

# A combined experimental and computational study on the adsorption and reactions of NO on rutile TiO<sub>2</sub>

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This supplementary information contains the geometry optimized coordinates and the absolute energies (SVP and TZVPP) in au of the calculated N<sub>x</sub>O<sub>y</sub> structures

Cluster

Atom	x	y	z
O	-6.172203002750	-0.004052241899	9.972259949149
O	-6.009743408145	0.000823061800	14.776537039486
O	0.004981774163	-5.668095120075	8.583508868893
O	0.000354230343	-0.002160887709	3.505944664751
O	-0.024159614553	0.000971495396	8.628051260035
O	6.116639690595	0.019594647569	9.965302632180
O	5.954881316573	0.004666289774	14.777319373595
O	0.016604767911	5.667766910152	8.582720492983
TI	-6.419343473729	-2.811878616207	12.886116344466
TI	-6.415813433045	2.817365475751	12.884462727246
TI	-6.120193134587	0.010333296293	6.631293672854
TI	0.031748631439	-5.522343341514	12.111619233042
TI	-0.005173809252	-2.801129063956	6.187099102597
TI	-0.178048930087	0.017603904792	12.119511431457
TI	0.022992323554	2.810265944685	6.195756672874
TI	6.415321754431	2.808584778150	12.882176340386
TI	6.136697938362	-0.009854005955	6.631715860785
TI	0.087830761641	5.516910456753	12.120905808646
O	-3.631103897400	-2.698241689503	6.252805509168
O	-9.950989540273	-2.682392810606	12.718566990880
O	-2.304530156377	-2.828576556897	12.597715200709
O	-3.642535344674	2.695349105434	6.256440590284
O	-9.949496294939	2.681528210413	12.714893779596
O	-2.305720817706	2.823954270909	12.591923157777
O	3.633439261786	-2.691380294035	6.254220694638
O	2.256312683689	-2.862758168307	12.613559025841
O	9.889585775546	-2.646663600292	12.657537664477
O	3.623200230391	2.695814362248	6.241623902130
O	2.259270621954	2.854746212294	12.612731705777
O	9.934587770304	2.699891472941	12.716894709563

SCF-energies:

SVP -50236.67280920

TZVPP -50248.41314117

NO( $N_{ad}$ )

Atom	x	y	z
O	-6.184108859283	-0.000891955663	9.976865798599
O	-5.973681021978	0.001289069197	14.772256973558
O	0.009966739297	-5.671022065500	8.577786685757
O	0.001109958397	-0.002448781394	3.516512031123
O	-0.017011416262	0.006243564630	8.630340843550
O	6.127754327875	0.019836868444	9.973476490832
O	5.912981944470	0.009766430937	14.781508553553
O	0.018683658171	5.666757268650	8.574086055728
TI	-6.421836891361	-2.814656258825	12.873022805229
TI	-6.420613016657	2.818870972163	12.869512197549
TI	-6.108955720893	0.011495463153	6.626423602311
TI	0.048690284112	-5.531809003025	12.089502574058
TI	-0.003925702111	-2.771139779779	6.225145359832
TI	-0.220559023522	0.012253798668	12.271145541466
TI	0.028212218452	2.776652409478	6.223438572144
TI	6.412111847361	2.809032232818	12.866674645989
TI	6.128922821017	-0.010879298750	6.630880134860
TI	0.104424205053	5.526927269989	12.091453375646
O	-3.641938322120	-2.701386039196	6.261046679119
O	-9.951530892576	-2.680775678387	12.728013961123
O	-2.318341684488	-2.851670548527	12.571194586930
O	-3.655626629884	2.698881387369	6.260932869571
O	-9.950821625913	2.680905000861	12.726233934706
O	-2.312500870921	2.844620188375	12.600792453875
O	3.647942014484	-2.694617544916	6.259691552120
O	2.264113891662	-2.894150289349	12.603347334764
O	9.888903522569	-2.645078367330	12.671471549999
O	3.638795523380	2.700575735679	6.244444853687
O	2.266425743452	2.889593711787	12.609689653582
O	9.932816302531	2.698451180773	12.725170241283
N	0.012355827447	-0.127907062075	16.910452384561
O	0.191520330556	1.420016648580	18.376247990698

