51
34	-555.93	90	-72.85	146	116.62	202	230.82
35	-547.68	91	-70.20	147	117.61	203	232.99
36	-536.49	92	-69.44	148	118.01	204	235.64
37	-530.30	93	-65.29	149	120.85	205	237.83
38	-528.14	94	-62.77	150	124.08	206	239.83
39	-518.73	95	-61.39	151	128.67	207	241.30
40	-504.14	96	-60.11	152	130.27	208	243.98
41	-502.77	97	-58.76	153	133.49	209	244.25
42	-393.26	98	-56.05	154	137.24	210	247.41
43	-207.69	99	-54.19	155	139.86	211	249.47
44	-204.03	100	-51.93	156	141.54	212	249.85
45	-198.53	101	-47.78	157	142.54	213	252.38
46	-191.95	102	-46.23	158	142.95	214	255.14
47	-185.84	103	-41.35	159	144.46	215	257.17
48	-185.62	104	-37.93	160	147.51	216	259.29
49	-180.61	105	-35.33	161	150.30	217	260.11
50	-179.73	106	-33.64	162	152.25	218	262.38
51	-177.76	107	-23.89	163	153.45	219	262.83
52	-173.54	108	-1.11	164	154.26	220	265.16
53	-170.82	109	-0.00	165	156.23	221	266.20
54	-167.38	110	-0.00	166	158.60	222	267.15
55	-166.27	111	-0.00	167	160.89	223	269.07
56	-165.40	112	0.00	168	163.80	224	269.77

225	272.54	283	374.49	341	591.36	399	835.84
226	274.16	284	375.68	342	595.24	400	836.68
227	275.91	285	378.83	343	596.60	401	838.65
228	278.05	286	381.60	344	596.86	402	839.55
229	280.04	287	381.87	345	599.84	403	842.11
230	280.88	288	384.36	346	602.57	404	842.61
231	284.03	289	386.25	347	609.94	405	844.87
232	286.78	290	387.12	348	612.34	406	845.90
233	288.22	291	389.10	349	615.82	407	846.58
234	289.89	292	391.52	350	618.91	408	848.89
235	290.77	293	395.43	351	619.96	409	849.52
236	293.47	294	398.32	352	622.33	410	854.04
237	295.55	295	403.27	353	632.79	411	856.66
238	296.36	296	406.58	354	633.37	412	858.75
239	297.38	297	409.93	355	637.85	413	859.59
240	300.55	298	447.41	356	644.87	414	861.86
241	301.51	299	457.73	357	645.79	415	863.71
242	302.96	300	468.19	358	647.08	416	868.55
243	304.48	301	474.97	359	658.43	417	868.73
244	307.52	302	479.40	360	664.19	418	869.11
245	308.19	303	481.60	361	673.45	419	871.31
246	310.81	304	488.24	362	678.86	420	875.83
247	313.24	305	491.79	363	681.89	421	877.71
248	313.47	306	492.98	364	683.78	422	881.15
249	315.38	307	497.39	365	688.65	423	882.06
250	317.81	308	500.85	366	692.73	424	884.48
251	319.04	309	504.35	367	699.69	425	887.84
252	321.46	310	509.54	368	704.23	426	889.01
253	322.90	311	514.27	369	709.76	427	892.25
254	324.68	312	516.76	370	710.80	428	893.25
255	326.42	313	520.06	371	713.30	429	895.65
256	327.13	314	522.90	372	716.37	430	896.42
257	328.82	315	526.57	373	719.15	431	896.81
258	329.41	316	526.84	374	730.34	432	898.60
259	333.46	317	527.50	375	737.84	433	903.93
260	336.06	318	529.61	376	742.84	434	906.38
261	336.96	319	532.77	377	745.87	435	907.02
262	337.67	320	534.91	378	749.81	436	909.13
263	341.51	321	536.99	379	752.10	437	909.16
264	342.02	322	539.62	380	756.41	438	910.16
265	343.75	323	543.01	381	761.93	439	913.54
266	344.79	324	545.46	382	765.05	440	914.66
267	346.15	325	546.40	383	768.11	441	917.60
268	348.15	326	548.90	384	776.98	442	917.88
269	349.90	327	553.21	385	777.97	443	918.82
270	352.35	328	553.74	386	781.37	444	920.81
271	354.49	329	559.80	387	785.02	445	922.83
272	354.94	330	563.66	388	788.52	446	932.36
273	358.03	331	566.08	389	805.02	447	935.84
274	358.90	332	567.24	390	806.08	448	938.06
275	360.02	333	573.39	391	813.95	449	939.55
276	360.88	334	575.46	392	817.64	450	944.10
277	363.11	335	575.77	393	823.29	451	946.67
278	364.37	336	577.79	394	824.40	452	952.86
279	367.55	337	579.75	395	829.08	453	961.86
280	368.48	338	581.64	396	830.06	454	964.80
281	369.60	339	587.02	397	833.19	455	980.54
282	372.51	340	588.26	398	834.83	456	991.46

