

Supporting Information for

DFT Study of Formation Mechanism of
Anthraquinone from Reaction of NO₂ and
Anthracene on NaCl Cluster: the Role of
NaNO₃

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Engineering, Nanchang University, Nanchang, Jiangxi, 330031 China.

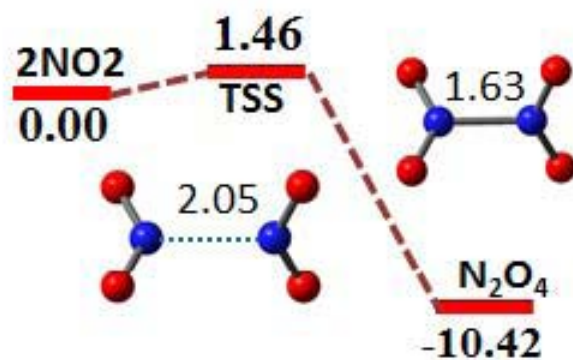


Fig. S1. The energy profile of the NO_2 to N_2O_4 .

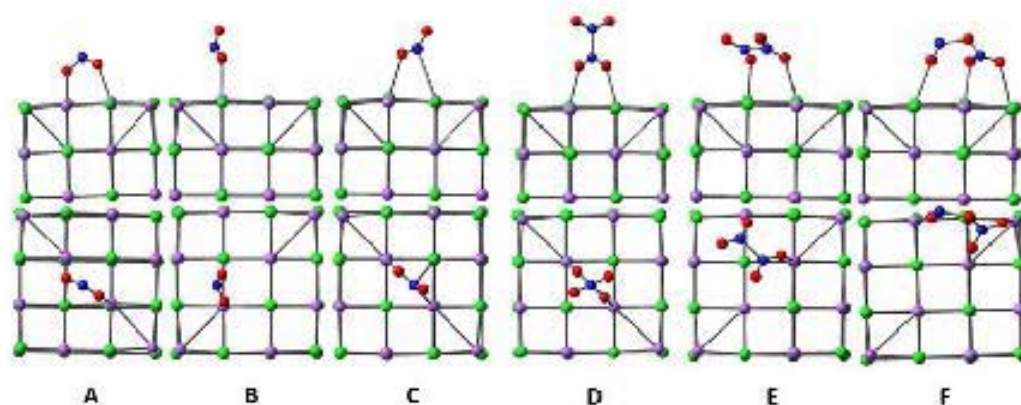


Fig. S2A Optimized various NO_2 and N_2O_4 adsorption geometries and positions on the NaCl surface (Top: side view; bottom: top view).

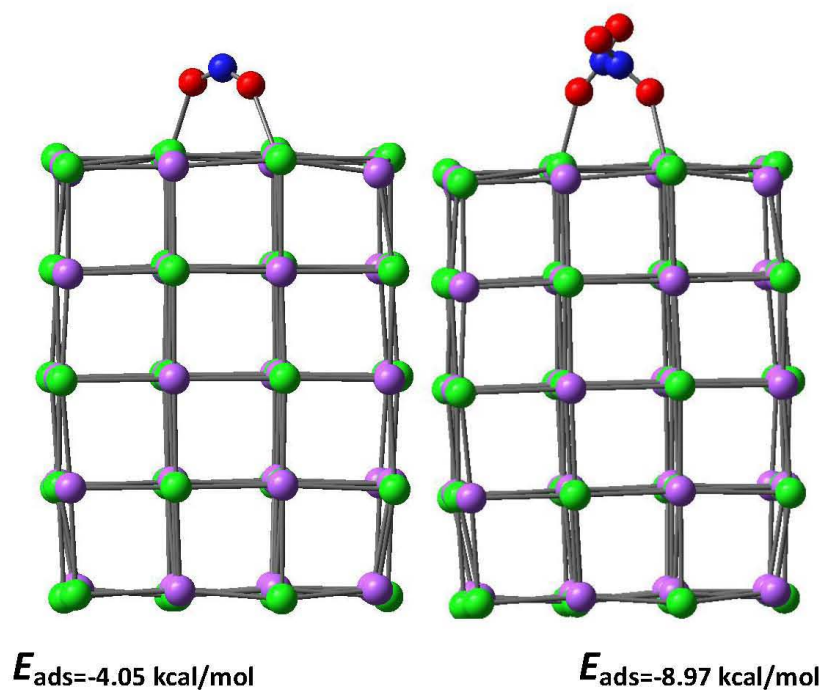


Fig. S2B. Optimized NO_2 and N_2O_4 adsorption geometries and on the 5-layers NaCl surface.