SCF-energies:

SVP -50366.43088903

TZVPP -50378.32275955

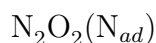
NO(O<sub>ad</sub>)

Atom	x	y	z
O	-6.181066438017	-0.002262275794	9.975144327923
O	-5.987364205648	0.002639210577	14.771921321518
O	0.008496365688	-5.670749543381	8.578438905913
O	0.000724663092	-0.002245580914	3.515173972940
O	-0.021828448999	0.004214875129	8.638259376153
O	6.125446798725	0.020584272503	9.971359350967
O	5.928435856252	0.009360904510	14.780174493877
O	0.018330725088	5.667713120855	8.575613884871
TI	-6.421092739100	-2.813759900039	12.875918834116
TI	-6.419463393826	2.819173928897	12.870334577308
TI	-6.111721022455	0.013137071061	6.626964971385
TI	0.046158870970	-5.528979643259	12.094562111671
TI	-0.007317763958	-2.779281950022	6.214145218671
TI	-0.210207874898	0.011950711543	12.228315596201
TI	0.029269762636	2.786657847540	6.216927989172
TI	6.413362397514	2.809014124104	12.868726350529
TI	6.130734978032	-0.012764977573	6.631053408528
TI	0.100326391050	5.523218192248	12.100023147558
O	-3.638062124537	-2.700599272269	6.258398285037
O	-9.951591880667	-2.681461499256	12.725637909436
O	-2.313958426047	-2.846367786088	12.576850365424
O	-3.653469838278	2.697393296269	6.260243356236
O	-9.950936972257	2.681623452986	12.722191454124
O	-2.310727725028	2.840927179376	12.595280312667
O	3.644729490949	-2.692758180456	6.259738063932
O	2.263575094256	-2.887467129064	12.601432714524
O	9.889601017113	-2.645988866817	12.667725050264
O	3.632861276056	2.698908157269	6.244732006592
O	2.265376723820	2.881567352168	12.611401228972
O	9.933967724523	2.699240090894	12.722598517575
N	0.119317738807	1.504491446017	18.374106357574
O	-0.013735895607	-0.104091406165	16.930089045112

SCF-energies:

SVP -50366.42432666

TZVPP -50378.31553368

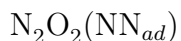


Atom	x	y	z
O	-6.189273082033	-0.005952185551	9.987153054345
O	-5.969142564806	-0.001636331514	14.777180000480
O	0.008424339251	-5.668064534660	8.574857980598
O	0.001464619643	-0.002398733877	3.519591237590
O	-0.008633483296	0.000412886987	8.597136305563
O	6.136588252582	0.013359703867	9.982929597955
O	5.905668672492	0.007830355762	14.788261477251
O	0.017059241096	5.668067346114	8.575472579252
TI	-6.423289306206	-2.809805231112	12.862522203918
TI	-6.414510539342	2.819406443041	12.863542400579
TI	-6.098183865823	0.009360769103	6.624351705242
TI	0.040785705219	-5.532895821613	12.065108335493
TI	0.000817017968	-2.734437841288	6.233965084334
TI	-0.206718406997	0.004608263275	12.405664430004
TI	0.029266791748	2.764025945517	6.259094986362
TI	6.407581327114	2.810144024821	12.860176425779
TI	6.121911093954	-0.009285368814	6.631046456793
TI	0.097370650254	5.519399603116	12.094873379086
O	-3.658979851427	-2.705311256601	6.265274784950
O	-9.954578230022	-2.683805359335	12.736450448501
O	-2.317270545702	-2.870015886740	12.601970970130
O	-3.668307511601	2.701070111303	6.269559536912
O	-9.951151032113	2.679804765705	12.730970634729
O	-2.315863469280	2.853165067886	12.591058873627
O	3.663899298577	-2.701282586688	6.262675463663
O	2.269952772016	-2.906655220304	12.615018091971
O	9.893770919539	-2.649361047805	12.683717815897
O	3.655481859142	2.704101770625	6.252800737913
O	2.278692757104	2.893927032522	12.578878782923
O	9.933688149062	2.697356353032	12.729644744745
N	0.119435017873	-2.574228452552	19.649840334188
O	0.211880065883	-1.248387413928	21.283853067115
N	0.037276747937	0.119670187963	16.720632513955
O	0.125253791474	1.950291228321	17.900281017109