457	1006.31	487	1370.90	517	1615.21	547	4120.62
458	1015.74	488	1372.43	518	3017.10	548	4124.36
459	1029.44	489	1374.11	519	3093.06	549	4125.13
460	1040.66	490	1377.34	520	3130.41	550	4126.41
461	1048.66	491	1378.93	521	3186.17	551	4127.57
462	1049.34	492	1380.81	522	3194.19	552	4129.56
463	1056.57	493	1381.81	523	3283.35	553	4132.18
464	1058.78	494	1383.52	524	3295.35	554	4135.22
465	1063.25	495	1385.21	525	3363.65	555	4136.53
466	1066.79	496	1386.79	526	3388.63	556	4141.19
467	1069.97	497	1389.43	527	3556.68	557	4141.37
468	1146.57	498	1391.79	528	3588.41	558	4142.19
469	1172.74	499	1395.64	529	3599.68	559	4144.13
470	1196.78	500	1396.17	530	3636.11	560	4145.01
471	1261.80	501	1397.56	531	3670.44	561	4152.36
472	1274.31	502	1399.53	532	3693.57	562	4153.14
473	1300.98	503	1402.65	533	3764.16	563	4157.04
474	1325.38	504	1405.83	534	3778.69	564	4157.21
475	1329.15	505	1409.30	535	3859.88	565	4158.50
476	1338.72	506	1410.84	536	4101.78	566	4159.74
477	1340.18	507	1418.16	537	4108.01	567	4162.15
478	1342.50	508	1419.65	538	4111.04	568	4162.23
479	1345.56	509	1427.08	539	4112.46	569	4163.25
480	1348.44	510	1431.08	540	4114.71	570	4164.25
481	1355.07	511	1459.73	541	4116.32	571	4166.38
482	1355.89	512	1460.95	542	4116.94	572	4168.19
483	1361.22	513	1560.61	543	4117.70	573	4169.89
484	1364.51	514	1576.77	544	4118.87	574	4170.65
485	1365.87	515	1579.70	545	4119.07	575	4171.44
486	1368.93	516	1612.45	546	4119.78	576	4171.85

100 Surface - DNT PBE/6-31G**

zpe= 1.0689853 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.19	21.13	104.04	2420.37	3052.94	2.24238
293.15	0.1000000	22.28	21.19	108.21	2397.61	3071.93	2.30858
298.15	0.1000000	22.32	21.21	110.29	2385.98	3081.59	2.34139
303.15	0.1000000	22.36	21.24	112.37	2374.20	3091.36	2.37402
313.15	0.1000000	22.44	21.28	116.50	2350.13	3111.20	2.43869
323.15	0.1000000	22.52	21.33	120.61	2325.42	3131.45	2.50260
333.15	0.1000000	22.60	21.38	124.70	2300.08	3152.09	2.56575

Table S13 Vibrational frequencies of DNT on the100 surface

1	-706.65	10	-668.99	19	-645.04	28	-599.25
2	-693.28	11	-666.25	20	-641.88	29	-596.28
3	-690.52	12	-664.82	21	-641.77	30	-592.70
4	-690.29	13	-663.11	22	-635.27	31	-580.86
5	-679.57	14	-661.75	23	-632.15	32	-580.52
6	-678.91	15	-654.28	24	-630.99	33	-571.16
7	-678.51	16	-651.25	25	-627.74	34	-556.75
8	-676.19	17	-647.07	26	-615.49	35	-542.89
9	-674.42	18	-646.71	27	-603.51	36	-534.32