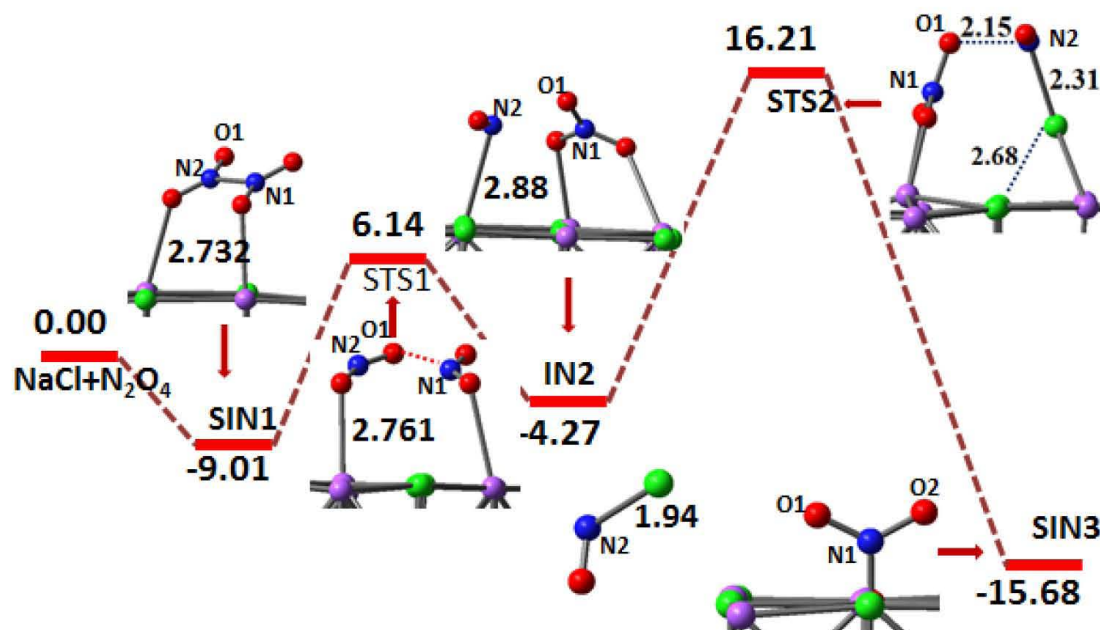
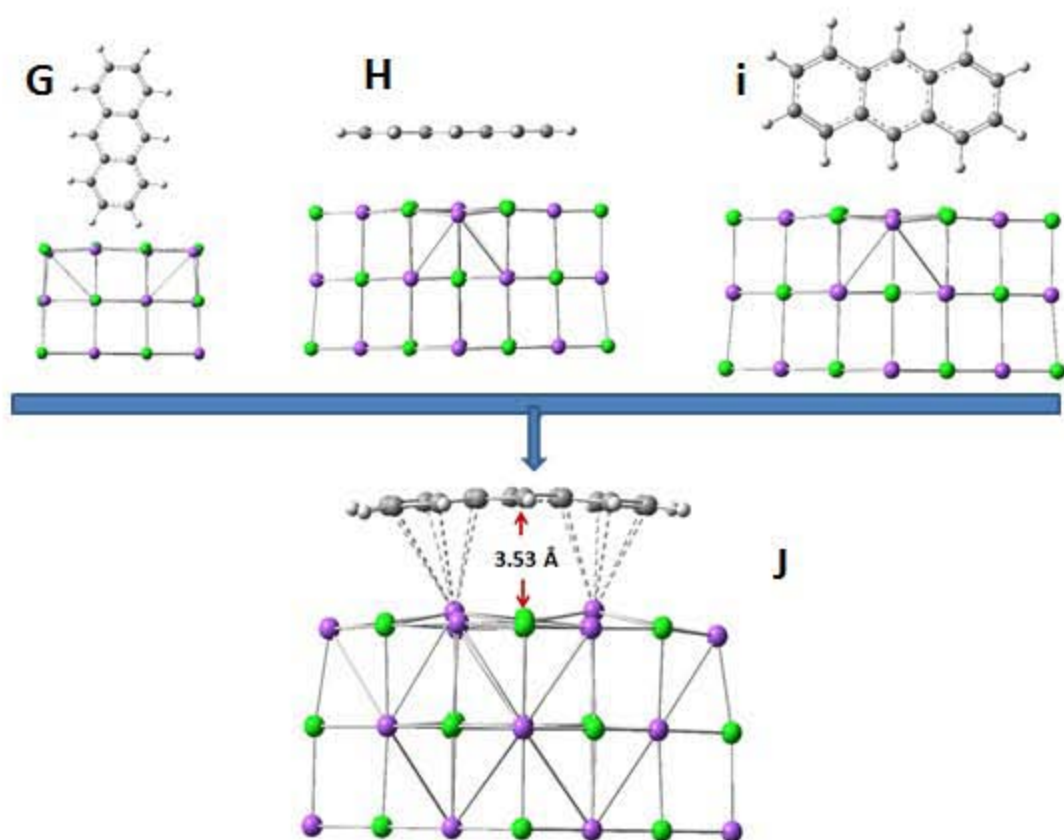


Fig. S3. The energy profile of the reaction of N_2O_4 on the NaCl surface in absence of H_2O calculated by singlet point energy at M06-2X/6-311++g(2d,p) level. (Unit of energy: kcal/mol) .



$$E_{\text{ads}} = -4.62 \text{ kcal/mol}$$

All initial structure G H and I were optimized, respectively. After optimization, the same geometry, structure J was obtained.

Fig. S4. The optimized structures of anthracene on NaCl.