SCF-energies:

SVP -50496.18438411

TZVPP -50508.23045700



Atom	x	y	z
O	-6.204010204492	0.004832450307	9.980874071246
O	-5.964316765801	-0.011901572780	14.769203619254
O	0.000524715110	-5.689628554718	8.589743130604
O	0.001649955276	0.015217933658	3.506895196018
O	-0.013221188115	0.026745254350	8.619591588170
O	6.144763663543	0.029867154855	9.981270001063
O	5.907134398158	0.001741499077	14.790741333854
O	0.015350900694	5.671543148911	8.576090378489
TI	-6.427483620186	-2.808763310996	12.842552909819
TI	-6.419240071843	2.814177753942	12.870318623645
TI	-6.098121197026	0.014389499301	6.619752769307
TI	0.008876795819	-5.489407456627	12.256851824402
TI	-0.006294049892	-2.865458947996	6.342971351593
TI	-0.150356019806	0.087694187058	12.243843676324
TI	0.036785599513	2.719056292710	6.145254696248
TI	6.415905251714	2.807493906749	12.871187056731
TI	6.125177514668	-0.016185827105	6.632973256295
TI	0.072299244119	5.553648508730	12.058837915445
O	-3.648702900980	-2.696923581477	6.280619104290
O	-9.954787852623	-2.683140433648	12.729596313533
O	-2.332822892108	-2.826399584075	12.498612995996
O	-3.664673669614	2.701151976732	6.259749482333
O	-9.951373476780	2.680061906367	12.736891975271
O	-2.315075451022	2.856363365543	12.580679708709
O	3.655672946258	-2.689991929128	6.283634325377
O	2.297310588413	-2.854578058111	12.526468611243
O	9.893869233008	-2.646850954911	12.677573064718
O	3.642713298035	2.704440806137	6.243601680728
O	2.263235480778	2.873791944473	12.600808466661
O	9.934093947681	2.698996208776	12.736498804681
N	-0.040400938048	-0.971205725879	16.672213761962
O	-0.007871880532	-0.295333710878	18.715840263665
N	-0.024476097481	-4.616137699997	16.729134007056
O	-0.000914986501	-5.223912412067	18.785466591321

SCF-energies:

SVP -50496.18223573

TZVPP -50508.22571953

N<sub>2</sub>O<sub>2</sub>(rec)

Atom	x	y	z
O	-6.187729930803	-0.004603038203	9.986744225754
O	-5.970024124554	0.001078781269	14.776854172625
O	0.008769823496	-5.668143610616	8.577792778837
O	0.001122099340	-0.002414345178	3.517099827184
O	-0.007892651979	0.003549185401	8.593073577104
O	6.140117844930	0.015805518032	9.982652357661
O	5.912105651996	0.010223922892	14.789081534835
O	0.016101015335	5.665697975641	8.573832848596
TI	-6.419341730156	-2.809985409881	12.862452441937
TI	-6.413484755076	2.818430969776	12.858814238661
TI	-6.094759170361	0.014765765705	6.623365601563
TI	0.040157327603	-5.528466342204	12.071617398291
TI	-0.007554826643	-2.735263845445	6.246210608522
TI	-0.208467459764	0.005638432951	12.438509739428
TI	0.037272859918	2.755160891609	6.255763213131
TI	6.406592836184	2.808469235289	12.854650801979
TI	6.118833660790	-0.015117251611	6.629871732172
TI	0.098039620488	5.517384809911	12.087574192092
O	-3.657118418397	-2.706338281813	6.261971100983
O	-9.954370543496	-2.682739857439	12.737491639893
O	-2.321139603015	-2.873024756901	12.598649286992
O	-3.673480225077	2.700965767800	6.264725003939
O	-9.951749635042	2.680940548948	12.731797831818
O	-2.315427959868	2.859555669386	12.606507736131
O	3.668313628245	-2.700293263031	6.260949545936
O	2.272255833258	-2.903623174609	12.613361368493
O	9.895220000714	-2.649304107895	12.685497270351
O	3.655302494402	2.705578951227	6.246447453255
O	2.281397799169	2.896624936029	12.583296374362
O	9.935110479785	2.698395168955	12.731116144267
N	0.051868138938	0.053562417339	16.724192300494
O	0.190497672792	1.919126761436	17.857220627399
N	0.303940375798	0.204991833356	21.723845695339
O	0.179591439158	-1.730173146688	20.939845004640