37	-528.63	95	-62.91	153	134.19	211	251.30
38	-523.24	96	-60.60	154	138.52	212	253.77
39	-514.21	97	-58.84	155	140.26	213	255.80
40	-501.13	98	-58.03	156	141.49	214	257.53
41	-500.61	99	-55.37	157	142.42	215	259.53
42	-388.59	100	-52.35	158	145.61	216	260.13
43	-208.58	101	-48.57	159	148.51	217	260.50
44	-204.83	102	-45.66	160	150.46	218	262.97
45	-197.89	103	-41.57	161	152.48	219	264.86
46	-191.12	104	-37.64	162	154.31	220	266.27
47	-186.38	105	-35.93	163	155.22	221	267.74
48	-185.11	106	-32.73	164	157.16	222	268.79
49	-181.00	107	-22.70	165	158.33	223	269.86
50	-180.25	108	-0.00	166	159.46	224	272.04
51	-177.33	109	-0.00	167	161.86	225	272.62
52	-174.15	110	0.00	168	163.04	226	274.58
53	-171.72	111	0.00	169	166.78	227	276.64
54	-167.96	112	0.00	170	168.53	228	278.44
55	-166.04	113	0.00	171	170.73	229	281.25
56	-164.81	114	4.95	172	173.48	230	282.91
57	-163.19	115	17.12	173	174.25	231	283.94
58	-162.49	116	20.53	174	177.68	232	286.95
59	-157.66	117	26.01	175	181.02	233	288.50
60	-153.44	118	28.22	176	181.76	234	290.29
61	-152.76	119	29.80	177	184.35	235	294.22
62	-151.58	120	35.51	178	185.97	236	296.06
63	-146.25	121	40.63	179	187.28	237	296.94
64	-144.88	122	44.78	180	188.91	238	300.00
65	-143.29	123	48.47	181	189.74	239	300.52
66	-140.49	124	52.00	182	191.98	240	302.52
67	-139.68	125	53.71	183	195.33	241	304.84
68	-132.86	126	55.56	184	195.45	242	305.15
69	-132.15	127	57.40	185	198.22	243	307.45
70	-126.03	128	62.12	186	198.80	244	309.41
71	-123.20	129	65.80	187	200.88	245	310.23
72	-121.98	130	66.81	188	203.30	246	312.59
73	-114.84	131	69.20	189	204.94	247	314.21
74	-108.65	132	71.77	190	208.07	248	315.89
75	-107.71	133	72.00	191	210.24	249	319.41
76	-103.89	134	77.28	192	211.35	250	321.10
77	-101.80	135	84.25	193	212.93	251	323.27
78	-100.36	136	92.32	194	215.25	252	324.38
79	-98.68	137	96.23	195	218.18	253	328.12
80	-95.07	138	100.99	196	223.01	254	330.54
81	-91.57	139	104.52	197	224.88	255	331.23
82	-89.49	140	108.30	198	226.61	256	333.98
83	-87.52	141	109.83	199	228.34	257	335.79
84	-85.46	142	111.84	200	231.70	258	336.65
85	-84.73	143	114.71	201	233.20	259	337.16
86	-81.89	144	116.14	202	235.20	260	338.82
87	-79.77	145	117.42	203	237.24	261	341.60
88	-77.46	146	118.74	204	238.80	262	343.45
89	-76.10	147	122.40	205	241.77	263	344.26
90	-73.85	148	125.19	206	243.43	264	345.20
91	-70.95	149	126.03	207	244.02	265	347.58
92	-69.51	150	127.09	208	246.88	266	349.35
93	-66.98	151	130.04	209	248.88	267	352.36
94	-64.54	152	131.97	210	250.18	268	353.37

269	356.10	327	570.51	385	811.47	443	940.99
270	356.87	328	573.82	386	815.68	444	942.81
271	359.40	329	576.45	387	818.02	445	948.05
272	360.54	330	577.39	388	820.75	446	952.84
273	362.55	331	578.47	389	822.94	447	961.64
274	363.62	332	580.58	390	824.09	448	963.48
275	363.92	333	581.57	391	829.50	449	969.97
276	367.42	334	587.01	392	830.05	450	984.27
277	369.59	335	589.87	393	831.41	451	991.48
278	369.93	336	593.48	394	834.40	452	1007.49
279	372.97	337	596.22	395	835.50	453	1016.66
280	374.77	338	596.48	396	836.47	454	1036.42
281	377.11	339	597.73	397	838.29	455	1043.54
282	378.17	340	600.14	398	838.89	456	1050.66
283	380.27	341	603.65	399	841.62	457	1058.57
284	383.05	342	609.67	400	842.02	458	1065.58
285	384.19	343	612.77	401	844.69	459	1066.38
286	387.22	344	616.24	402	845.54	460	1099.25
287	388.88	345	618.96	403	847.19	461	1128.10
288	389.38	346	620.01	404	848.84	462	1149.11
289	395.85	347	622.48	405	849.74	463	1163.28
290	397.21	348	624.81	406	854.04	464	1207.61
291	403.63	349	632.35	407	855.03	465	1256.76
292	407.62	350	636.09	408	858.22	466	1261.39
293	410.45	351	643.63	409	860.68	467	1274.34
294	415.09	352	646.47	410	861.97	468	1300.92
295	426.97	353	654.13	411	867.24	469	1321.64
296	456.52	354	658.82	412	868.83	470	1338.94
297	477.38	355	662.14	413	869.39	471	1339.96
298	480.44	356	663.99	414	871.81	472	1340.28
299	482.13	357	672.34	415	875.10	473	1343.03
300	488.95	358	678.25	416	875.94	474	1355.20
301	489.77	359	681.55	417	880.02	475	1356.11
302	494.41	360	688.89	418	881.33	476	1361.60
303	497.26	361	692.24	419	881.87	477	1364.75
304	502.50	362	695.20	420	883.68	478	1369.11
305	504.77	363	698.05	421	888.43	479	1370.43
306	508.51	364	703.72	422	892.71	480	1371.22
307	520.29	365	708.49	423	893.84	481	1372.84
308	522.81	366	709.84	424	895.59	482	1374.74
309	526.16	367	713.60	425	897.39	483	1376.31
310	526.74	368	714.01	426	899.42	484	1377.31
311	528.23	369	727.78	427	902.29	485	1379.35
312	530.65	370	730.44	428	906.60	486	1381.03
313	534.60	371	738.67	429	907.07	487	1381.64
314	538.40	372	742.66	430	908.02	488	1383.64
315	541.28	373	745.76	431	909.41	489	1385.41
316	542.65	374	746.59	432	912.36	490	1386.84
317	543.02	375	754.37	433	913.88	491	1389.39
318	545.33	376	760.58	434	914.87	492	1392.10
319	549.00	377	761.97	435	917.12	493	1396.07
320	551.31	378	765.57	436	918.16	494	1396.62
321	553.70	379	777.05	437	920.82	495	1397.77
322	557.37	380	777.92	438	922.20	496	1402.64
323	559.81	381	783.49	439	931.16	497	1406.41
324	562.07	382	784.44	440	932.93	498	1409.07
325	567.13	383	787.35	441	936.56	499	1409.74
326	567.87	384	802.61	442	939.67	500	1411.02