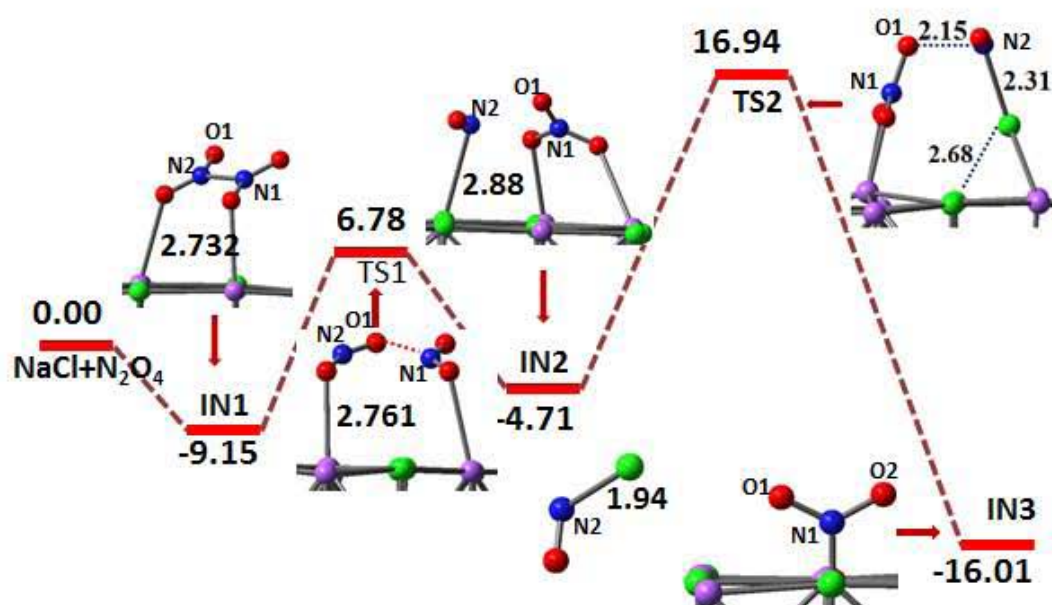


Fig. S5. The energy profile of the reaction of N_2O_4 on the NaCl surface in absence of H_2O (Unit of energy: kcal/mol; Unit of length: Å)

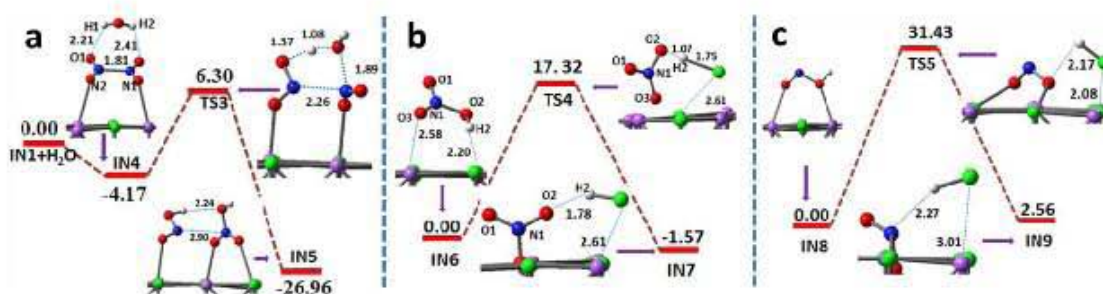


Fig. S6 The energy profile of conversion of N_2O_4 on NaCl in present of H_2O , the energy profile of the reaction of HNO_3 (a) and HNO_2 (b) and NaCl to form the NaNO_3 and NaNO_2 ((Unit of energy: kcal/mol; Unit of length: Å).

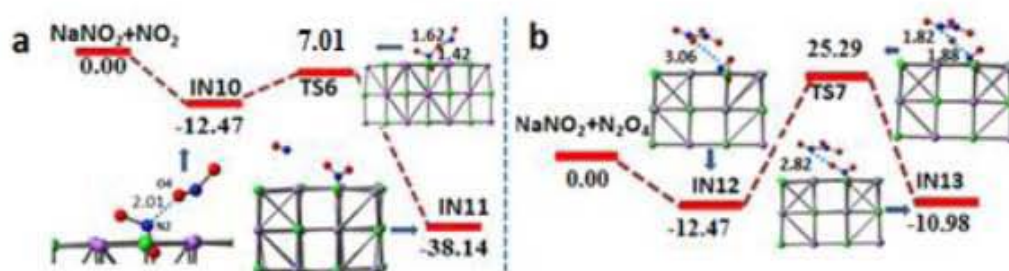


Fig. S7. The energy profile of conversion of NaNO_2 to NaNO_3 in present of NO_2 (a) and N_2O_4 (b) (Unit of energy: kcal/mol; Unit of length: Å).

