

付録 1

●安定構造・Adduct・遷移状態の原子座標と振動状態

CBS-QB3 法で最適化した分子構造の原子座標[Å]と振動状態[cm<sup>-1</sup>]について記載する。

(1) Al/O<sub>2</sub> 反応系

(1-2-1) O<sub>2</sub>

O	0.00000000	0.00000000	0.60281700
O	-0.00000000	0.00000000	-0.60281700
Frequencies --	1640.7		

(1-4-1) AlO

Al	0.00000000	0.00000000	0.62082819
O	0.00000000	0.00000000	-1.00884581
Frequencies --	952.5		

(1-5-1) AlO<sub>2</sub>

Al	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.65377500
O	-0.00000000	0.00000000	-1.65377500
Frequencies --	168.9, 198.6, 775.0, 820.7		

(1-5-2) AlO<sub>2</sub>-2

O	0.00000000	0.67324300	-0.82483924
O	0.00000000	-0.67324300	-0.82483924
Al	0.00000000	0.00000000	1.01518676
Frequencies --	320.3, 493.6, 1169.9		

(1-5-3) AlO<sub>2</sub>-3

O	0.00000000	0.81707100	-0.67649310
O	0.00000000	-0.81707100	-0.67649310
Al	0.00000000	0.00000000	0.83260690
Frequencies --	589.9, 716.3, 917.1		

(1-5-4) AlO<sub>2</sub>-4

O	0.07821054	1.72125033	0.00000000
O	-0.13635810	0.42423437	0.00000000
Al	0.03578311	-1.32029828	0.00000000
Frequencies --	56.2, 557.1, 1229.0		

(1-5-5) AlO<sub>2</sub>-5

O	0.00000000	-0.00000000	1.73509458
O	0.00000000	0.00000000	0.42258358
Al	0.00000000	0.00000000	-1.32780194
Frequencies --	26.7, 551.4, 1236.9		

(1-5-6) AlO<sub>2</sub>-TS1

Al	0.04502133	0.76111873	0.00000000
O	0.99168352	-0.66748480	0.00000000
O	-1.06484317	-0.56933313	0.00000000
Frequencies --	-368.9, 727.7, 834.5		

(1-5-7) AlO<sub>2</sub>-TS2

Al	0.08239812	-1.29056328	0.00000000
O	-0.32255962	0.43592451	0.00000000
O	0.18866267	1.66124082	0.00000000
Frequencies --	-71.0, 568.4, 1195.6		
(1-5-8) AlO <sub>2</sub> -TS3			
O	0.74473030	-0.67718103	0.00000000
O	-0.65559133	-0.90133319	0.00000000
Al	-0.05485475	0.97139337	0.00000000
Frequencies --	-881.6, 264.3, 882.5		
(1-5-9) AlO <sub>2</sub> -TS4			
Al	-0.17091656	0.84775527	0.00000000
O	0.99676191	-0.44007394	0.00000000
O	-0.71902250	-0.93752837	0.00000000
Frequencies --	-1102.8, 459.7, 807.6		
(1-6-1) AlO <sub>3</sub>			
O	0.00000000	0.68487800	-1.32008595
O	0.00000000	-0.68487800	-1.32008595
Al	0.00000000	0.00000000	0.39683005
O	0.00000000	0.00000000	1.99532305
Frequencies --	176.2, 193.1, 446.4, 546.8, 1105.1, 1150.9		
(1-7-1) Al <sub>2</sub> (1)			
Al	0.00000000	0.00000000	1.53747000
Al	-0.00000000	0.00000000	-1.53747000
Frequencies --	209.1		
(1-8-1) Al <sub>2</sub> (3)			
Al	0.00000000	0.00000000	1.38173000
Al	-0.00000000	0.00000000	-1.38173000
Frequencies --	253.6		
(1-9-1) Al <sub>2</sub> O(1)			
Al	0.00000000	0.00000000	1.71580500
Al	-0.00000000	0.00000000	-1.71580500
O	0.00000000	0.00000000	0.00000000
Frequencies --	110.7, 110.7, 505.6, 984.0		
(1-9-2) Al <sub>2</sub> O(1)-2			
Al	0.00000000	0.00000000	2.12137803
Al	0.00000000	0.00000000	-0.69809497
O	0.00000000	0.00000000	-2.31283497
Frequencies --	78.8, 78.8, 239.5, 1057.9		
(1-9-3) Al <sub>2</sub> O(1)-TS1			
Al	0.16335898	-1.88588029	0.00000000
Al	-0.55522297	0.74900334	0.00000000
O	0.63677898	1.84742503	0.00000000
Frequencies --	-98.6, 278.9, 1036.2		
(1-10-1) Al <sub>2</sub> O(3)			
Al	0.00000000	1.30277900	-0.27213812