501	1419.04	518	3279.97	535	4116.41	553	4144.39
502	1420.69	519	3306.94	536	4116.83	554	4144.78
503	1442.51	520	3349.65	537	4117.68	555	4152.45
504	1452.52	521	3353.40	538	4118.77	556	4153.15
505	1461.21	522	3474.29	539	4119.04	557	4157.05
506	1472.77	523	3631.04	540	4119.76	558	4157.12
507	1559.74	524	3668.79	541	4120.57	559	4158.46
508	1572.42	525	3676.12	542	4124.34	560	4160.04
509	1603.32	526	3763.84	543	4125.12	561	4161.98
510	1615.63	527	3778.47	544	4126.46	562	4162.19
511	2996.40	528	3796.12	545	4127.91	563	4162.82
512	3069.56	529	3864.04	546	4129.30	564	4164.09
513	3089.88	530	4101.82	547	4132.68	565	4166.59
514	3157.88	531	4107.36	548	4135.46	566	4168.10
515	3171.77	532	4111.20	549	4137.03	567	4169.74
516	3185.84	533	4112.84	550	4141.05	568	4170.73
517	3254.44	534	4114.20	551	4141.59	569	4171.53
				552	4142.47	570	4171.75

100 Surface - DNAN PBE/6-31G**

zpe= 1.0736769 Hartree * 0.986

T (K)	p (MPa)	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot. (kJ/mol)	energy (kJ/mol)	entropy (kJ/mol/K)
283.15	0.1000000	22.20	21.14	101.82	2437.70	3065.51	2.22554
293.15	0.1000000	22.29	21.19	106.00	2415.11	3084.57	2.29199
298.15	0.1000000	22.33	21.22	108.08	2403.57	3094.26	2.3249
303.15	0.1000000	22.37	21.24	110.16	2391.86	3104.06	2.35766
313.15	0.1000000	22.45	21.29	114.30	2367.96	3123.98	2.42257
323.15	0.1000000	22.53	21.34	118.42	2343.41	3144.30	2.48671
333.15	0.1000000	22.61	21.38	122.52	2318.22	3165.02	2.55010

Table S14 Vibrational frequencies of DNAN on the 100 surface

1	-707.16	19	-645.53	37	-528.60	55	-166.03
2	-692.96	20	-641.56	38	-524.78	56	-165.33
3	-690.43	21	-636.13	39	-515.47	57	-162.81
4	-688.93	22	-634.42	40	-500.92	58	-161.94
5	-679.32	23	-630.73	41	-499.71	59	-157.62
6	-679.02	24	-630.03	42	-390.65	60	-153.67
7	-677.90	25	-628.79	43	-208.60	61	-153.38
8	-674.52	26	-615.71	44	-204.92	62	-151.42
9	-669.55	27	-603.28	45	-198.06	63	-145.65
10	-668.81	28	-602.24	46	-191.16	64	-144.23
11	-664.81	29	-595.92	47	-187.62	65	-143.14
12	-662.46	30	-592.24	48	-185.76	66	-140.23
13	-661.46	31	-580.57	49	-180.77	67	-139.39
14	-659.66	32	-580.13	50	-180.22	68	-133.19
15	-654.00	33	-571.00	51	-176.78	69	-131.50
16	-652.04	34	-556.71	52	-174.80	70	-125.69
17	-647.64	35	-542.73	53	-171.28	71	-122.73
18	-646.88	36	-534.89	54	-167.60	72	-121.62