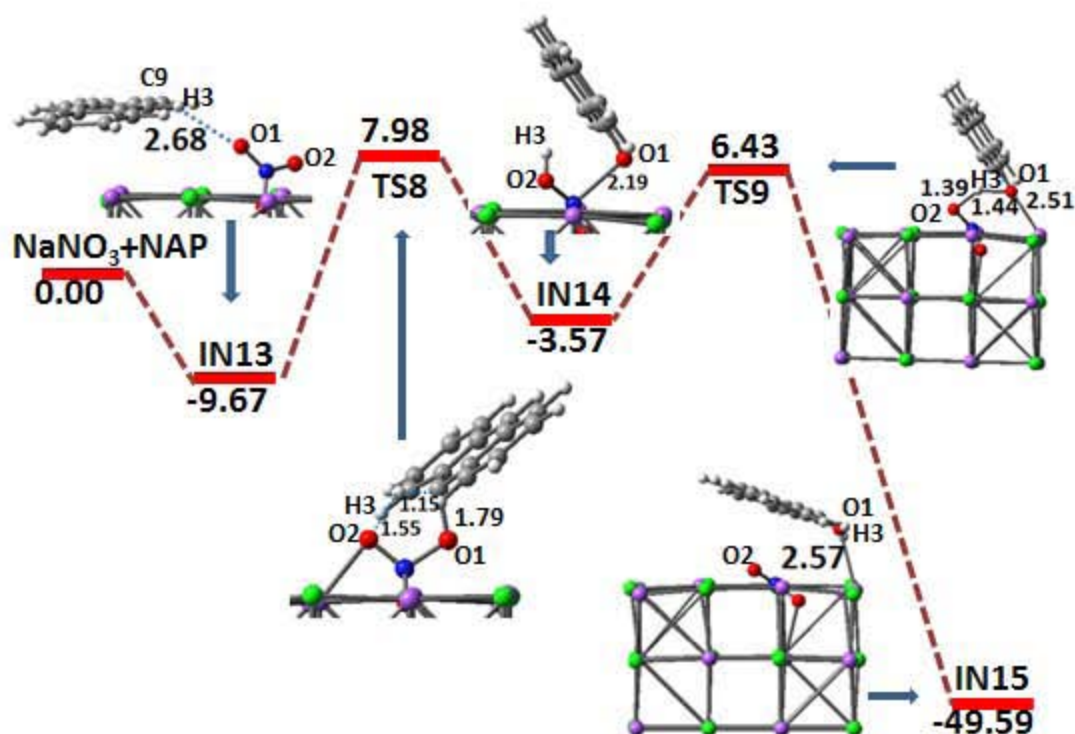


Fig. S8. The reaction energy profile of anthranol on the surface of NaCl in present of NO_2 via channel I (Unit of energy: kcal/mol; Unit of length: Å).

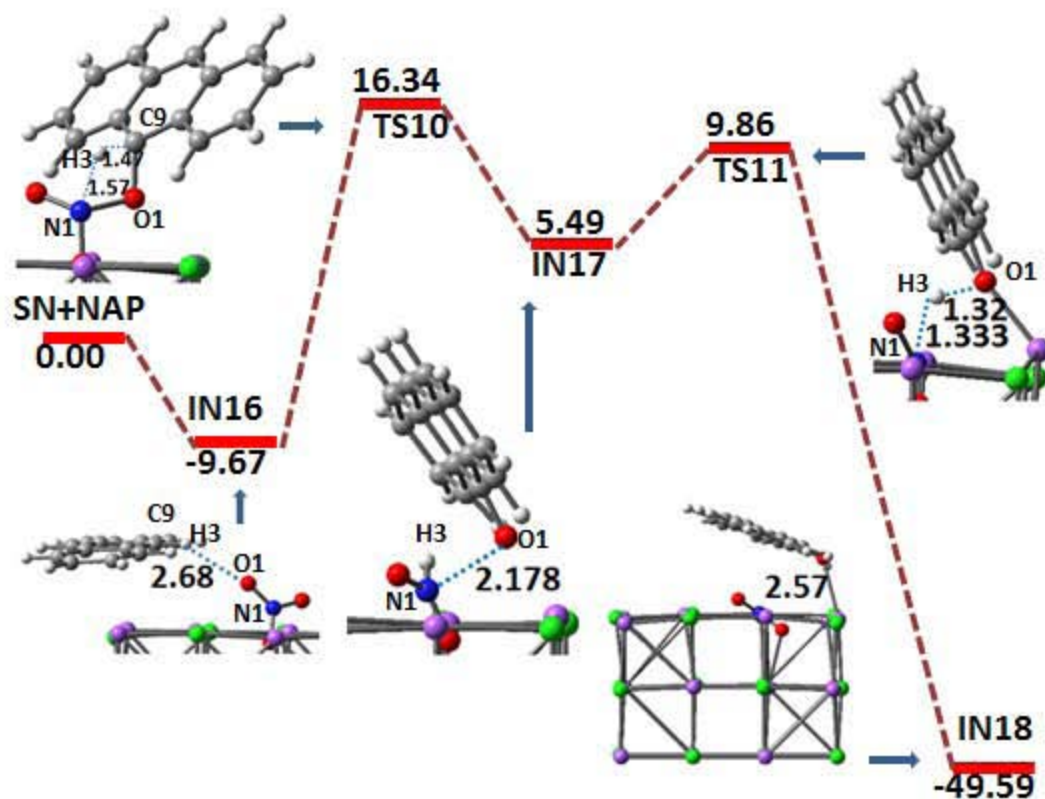


Fig. S9. The reaction energy profile of anthranol on the surface of NaCl in present of NO₂ via channel II (Unit of energy: kcal/mol; Unit of length: Å).