SCF-energies:

SVP -50496.17758476

TZVPP -50508.22284113

$N_2O(N_{ad})$

Atom	x	y	z
O	-6.195663702015	0.002962421899	9.978817910443
O	-5.963262577062	0.001803220050	14.769790335030
O	0.014878179047	-5.674227787431	8.571657725320
O	0.001554238593	-0.001519628994	3.524322734205
O	-0.026513149331	0.007222624810	8.655794376520
O	6.132876204587	0.020947388169	9.970953228571
O	5.938620020209	0.008990359879	14.776472803293
O	0.021181967985	5.670207777983	8.569324121596
TI	-6.421733616733	-2.817061514696	12.862493795925
TI	-6.426665218345	2.819944618703	12.858496290125
TI	-6.100099695212	0.012160127459	6.623491594829
TI	0.066218273563	-5.527509704397	12.084533759133
TI	0.002070037461	-2.768952815845	6.245783106444
TI	-0.249035784112	0.018398025635	12.340694827502
TI	0.036613742691	2.764905548096	6.235135669023
TI	6.413340395628	2.806395858215	12.868933036028
TI	6.135835630334	-0.011794927942	6.632542868183
TI	0.124955255827	5.528728573933	12.077613003599
O	-3.645609503874	-2.701867113089	6.265728520887
O	-9.951385967830	-2.679811572229	12.731660392135
O	-2.326605656364	-2.856662987178	12.522007579365
O	-3.660524713454	2.700593750338	6.264466756142
O	-9.952523310668	2.682231588015	12.733564981347
O	-2.315665752363	2.849932802143	12.583281742685
O	3.646527633602	-2.692481640491	6.263347740188
O	2.266848758777	-2.899002523396	12.582979860564
O	9.892291847449	-2.647377977150	12.667394193165
O	3.636633103999	2.700176284178	6.247519603261
O	2.269854480446	2.894971711383	12.589404857574
O	9.935730881864	2.700902832986	12.722495708513
N	-1.263411058015	0.991237351068	18.192778324563
O	-1.503953592270	0.780479572503	20.371728041488
O	-0.137947530110	-0.264298578743	16.614728705507

SCF-energies:

SVP -50421.13973781

TZVPP -50433.09406376



N<sub>2</sub>O(O<sub>ad</sub>)