73	-115.01	131	68.77	189	203.57	247	310.15
74	-108.99	132	71.68	190	204.91	248	311.92
75	-106.24	133	72.38	191	206.29	249	314.98
76	-103.20	134	78.03	192	208.50	250	316.34
77	-101.98	135	87.90	193	211.38	251	318.93
78	-98.82	136	93.24	194	213.06	252	321.32
79	-97.70	137	98.17	195	216.35	253	321.73
80	-94.81	138	102.22	196	222.14	254	323.92
81	-91.27	139	102.54	197	222.72	255	326.51
82	-88.73	140	106.32	198	223.35	256	329.64
83	-87.47	141	109.46	199	226.34	257	330.94
84	-85.23	142	113.24	200	227.72	258	333.46
85	-83.47	143	113.64	201	230.73	259	334.59
86	-81.73	144	115.70	202	232.08	260	337.05
87	-80.68	145	117.23	203	234.26	261	338.69
88	-78.23	146	117.99	204	234.62	262	340.80
89	-74.97	147	119.47	205	237.23	263	342.54
90	-73.58	148	122.50	206	239.88	264	343.03
91	-71.22	149	125.83	207	241.15	265	343.45
92	-69.37	150	126.46	208	242.49	266	346.79
93	-67.71	151	130.38	209	245.02	267	347.58
94	-65.07	152	132.74	210	246.94	268	350.09
95	-63.57	153	134.62	211	247.04	269	351.77
96	-60.38	154	135.79	212	250.05	270	353.12
97	-58.96	155	138.69	213	250.80	271	356.19
98	-58.05	156	141.92	214	253.65	272	357.63
99	-55.66	157	142.84	215	254.56	273	360.20
100	-52.42	158	143.84	216	257.04	274	361.24
101	-48.97	159	145.19	217	259.94	275	362.74
102	-45.44	160	147.56	218	260.29	276	363.31
103	-42.31	161	153.47	219	261.71	277	364.43
104	-38.12	162	154.08	220	263.41	278	366.73
105	-34.50	163	155.95	221	266.77	279	367.43
106	-32.90	164	157.04	222	267.33	280	369.03
107	-23.67	165	159.07	223	268.62	281	370.41
108	-2.19	166	160.43	224	269.56	282	373.51
109	-0.00	167	161.56	225	270.53	283	377.29
110	-0.00	168	162.95	226	271.42	284	378.77
111	-0.00	169	164.85	227	274.60	285	380.50
112	-0.00	170	168.50	228	275.04	286	381.96
113	0.00	171	170.98	229	277.12	287	384.08
114	0.00	172	172.67	230	279.92	288	385.82
115	16.25	173	175.43	231	282.86	289	390.43
116	19.27	174	176.96	232	283.83	290	392.32
117	24.51	175	179.02	233	285.87	291	395.81
118	26.17	176	179.95	234	287.48	292	397.14
119	29.07	177	182.14	235	289.70	238	297.64
120	32.16	178	184.61	236	293.74	239	299.67
121	39.33	179	186.58	237	296.13	240	300.21
122	41.56	180	188.41	238	297.64	241	301.74
123	45.42	181	189.69	239	299.67	242	302.35
124	49.58	182	192.02	240	300.21	243	304.26
125	50.44	183	193.43	241	301.74	244	304.57
126	54.46	184	195.81	242	302.35	245	306.73
127	57.57	185	197.99	243	304.26	246	309.49
128	61.43	186	198.61	244	304.57	247	310.15
129	65.91	187	200.83	245	306.73	248	311.92
130	66.68	188	201.91	246	309.49	249	314.98