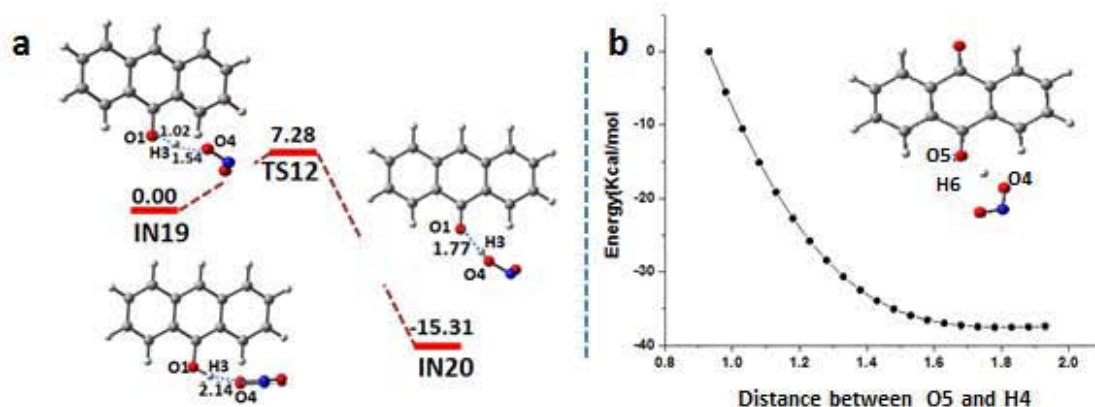


Fig. S10. The reaction energy profile of 9-anthranol and 10- anthranol with NO₂ (Unit of energy: kcal/mol; Unit of length: Å).

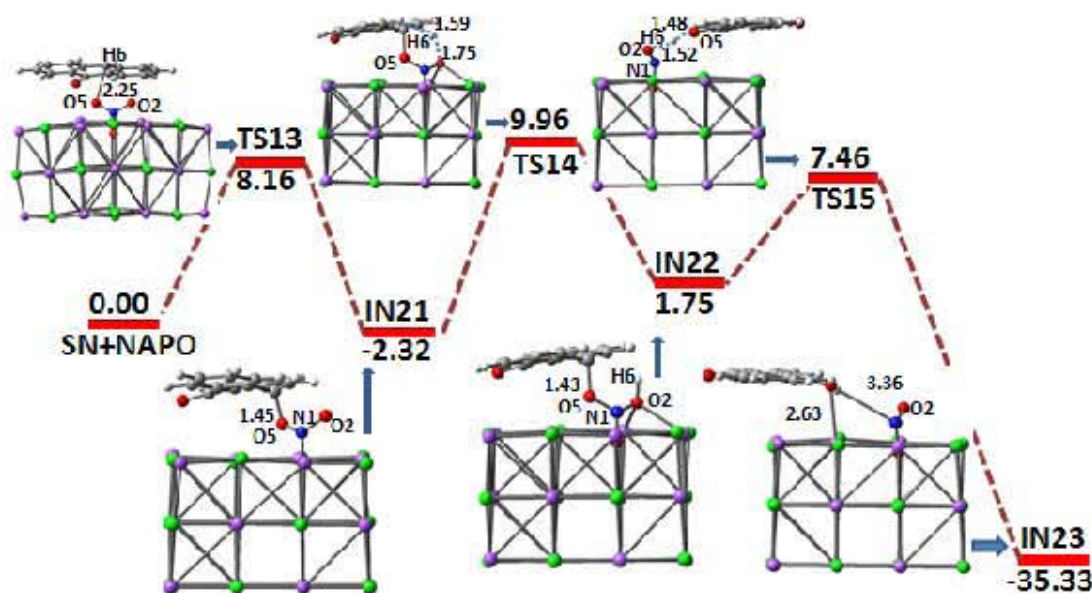


Fig. S11. The energy profile of the oxidation of 9-anthranol-10-one on the surface of NaCl in present of NO₂ via channel II (Unit of energy: kcal/mol; Unit of length: Å).