Atom	x	y	z
O	-6.196852794811	-0.003022838885	9.971056046809
O	-5.994835489231	0.001143446359	14.761113746293
O	0.010906610783	-5.672078259736	8.572018500150
O	0.001418412833	-0.001331530841	3.527514518012
O	-0.013000508304	0.000143724046	8.670366830767
O	6.134967767079	0.019715750832	9.979071735173
O	5.899103336086	0.013055046399	14.783237388105
O	0.021438440633	5.673037496850	8.570744489497
TI	-6.424149950905	-2.815359802074	12.872150914927
TI	-6.424285120320	2.819916464919	12.870869190025
TI	-6.117295937200	0.011721566365	6.628266718908
TI	0.053162321817	-5.527790166302	12.080224988839
TI	-0.013427236827	-2.764056697440	6.242688468669
TI	-0.234514161193	0.023183590776	12.354258947992
TI	0.020309115605	2.769359056018	6.245706982641
TI	6.413829662924	2.811603937085	12.853914773430
TI	6.118886902954	-0.012575240607	6.630498707714
TI	0.107035220884	5.527893446197	12.084259691078
O	-3.639608073111	-2.701300680485	6.263875405760
O	-9.954883889886	-2.683275504380	12.726291246431
O	-2.317147567729	-2.842911707352	12.545641774820
O	-3.651483944916	2.698313466760	6.267510056906
O	-9.954540025179	2.683424924503	12.723888565185
O	-2.319644952521	2.839869898128	12.541051654567
O	3.652989029164	-2.694247807254	6.263612708199
O	2.276075086573	-2.919480765390	12.601938211490
O	9.889835706580	-2.644501376878	12.679428245284
O	3.640849167015	2.700717276272	6.252197680753
O	2.274379124318	2.907155521867	12.593651005617
O	9.932191557567	2.699174964449	12.729341531695
O	-0.112420352322	0.001715193384	16.643858927506
N	1.438844641580	0.022869010218	18.311728007707
N	2.802493429472	0.039599590517	19.927905970417

SCF-energies:

SVP -50421.13973781

TZVPP -50433.09157916

NO<sub>2</sub>(O<sub>ad</sub>)

Atom	x	y	z
O	-6.195663702015	0.002962421899	9.978817910443
O	-5.963262577062	0.001803220050	14.769790335030
O	0.014878179047	-5.674227787431	8.571657725320
O	0.001554238593	-0.001519628994	3.524322734205
O	-0.026513149331	0.007222624810	8.655794376520
O	6.132876204587	0.020947388169	9.970953228571
O	5.938620020209	0.008990359879	14.776472803293
O	0.021181967985	5.670207777983	8.569324121596
TI	-6.421733616733	-2.817061514696	12.862493795925
TI	-6.426665218345	2.819944618703	12.858496290125
TI	-6.100099695212	0.012160127459	6.623491594829
TI	0.066218273563	-5.527509704397	12.084533759133
TI	0.002070037461	-2.768952815845	6.245783106444
TI	-0.249035784112	0.018398025635	12.340694827502
TI	0.036613742691	2.764905548096	6.235135669023
TI	6.413340395628	2.806395858215	12.868933036028
TI	6.135835630334	-0.011794927942	6.632542868183
TI	0.124955255827	5.528728573933	12.077613003599
O	-3.645609503874	-2.701867113089	6.265728520887
O	-9.951385967830	-2.679811572229	12.731660392135
O	-2.326605656364	-2.856662987178	12.522007579365
O	-3.660524713454	2.700593750338	6.264466756142
O	-9.952523310668	2.682231588015	12.733564981347
O	-2.315665752363	2.849932802143	12.583281742685
O	3.646527633602	-2.692481640491	6.263347740188
O	2.266848758777	-2.899002523396	12.582979860564
O	9.892291847449	-2.647377977150	12.667394193165
O	3.636633103999	2.700176284178	6.247519603261
O	2.269854480446	2.894971711383	12.589404857574
O	9.935730881864	2.700902832986	12.722495708513
N	-1.263411058015	0.991237351068	18.192778324563
O	-1.503953592270	0.780479572503	20.371728041488
O	-0.137947530110	-0.264298578743	16.614728705507

SCF-energies:

SVP -50441.53375431

TZVPP -50453.51256224

NO<sub>2</sub>(OO<sub>ad</sub>)