250	316.34	307	507.84	309	516.43	367	705.63
251	318.93	308	513.89	310	520.78	368	709.74
252	321.32	309	516.43	311	524.62	369	713.21
253	321.73	310	520.78	312	525.76	370	716.83
254	323.92	311	524.62	313	527.55	371	725.01
255	326.51	312	525.76	314	528.69	372	732.28
256	329.64	313	527.55	315	531.13	373	735.05
257	330.94	314	528.69	316	534.93	374	741.76
258	333.46	315	531.13	317	538.53	375	745.34
259	334.59	316	534.93	318	541.90	376	746.74
260	337.05	317	538.53	319	543.50	377	751.27
261	338.69	318	541.90	320	546.18	378	762.96
262	340.80	319	543.50	321	550.32	379	765.19
263	342.54	320	546.18	322	551.56	380	765.78
264	343.03	321	550.32	323	554.63	381	777.70
265	343.45	322	551.56	324	559.66	382	780.99
266	346.79	323	554.63	325	561.45	383	783.40
267	347.58	324	559.66	326	563.03	384	785.05
268	350.09	325	561.45	327	567.57	385	795.29
269	351.77	326	563.03	328	568.43	386	803.90
270	353.12	327	567.57	329	572.62	387	805.15
271	356.19	328	568.43	330	576.68	388	812.98
272	357.63	329	572.62	331	577.09	389	815.59
273	360.20	330	576.68	332	578.07	390	818.05
274	361.24	331	577.09	333	578.91	391	822.07
275	362.74	332	578.07	334	581.11	392	825.28
276	363.31	333	578.91	335	582.69	393	826.15
277	364.43	334	581.11	336	587.43	394	826.57
278	366.73	335	582.69	337	589.90	395	829.68
279	367.43	336	587.43	338	593.17	396	831.26
280	369.03	337	589.90	339	596.21	397	834.75
281	370.41	338	593.17	340	596.54	398	835.39
282	373.51	339	596.21	341	597.55	399	836.55
283	377.29	340	596.54	342	600.69	400	838.11
284	378.77	341	597.55	343	603.43	401	838.75
285	380.50	342	600.69	344	605.41	402	841.73
286	381.96	343	603.43	345	610.39	403	844.07
287	384.08	344	605.41	346	613.10	404	844.86
288	385.82	345	610.39	347	616.67	405	845.50
289	390.43	346	613.10	348	619.42	406	847.65
290	392.32	347	616.67	349	622.00	407	848.73
291	395.81	348	619.42	350	622.77	408	850.18
292	397.14	293	402.16	351	627.66	409	854.43
293	402.16	294	402.60	352	637.55	410	854.53
293	402.16	295	404.01	353	638.22	411	857.26
294	402.60	296	406.75	354	644.95	412	860.71
295	404.01	297	466.91	355	647.53	413	862.04
296	406.75	298	468.86	356	658.83	414	866.90
297	466.91	299	479.08	357	664.25	415	869.03
298	468.86	300	482.02	358	668.81	416	869.59
299	479.08	301	483.75	359	672.63	417	871.37
300	482.02	302	488.37	360	677.97	418	872.37
301	483.75	303	494.64	361	681.02	419	877.00
302	488.37	304	497.00	362	688.56	420	879.29
303	494.64	305	501.51	363	689.68	421	881.69
304	497.00	306	504.26	364	693.54	422	884.57
305	501.51	307	507.84	365	700.26	423	887.24
306	504.26	308	513.89	366	703.83	424	888.86

425	892.72	462	1139.06	499	1405.63	536	4112.76
426	895.74	463	1145.54	500	1409.20	537	4114.23
427	896.53	464	1159.93	501	1410.75	538	4116.25
428	898.10	465	1169.04	502	1418.27	539	4116.66
429	901.17	466	1182.44	503	1419.28	540	4117.69
430	904.78	467	1238.49	504	1425.81	541	4118.84
431	905.61	468	1261.58	505	1441.97	542	4119.21
432	907.64	469	1274.53	506	1460.52	543	4119.74
433	908.40	470	1301.08	507	1462.05	544	4120.34
434	912.85	471	1306.76	508	1465.86	545	4124.37
435	914.20	472	1318.09	509	1494.85	546	4125.25
436	915.80	473	1338.61	510	1534.73	547	4126.31
437	917.37	474	1339.57	511	1569.07	548	4127.91
438	918.30	475	1340.47	512	1589.14	549	4129.21
439	919.46	476	1342.80	513	1622.12	550	4132.65
440	921.14	477	1354.76	514	2977.55	551	4133.26
441	929.80	478	1355.95	515	3071.37	552	4137.20
442	933.18	479	1361.41	516	3122.19	553	4140.91
443	936.71	480	1364.44	517	3160.15	554	4141.47
444	938.82	481	1369.10	518	3184.18	555	4142.33
445	940.52	482	1370.86	519	3189.96	556	4144.78
446	941.65	483	1372.81	520	3270.15	557	4145.07
447	948.22	484	1374.47	521	3285.25	558	4152.23
448	949.33	485	1377.38	522	3299.56	559	4153.05
449	954.75	486	1379.42	523	3357.01	560	4157.02
450	955.49	487	1380.93	524	3379.91	561	4157.08
451	974.99	488	1381.43	525	3532.09	562	4158.37
452	975.31	489	1383.18	526	3634.50	563	4159.91
453	987.23	490	1383.53	527	3644.83	564	4161.53
454	996.38	491	1385.23	528	3710.48	565	4162.25
455	1032.87	492	1386.86	529	3766.37	566	4162.75
456	1044.01	493	1389.49	530	3789.94	567	4164.24
457	1060.68	494	1392.01	531	3793.92	568	4166.45
458	1062.85	495	1395.95	532	3865.51	569	4168.08
459	1071.70	496	1396.70	533	4101.74	570	4169.80
460	1076.31	497	1397.77	534	4107.27	571	4170.77
461	1136.86	498	1402.76	535	4111.14	572	4171.48
						573	4171.74