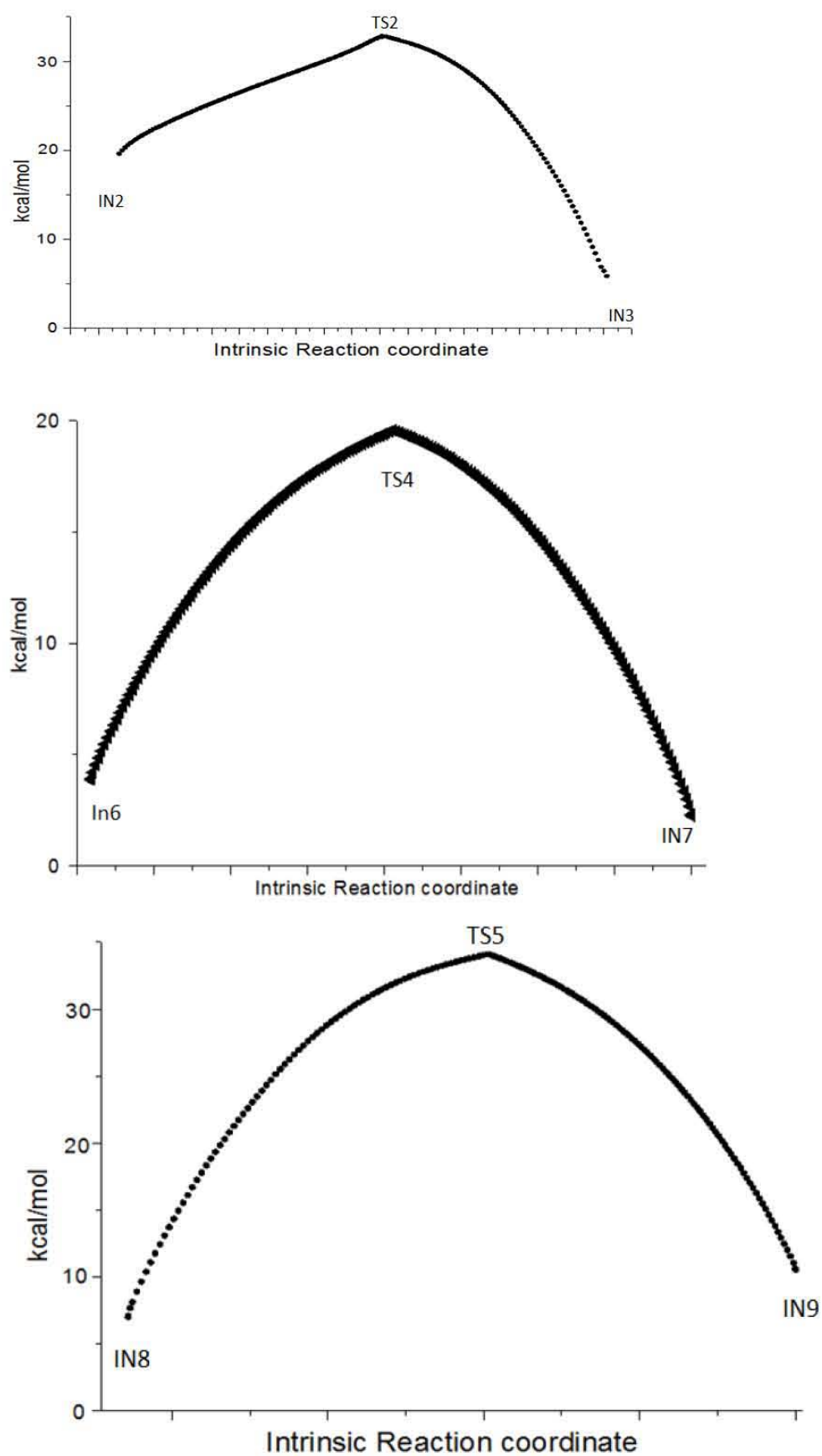


Fig. S12. IRC energy profile for TS2, TS4 and TS5.

Cartesian coordinates of some important structure optimized in our calculations

NO₂ -204.98312

N	0.00000000	-0.00000000	0.32072109
O	0.00000000	1.09708104	-0.14031548
O	-0.00000000	-1.09708104	-0.14031548

N₂O - 409.98289

N	0.81755055	-0.00336587	0.00475771
O	1.31035435	-0.83583043	-0.68652488
O	1.26258685	0.85343523	0.69841125
N	-0.81739655	-0.00592667	-0.00810481
O	-1.28868730	-0.86045197	0.67912349
O	-1.28438865	0.85097815	-0.68808115

TSS -409.96393

N	-1.02941800	-0.00609400	-0.00632200
O	-1.49125000	0.81488600	-0.72678800
O	-1.48956300	-0.81669000	0.72660800
N	1.02944300	-0.00085300	0.00017700
O	1.47957100	0.82520900	0.72459400
O	1.50122000	-0.81732600	-0.71903800

NaCl -14941.61537

Na	0	3.84540519	-1.85707595	2.65761452
Na	0	3.84543876	1.85696488	2.65758568
Cl	0	1.88877639	-0.00002956	2.81410359
Cl	0	5.72307719	-0.00008243	2.63974966
Na	0	0.00004639	1.94006517	2.73520735
Na	0	0.00008051	5.50678276	2.55070482
Cl	0	-1.99252758	3.85426900	2.75731116
Cl	0	1.99271704	3.85428120	2.75730402
Na	0	-0.00013518	-5.50669127	2.55073127
Na	0	-0.00006377	-1.94002406	2.73522770
Cl	0	-1.99272602	-3.85416761	2.75734157
Cl	0	1.99255819	-3.85429217	2.75732254
Na	0	-3.84552240	-1.85693552	2.65758904
Na	0	-3.84545859	1.85713922	2.65760028
Cl	0	-5.72312196	0.00012808	2.63974809
Cl	0	-1.88882311	0.00005626	2.81410154
Na	0	5.71451097	-0.00010741	-0.03849483

Cl	0	2.18020642	-3.87901370	2.37394770
Na	0	-3.86724128	-2.11562286	2.28459743
Na	0	-4.02262407	1.79574963	2.29402660
Cl	0	-5.80927746	-0.23591438	2.23817954
Cl	0	-1.98160306	-0.08371785	2.45094154
Na	0	5.88678188	0.23162882	-0.48007112
Na	-1	4.04902514	-1.82666746	-3.21289551
Na	0	1.99236410	0.08016803	-0.40201352
Na	-1	3.89651707	2.14433421	-3.20569399
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Cl	0	3.90332264	2.21999078	-0.45378615
Cl	-1	5.95829447	0.23506717	-3.20813944
Cl	0	4.06761136	-1.90245794	-0.46072917
Na	0	1.85013228	4.03451398	-0.44047688
Na	-1	-0.07428337	1.99182502	-3.20803820
Na	0	-2.16152155	3.87783939	-0.44299319
Na	-1	-0.22692685	5.96283819	-3.20079536
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Cl	0	-0.07930148	2.00072012	-0.36999701
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Na	-1	-4.04539880	1.83936778	-3.21037793
Cl	-1	-5.95471786	-0.22234176	-3.21521800
Cl	0	-4.06750366	1.90476583	-0.45788703
Cl	-1	-1.98369925	-0.06974608	-3.21298846
Cl	0	-3.90235406	-2.21737680	-0.46602838
N	0	-0.00268359	-0.01690028	5.50020213
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O	0	-0.04618349	1.11551100	5.00984016
N	0	-0.00447374	-0.00802899	7.30956926
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O	0	1.06493550	-0.35521536	7.80238494