Atom	x	y	z
O	-6.193120703471	-0.000746977212	9.972556957439
O	-5.984806869239	-0.010160624567	14.765400516837
O	0.007181794933	-5.675712729677	8.587445032785
O	0.001260492908	0.001071978335	3.514618897964
O	-0.022340255377	0.006554574743	8.642375329174
O	6.132816907247	0.022208864455	9.973624000053
O	5.928935020788	0.000557679943	14.784852453456
O	0.019488682154	5.671323770670	8.576444230616
TI	-6.428565320313	-2.815747925923	12.856749041059
TI	-6.419280276312	2.817085395540	12.876568096367
TI	-6.109532414379	0.011317031909	6.624392811053
TI	0.042999551288	-5.517295426103	12.140897935115
TI	-0.002438876700	-2.803403784295	6.248438008441
TI	-0.209370309862	0.045071015008	12.232737082387
TI	0.027437459822	2.774243238231	6.203516441764
TI	6.412027089990	2.806883126583	12.877470623535
TI	6.131667917309	-0.010324861483	6.634152586032
TI	0.102184030411	5.532410825724	12.094359771147
O	-3.640135465218	-2.699919064653	6.263908132469
O	-9.955236638190	-2.683888429961	12.724881163174
O	-2.321605879921	-2.836120662934	12.540565211854
O	-3.651713273946	2.698333277894	6.260431189384
O	-9.951056443959	2.680379610598	12.727352061553
O	-2.317413442753	2.843110714262	12.562963717037
O	3.642914190225	-2.691781437072	6.265069000170
O	2.276819868408	-2.880119267376	12.570774938633
O	9.892338771942	-2.646944745314	12.669664519892
O	3.633465020366	2.698361243531	6.246187804418
O	2.263919441343	2.876783996002	12.590981062174
O	9.932603195553	2.698942618011	12.726567389751
N	-0.073905080887	-2.326548097025	17.866621595633
O	-0.070697505683	-4.473036273361	17.252060851993
O	-0.076488685558	-0.362672859267	16.738223951568

SCF-energies:

SVP -50441.53296841

TZVPP -50453.51032511

TS1

Atom	x	y	z
O	-6.187126232801	-0.009907312301	9.977978671813
O	-5.990805271497	0.006011035698	14.766739725634
O	0.001596234016	-5.670103581990	8.570428767328
O	0.001977556918	0.000244906264	3.526556556991
O	-0.021287483540	-0.000313978838	8.649970404167
O	6.132696320302	0.027518814359	9.979563528471
O	5.923206708149	0.004931767498	14.786878391687
O	0.029784051070	5.671947263538	8.572716562835
TI	-6.425940305494	-2.814525660967	12.871213259372
TI	-6.427388092937	2.820022783820	12.862393517157
TI	-6.104924211175	0.004684593302	6.625190517237
TI	0.080706187491	-5.531628608421	12.075815593067
TI	0.005060275081	-2.760370128145	6.248706447091
TI	-0.254277413636	0.038829873443	12.379358939787
TI	0.020653496243	2.757269976567	6.242304379417
TI	6.413900880580	2.805472091371	12.869312019723
TI	6.126459049990	-0.005860067339	6.634006201107
TI	0.107067721653	5.540531094858	12.076005704379
O	-3.650262812494	-2.701528905828	6.261738448131
O	-9.953984575864	-2.682431296273	12.733155477565
O	-2.295771069786	-2.844837927203	12.645632193267
O	-3.654405748421	2.702274485307	6.266468119977
O	-9.955218237962	2.683225234158	12.723288525622
O	-2.333968828646	2.860170887293	12.518981157221
O	3.650096594309	-2.695396181116	6.263653955330
O	2.292195991936	-2.929404761349	12.545280556161
O	9.893557556967	-2.646336151444	12.671706210080
O	3.644567454409	2.700047146210	6.251037050593
O	2.250110805433	2.898423261144	12.651017623969
O	9.933408936270	2.700364903868	12.732790984430
N	-0.010641562171	-0.016679095955	16.648013248709
O	0.984034374117	1.485654913656	18.433391117610
N	0.631204818308	-0.268824131884	20.196262510347
O	-0.341951843423	-1.783524880536	18.440174372185

SCF-energies:

SVP -50496.09174532

TS2

Atom	x	y	z
O	-6.200637334439	-0.003054820903	9.972967724182
O	-5.965605006028	0.001323746231	14.756166132975
O	0.011912053506	-5.671227543701	8.574536822727
O	0.001511524108	-0.001099569637	3.527809345730
O	-0.020163295411	-0.000359106493	8.655486119702
O	6.136483404063	0.019742682938	9.973655389330
O	5.919031028967	0.010768746531	14.775017832351
O	0.022887938870	5.672008860212	8.574474461140
TI	-6.426558092662	-2.817018858804	12.860352809131
TI	-6.427183274153	2.821731166219	12.859033258577
TI	-6.104782254806	0.011291234176	6.622189527768
TI	0.062600142965	-5.528813447382	12.077121474406
TI	-0.002974250371	-2.756288587975	6.246528739053
TI	-0.244901216420	0.023822677681	12.386254492448
TI	0.030378262961	2.761995753233	6.250220166050
TI	6.415155548214	2.809651654683	12.861248036725
TI	6.128112800819	-0.012217182819	6.630832851249
TI	0.116768146543	5.528612960199	12.082733882271
O	-3.646758057552	-2.703997319375	6.263393308617
O	-9.954229617224	-2.681845761963	12.732571937308
O	-2.321222323167	-2.849734892888	12.559712015389
O	-3.658576286223	2.701195216658	6.267442901578
O	-9.954028120276	2.682165097552	12.730449053210
O	-2.324156366934	2.846253126839	12.552275783758
O	3.652176692005	-2.695523666664	6.262496164779
O	2.271880189980	-2.906994707796	12.599206895393
O	9.891873182789	-2.646526892561	12.674123834988
O	3.640518134984	2.701665765580	6.251105842838
O	2.269943692127	2.892593768041	12.593485299734
O	9.934970906146	2.700482232011	12.726982987911
N	-0.091325410055	0.011084390077	16.763695096054
O	1.714013808870	-0.017387794453	18.557490934257
O	-1.815086018192	-0.048194638383	18.636026280529
N	-0.010748426338	-0.072602191956	20.378751805710

SCF-energies:

SVP -50496.09054328

TS3

Atom	x	y	z
O	-6.194732264282	-0.001308818198	9.972866185461
O	-5.993771072414	0.001340075013	14.764357671698
O	0.007430427966	-5.674155768323	8.577525150303
O	0.001586081930	0.000902066530	3.523573579466
O	-0.008061399600	0.004513316703	8.644002730404
O	6.132853956741	0.024915598654	9.983270039559
O	5.896256083456	0.004175582997	14.790516860139
O	0.025251848557	5.672692497990	8.573893946719
TI	-6.421480409585	-2.816638091961	12.873783129407
TI	-6.424264881389	2.818236175324	12.872972573612
TI	-6.117149035849	0.003758422114	6.628581583168
TI	0.050896310607	-5.519937825653	12.106169164315
TI	-0.001513833260	-2.781832053640	6.251390332892
TI	-0.218512926262	0.041795582087	12.308780142723
TI	0.010120178580	2.761933174350	6.222676453356
TI	6.412776296396	2.808287173181	12.866838380922
TI	6.119639634092	-0.003923461675	6.632807760299
TI	0.092270956349	5.537729282030	12.082020683249
O	-3.644720870114	-2.699308547506	6.268759300925
O	-9.953628399756	-2.683004517626	12.723830277803
O	-2.311632817754	-2.836473328993	12.553706917730
O	-3.648017368626	2.701271745657	6.267454669408
O	-9.954947270934	2.684121531489	12.723033007205
O	-2.325897812248	2.850421651287	12.530355211968
O	3.650546141085	-2.695160385196	6.267070244387
O	2.285315533078	-2.910832533236	12.562736554322
O	9.891276449689	-2.644033352555	12.677896625694
O	3.647929671736	2.701268828890	6.252164287441
O	2.258013747431	2.892533354758	12.627858029799
O	9.930616749761	2.698659805609	12.733960736943
N	-0.031775348673	-0.235503873339	16.727222482184
O	-0.085067068091	-3.043644902741	17.977726018093
N	1.439804310635	-0.984151515974	18.429372739425
O	3.082991224069	-0.522118639790	19.811312847247

SCF-energies:

SVP -50496.09252249