100 Surface - NTO PBE/6-31G**

zpe= 1.0042609 Hartree * 0.986

T	p	ln(qtrans)	ln(qrot)	ln(qvib)	chem.pot.	energy	entropy
(K)	(MPa)				(kJ/mol)	(kJ/mol)	(kJ/mol/K)
283.15	0.1000000	22.16	21.11	95.72	2272.54	2872.98	2.12891
293.15	0.1000000	22.25	21.16	99.71	2250.93	2891.22	2.19251
298.15	0.1000000	22.29	21.18	101.70	2239.89	2900.50	2.22402
303.15	0.1000000	22.33	21.21	103.68	2228.69	2909.88	2.25535
313.15	0.1000000	22.41	21.26	107.63	2205.82	2928.93	2.31745
323.15	0.1000000	22.49	21.30	111.56	2182.34	2948.36	2.37881
333.15	0.1000000	22.57	21.35	115.47	2158.25	2968.17	2.43943

Table S15 Vibrational frequencies of NTO on the 001 surface

1	-709.14	57	-162.36	113	0.00	169	172.31
2	-693.90	58	-160.50	114	0.00	170	174.18
3	-689.17	59	-156.74	115	22.27	171	180.63
4	-682.23	60	-154.84	116	22.96	172	182.81
5	-679.86	61	-152.19	117	29.26	173	184.81
6	-677.97	62	-149.80	118	30.90	174	185.82
7	-677.31	63	-148.50	119	32.25	175	188.06
8	-674.87	64	-146.28	120	37.71	176	189.79
9	-671.86	65	-143.43	121	41.92	177	190.42
10	-669.98	66	-141.84	122	42.79	178	193.39
11	-665.90	67	-138.40	123	43.94	179	195.32
12	-664.46	68	-133.86	124	50.66	180	195.58
13	-663.19	69	-130.89	125	59.61	181	198.19
14	-661.85	70	-128.10	126	60.96	182	198.95
15	-657.26	71	-125.66	127	64.14	183	200.36
16	-652.56	72	-121.46	128	66.23	184	204.00
17	-649.12	73	-114.99	129	66.96	185	204.75
18	-647.48	74	-109.98	130	67.86	186	205.79
19	-645.97	75	-107.78	131	71.31	187	207.56
20	-643.93	76	-105.13	132	72.97	188	209.09
21	-641.20	77	-103.93	133	78.90	189	212.16
22	-637.91	78	-99.78	134	85.50	190	214.09
23	-636.40	79	-97.50	135	88.25	191	215.40
24	-632.04	80	-96.82	136	95.82	192	218.83
25	-623.14	81	-92.72	137	102.75	193	223.19
26	-619.04	82	-90.76	138	106.44	194	226.09
27	-602.62	83	-87.92	139	108.73	195	227.85
28	-601.65	84	-85.85	140	110.73	196	229.23
29	-595.27	85	-84.10	141	111.78	197	231.00
30	-593.13	86	-82.50	142	114.38	198	234.23
31	-585.28	87	-80.63	143	115.75	199	235.13
32	-582.29	88	-79.54	144	117.34	200	238.10
33	-573.86	89	-76.34	145	119.51	201	240.67
34	-551.96	90	-74.95	146	121.86	202	242.76
35	-547.31	91	-72.21	147	125.21	203	244.61
36	-533.82	92	-69.79	148	127.77	204	246.08
37	-526.34	93	-68.00	149	130.41	205	246.62
38	-517.68	94	-66.51	150	131.38	206	247.46
39	-512.23	95	-63.58	151	134.70	207	249.69
40	-507.83	96	-60.90	152	136.85	208	251.66
41	-501.20	97	-60.00	153	139.31	209	253.50
42	-392.92	98	-56.54	154	142.73	210	256.15
43	-209.17	99	-54.70	155	144.48	211	258.24
44	-205.25	100	-53.43	156	146.89	212	260.14
45	-197.53	101	-49.84	157	150.14	213	261.80
46	-192.89	102	-45.23	158	151.53	214	263.90
47	-186.16	103	-43.93	159	153.27	215	264.70
48	-184.07	104	-38.80	160	155.90	216	265.31
49	-182.85	105	-35.93	161	158.25	217	266.81
50	-180.24	106	-29.44	162	159.88	218	268.96
51	-177.71	107	-23.17	163	160.92	219	271.67
52	-174.33	108	-3.17	164	161.33	220	272.19
53	-172.24	109	-0.00	165	163.43	221	274.20
54	-167.51	110	-0.00	166	166.91	222	276.23
55	-166.54	111	0.00	167	170.33	223	279.03
56	-164.95	112	0.00	168	170.45	224	279.18