structure E -15351.61283

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Na	0	-2.61864849	-2.99253713	3.13803596
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Cl	0	-4.85561543	-1.61737937	3.78456467
Na	0	1.09532803	-2.00218670	2.27425864
Na	0	1.88818330	-5.57123200	1.55067997
Cl	0	3.39384163	-3.39438432	1.34548126
Cl	0	-0.34290770	-4.44236207	2.47742512
Na	0	-0.93403605	5.43109735	2.76493357
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Na	0	-1.13168935	-4.32609697	-0.22454159
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Na	0	5.18119061	1.59130396	-1.92058389
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Cl	-1	4.48271503	1.70610535	-4.57362691
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Cl	0	2.91289868	3.07764418	-1.19174604
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N	0	4.52030374	-0.13753695	4.55768459
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O	0	4.99761958	-0.92725949	3.74351742
Structure A -15146.60529				
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Na	0	-3.94304404	1.95609831	2.55039859
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Na	0	-1.98619525	-0.00042501	-0.14663454
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Structure f -15351.60576

Na	0	2.01490989	-3.22785112	-3.42413142
Na	0	-1.37855992	-4.34146195	-1.90895972
Cl	0	-0.27414353	-1.87321036	-2.61568023
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Na	0	-2.56832742	-0.58227073	-1.69344149
Na	0	-5.65576674	-1.61205495	-0.00314514
Cl	0	-4.76658278	0.92400423	-0.50534151
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Na	0	0.94768361	0.54117807	-3.09811975
Cl	0	2.21143940	3.04290583	-3.61173808
Cl	0	3.25870531	-0.81773467	-4.05355622
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Na	0	-3.40801424	3.25596372	-1.01561891
Cl	0	-2.18545663	5.59864582	-1.56686794
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Na	0	1.95150144	-5.64347258	-0.34171346
Na	-1	4.29527564	-3.23157159	1.60719109
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Na	-1	0.80156994	-4.35017306	3.13523041
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Na	0	-2.55930378	-3.03523491	1.58692210
Na	-1	-0.23092386	-0.53713786	3.56583813
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Na	-1	-3.72469030	-1.65564089	5.09386745
Cl	-1	-2.49409324	0.81030575	4.54534002
Cl	0	-4.87752326	-1.67396557	2.61786779
Cl	-1	-1.46154816	-3.00296982	4.11469587
Cl	0	-1.39098192	-0.54355344	0.96618400
Na	0	4.40174790	-0.80259963	-1.46766931
Na	-1	6.75634112	1.70023606	0.50975232
Na	0	3.36008241	3.05073396	-1.02706741
Na	-1	3.26276680	0.58167184	2.03779237
Cl	-1	4.49332719	3.04759916	1.48924321
Cl	0	2.13083818	0.57290096	-0.55058000
Cl	-1	5.52595602	-0.76569208	1.05856919
Cl	0	5.71096924	1.70867038	-2.00720798
Na	0	-0.14578106	1.90885821	0.45123407
Na	-1	2.23011318	4.39478388	2.46848323
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Na	-1	-1.26355491	3.27613434	3.99649878
Cl	-1	-0.03300999	5.74209349	3.44786727
Cl	0	-2.42078239	3.27438885	1.52340048
Cl	-1	0.99952153	1.92884963	3.01737925
Cl	0	1.17515892	4.40615364	-0.08102388
N	0	-5.76957451	-0.90154158	-3.29106137
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O	0	-6.40230704	-1.36215961	-2.31816780
N	0	-6.20170939	0.94454870	-5.21842527
O	0	-6.57934826	-0.54038440	-4.42442535
O	0	-5.35591592	1.57863585	-4.74835993

Structure C -15146.59849

Na	0	4.20799780	-1.57061739	2.33400425
Na	0	3.70985341	2.27990844	2.60114961
Cl	0	1.99180014	0.09419555	2.67723658
Cl	0	5.81275056	0.60283473	2.37857743
Na	0	-0.19765652	1.78829929	2.78988479
Na	0	-0.66652223	5.49417400	2.77442477
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Cl	0	3.67287459	2.58043815	-0.14589604
Cl	-1	5.83274738	0.97804302	-3.06809411
Cl	0	4.18766899	-1.48296797	-0.42911298
Na	0	1.47983475	4.21975588	0.01195033
Na	-1	-0.32708021	2.19792516	-2.84808086
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Cl	-1	-2.54480361	3.91588264	-2.68427588
Cl	0	-0.77128312	6.00740757	0.14266915
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Cl	0	-0.26090569	2.01109625	-0.02859672
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Cl	0	-3.70897329	-2.49944971	-0.31951862
N	0	0.32822350	-1.37426247	6.08354458
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TS1 -15351.58459				
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Cl	-3.28324320	3.64871270	-2.36478494
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N	3.61517547	-0.18859040	4.68709038
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IN2 -15351.60221

Na	0	-3.92115469	1.68403586	2.39162339
Na	0	-3.77587976	-2.03829129	2.33817833
Cl	0	-1.90874814	-0.10502246	2.36956599
Cl	0	-5.72199343	-0.25047232	2.36308548
Na	0	0.05656522	-1.93477343	2.41232317
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IN3 -15351.62031

Na	0	2.30736402	3.30966324	-3.03450583
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Cl	0	1.25673930	0.82538297	-2.82940435
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TS3 -15427.96856