225	281.63	283	391.97	341	623.21	399	862.31
226	283.07	284	396.71	342	630.47	400	864.48
227	285.96	285	401.48	343	635.76	401	868.66
228	286.84	286	402.91	344	643.61	402	869.66
229	286.93	287	410.05	345	645.78	403	871.24
230	292.12	288	415.30	346	659.66	404	872.30
231	294.34	289	446.38	347	663.77	405	873.66
232	294.99	290	452.19	348	674.56	406	877.22
233	298.38	291	459.85	349	679.18	407	878.71
234	299.80	292	480.62	350	682.02	408	881.82
235	301.97	293	482.93	351	687.47	409	885.38
236	304.14	294	489.80	352	692.87	410	887.25
237	305.32	295	492.14	353	698.43	411	889.74
238	307.51	296	494.96	354	700.68	412	893.33
239	308.84	297	501.45	355	702.42	413	894.33
240	310.62	298	504.55	356	710.55	414	895.49
241	311.49	299	507.84	357	710.82	415	896.33
242	314.46	300	518.40	358	713.47	416	898.04
243	316.59	301	523.50	359	715.52	417	902.47
244	317.54	302	524.25	360	720.82	418	905.47
245	319.81	303	526.17	361	726.88	419	908.14
246	322.24	304	527.49	362	730.57	420	909.44
247	323.70	305	531.67	363	733.93	421	914.81
248	326.31	306	534.41	364	736.52	422	915.06
249	327.27	307	538.72	365	738.74	423	915.25
250	329.21	308	541.72	366	746.59	424	917.62
251	330.49	309	542.71	367	750.58	425	921.23
252	332.04	310	543.83	368	759.22	426	922.65
253	335.46	311	545.18	369	766.81	427	923.35
254	337.07	312	550.55	370	769.70	428	930.05
255	339.96	313	552.86	371	772.85	429	934.37
256	341.18	314	553.57	372	775.28	430	934.98
257	342.70	315	558.48	373	780.43	431	937.56
258	343.74	316	560.85	374	785.77	432	939.26
259	345.62	317	561.65	375	792.11	433	941.27
260	347.81	318	563.34	376	805.17	434	944.00
261	348.05	319	566.40	377	810.59	435	948.96
262	349.72	320	572.49	378	817.46	436	956.50
263	351.49	321	572.91	379	820.92	437	959.07
264	353.65	322	575.65	380	823.45	438	978.46
265	354.74	323	578.24	381	823.90	439	998.30
266	358.95	324	579.71	382	824.34	440	1006.10
267	360.86	325	581.42	383	828.99	441	1007.89
268	361.87	326	584.41	384	830.67	442	1016.72
269	362.96	327	588.15	385	833.01	443	1033.45
270	366.16	328	588.76	386	835.55	444	1045.84
271	368.47	329	594.56	387	836.36	445	1053.78
272	369.60	330	596.08	388	836.71	446	1069.10
273	371.75	331	596.74	389	839.25	447	1112.20
274	372.78	332	597.61	390	840.87	448	1171.54
275	376.16	333	600.72	391	841.15	449	1190.64
276	376.47	334	602.77	392	842.95	450	1192.67
277	377.84	335	606.12	393	845.11	451	1256.90
278	381.61	336	608.74	394	845.89	452	1261.42
279	382.87	337	611.67	395	854.15	453	1274.20
280	384.45	338	616.91	396	855.12	454	1301.26
281	387.28	339	619.53	397	857.13	455	1331.82
282	389.32	340	622.12	398	860.40	456	1337.90

457	1340.00	479	1399.76	501	3673.68	524	4137.10
458	1342.19	480	1402.31	502	3695.91	525	4137.16
459	1354.71	481	1406.21	503	3788.21	526	4140.79
460	1356.09	482	1409.57	504	3791.90	527	4141.47
461	1361.58	483	1410.45	505	3864.14	528	4142.74
462	1364.78	484	1418.63	506	4102.00	529	4144.79
463	1368.95	485	1420.77	507	4106.43	530	4144.97
464	1370.95	486	1452.31	508	4110.78	531	4151.32
465	1372.33	487	1462.97	509	4112.53	532	4153.39
466	1374.18	488	1577.76	510	4114.69	533	4156.72
467	1377.17	489	1596.46	511	4116.08	534	4157.36
468	1379.37	490	1794.57	512	4116.80	535	4157.70
469	1380.59	491	3196.69	513	4118.14	536	4160.19
470	1381.95	492	3201.94	514	4118.19	537	4162.23
471	1383.63	493	3273.83	515	4119.03	538	4162.34
472	1384.72	494	3331.49	516	4119.50	539	4163.19
473	1386.99	495	3393.23	517	4119.57	540	4163.90
474	1389.22	496	3416.49	518	4124.85	541	4166.10
475	1392.70	497	3428.56	519	4125.64	542	4168.55
476	1394.69	498	3579.75	520	4125.97	543	4169.82
477	1396.08	499	3632.92	521	4127.01	544	4170.93
478	1396.46	500	3667.56	522	4128.86	545	4171.35
				523	4132.77	546	4171.89