Na	2.72477485	-2.94066174	2.67679047
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Na	-1.98306318	-5.19996807	1.81605316
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Cl	3.11906237	-3.12558410	0.02205668
Na	3.08748176	3.07170552	0.03926302
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H		-2.75343448	-0.41062065	7.19770310
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Cl	0	3.96442881	-3.70322037	3.12696539
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Na	0	3.06997637	4.22939629	3.14043309
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Na	0	-3.75887800	-4.29870596	1.42798808
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Cl	0	-1.26724522	-4.33121297	2.11442010
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Na	0	1.66103957	-1.22914386	0.04606937
Na	-1	4.97421835	-0.90538480	-2.04157594
Cl	-1	2.23318116	-1.15150688	-2.60936028
Cl	0	4.38251901	-0.90350512	0.58882227
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Cl	0	1.37719159	1.52708685	0.09302282
Na	0	-0.77950229	-4.16073762	-0.58752760
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Cl	-1	-3.24901612	-1.64361696	-3.74446789
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IN9 -15147.24458				
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Na	0	-2.91649383	-3.36265052	2.00748939
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Na	0	5.28475280	2.29857763	0.74147046
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Cl	0	2.85390628	3.44596021	0.33996423
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Cl	0	4.46826690	-0.28143027	0.55073099
Na	0	0.33719369	4.33899664	-0.04877149
Na	-1	-0.16241366	1.88642296	-2.91530535
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O	0	-1.76785203	-1.61821538	3.61958808
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TS4 -15147.22239

Na	0	2.12814714	3.25218816	2.84279718
Na	0	-1.54979632	3.39971488	3.01259922
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Na	0	5.79974624	-0.48418405	1.96208765
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C	0	4.61692740	-2.29628168	-2.25164417
C	0	3.66204818	-3.33734326	-2.07410334
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Na	0	-1.13295746	-3.22011599	-3.30153188
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Cl	-1	-4.29040103	0.08393764	0.48088773
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Na	-0.63928910	-4.28878310	-2.04529323
Na	-2.04554749	-1.60486803	-4.17951625
Cl	-0.10184192	-1.66595537	-2.29580679
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Cl	-1.67502742	1.50323663	-0.76460020
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Na	0.26775032	1.44344932	1.15318892
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Cl	0.53388428	4.18857915	0.84330186
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TS13 -15375.49445

Na	-1.42013772	-4.10294500	0.13576636
Na	-3.87962477	-1.71626105	1.54225179
Cl	-1.77196822	-1.47315016	-0.46842475
Cl	-3.22989970	-4.28008010	2.02490716
Na	-2.53253885	1.10759429	-0.70161205
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Na	2.62578732	-4.39209514	-3.27688875
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Cl	2.25208303	-1.98700129	-4.13726023
Cl	0.60806086	-4.53570128	-1.65357776
Na	1.46703494	0.54104156	-4.42019929
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Cl	1.07189837	4.96573360	2.51023803
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Cl	5.81241093	-0.35009480	-0.32183350
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C	-2.59778950	-4.63121378	-3.17031272
C	-5.13863343	-1.81789308	-1.22139461
C	-3.92816410	-1.19550117	-3.74663831
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C	-6.49390752	1.61797730	-1.90838662
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IN22 -15375.50516			
Na	0.44767197	-4.40697888	-0.94738815
Na	-2.66081014	-3.44262642	0.75260368
Cl	-0.96567907	-2.10567648	-1.02566638
Cl	-1.21664792	-5.66244925	0.63805349
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Cl	2.33350173	-3.50195503	-2.68607430
Na	1.18349780	2.30304315	-4.01202213
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Na	0.43909875	-1.48816918	1.27780330
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Na	3.70628863	0.51151910	1.74803373
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Cl	2.21532043	-0.24868557	-0.45103500
Cl	5.23253021	-1.81368253	1.64734787
Cl	5.63139025	-1.40689290	-2.16435312
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Cl	2.48633240	6.36697414	0.33142565
Cl	-0.83638993	4.38827210	0.00471442
Cl	2.22457511	2.83375083	1.92865267
Cl	2.61940667	3.19751546	-1.94283704
N	-1.30372870	1.03435673	-3.00305208
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O	-0.74035088	1.53142055	-1.98887505
O	-0.41190888	0.44389816	-3.87880125
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C	-2.58390980	-1.77841555	-4.03342627
C	-1.52979423	-2.10641266	-4.90318302
C	-0.93932814	-3.36495784	-4.91052652
C	-4.18216424	-2.57545528	-2.26835899
C	-3.16764297	-0.38414284	-4.03470168
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H	-6.33259810	-1.85131867	-0.90188193
C	-6.72341566	0.13615941	-1.67182774
C	-6.35163403	1.08235282	-2.63344227
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H	-1.20245004	-1.37394089	-5.63969738
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C	-3.33519117	-2.22515596	-0.18396835
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TS6 -14891.44742

Na	0.10485212	4.01691445	2.70702162
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Cl	-0.04019633	4.39253418	0.05367709
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TS7 -15096.39434

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Cl	-4.45407349	4.04987657	-0.98203280
Cl	-5.15313386	1.32066168	1.64763225
Cl	-1.58083146	1.34227363	-0.22582642
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Cl	2.98004971	-1.19357200	4.13656260
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Cl	3.77706515	-4.00728846	1.64546433
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Cl	3.77519566	1.49406664	1.54508047
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