O	0.00000000	0.00000000	0.88444888
Al	0.00000000	-1.30277900	-0.27213812
Frequencies --	247.1, 673.0, 734.3		
(1-10-2) Al <sub>2</sub> O(3)-2			
Al	0.00000000	0.00000000	1.71506500
O	0.00000000	0.00000000	0.00000000
Al	-0.00000000	0.00000000	-1.71506500
Frequencies --	145.1, 204.2, 502.4, 884.4		
(1-10-3) Al <sub>2</sub> O(3)-3			
Al	0.00000000	0.00000000	1.97186515
O	0.00000000	0.00000000	-2.22112685
Al	0.00000000	0.00000000	-0.60501785
Frequencies --	106.0, 126.1, 265.4, 1032.2		
(1-10-4) Al <sub>2</sub> O(3)-TS1			
Al	0.00000000	-1.58960394	0.15528853
O	0.00000000	0.00000000	-0.50639913
Al	-0.00000000	1.58960394	0.15528853
Frequencies --	-147.9, 594.2, 874.8		
(1-10-5) Al <sub>2</sub> O(3)-TS2			
O	0.83501051	1.45408713	0.00000000
Al	-0.65378638	0.78361443	0.00000000
Al	0.13993376	-1.67843728	0.00000000
Frequencies --	-127.2, 233.9, 949.4		
(1-10-6) Al <sub>2</sub> O(3)-TS3			
Al	-0.62260513	0.91834170	0.00000000
O	0.78300377	1.77372350	0.00000000
Al	0.14075665	-2.00986385	0.00000000
Frequencies --	-289.5, 105.3, 892.6		
(1-11-1) Al <sub>2</sub> O <sub>2</sub> (1)			
Al	0.00000000	0.00000000	1.21817700
Al	-0.00000000	0.00000000	-1.21817700
O	0.00000000	1.26551000	0.00000000
O	0.00000000	-1.26551000	0.00000000
Frequencies --	298.8, 516.6, 616.7, 627.3, 747.1, 785.6		
(1-11-2) Al <sub>2</sub> O <sub>2</sub> (1)-2			
Al	0.00000000	0.00000000	-1.06601512
Al	0.00000000	0.00000000	2.33387988
O	0.00000000	0.00000000	0.60942288
O	0.00000000	0.00000000	-2.66970312
Frequencies --	72.3, 72.3, 231.3, 231.3, 459.5, 945.4, 1184.5		
(1-11-3) Al <sub>2</sub> O <sub>2</sub> (1)-3			
Al	0.00000000	0.00000000	1.75811800
Al	-0.00000000	0.00000000	-1.75811800
O	0.00000000	0.78288100	0.00000000
O	0.00000000	-0.78288100	0.00000000
Frequencies --	11.2, 232.3, 279.9, 407.9, 576.5, 823.4		

(1-11-4) Al<sub>2</sub>O<sub>2</sub>(1)-4

Al	0.00000000	0.00000000	-0.28669210
Al	0.00000000	0.00000000	2.52571990
O	0.00000000	0.80181900	-1.81921010
O	0.00000000	-0.80181900	-1.81921010

Frequencies -- 70.1, 86.7, 230.2, 610.8, 687.9, 921.3

(1-11-5) Al<sub>2</sub>O<sub>2</sub>(1)-TS1

Al	-0.52060517	1.00459701	0.00000000
Al	0.50996486	-1.43744659	0.00000000
O	-1.06020436	-0.60026463	0.00000000
O	1.07749485	1.30364521	0.00000000

Frequencies -- -207.6, 243.9, 346.7, 627.2, 802.5, 1034.1

(1-11-6) Al<sub>2</sub>O<sub>2</sub>(1)-TS2

Al	-0.04739293	1.65990285	0.00000000
Al	0.04739293	-1.65990285	0.00000000
O	0.89791256	0.14236905	0.00000000
O	-0.89791256	-0.14236905	0.00000000

Frequencies -- -631.3, 70.5, 285.1, 372.7, 600.9, 671.0

(1-11-7) Al<sub>2</sub>O<sub>2</sub>(1)-TS3

Al	-0.36592531	0.60510691	0.00000000
Al	2.25332479	-0.08627975	0.00000000
O	-1.02016954	-1.02266096	0.00000000
O	-2.04685461	0.17956683	0.00000000

Frequencies -- -94.7, 25.2, 267.8, 593.6, 656.2, 900.8

(1-12-1) Al<sub>2</sub>O<sub>2</sub>(3)

Al	0.00000000	0.00000000	1.21639500
Al	-0.00000000	0.00000000	-1.21639500
O	0.00000000	1.27008200	0.00000000
O	0.00000000	-1.27008200	0.00000000

Frequencies -- 279.1, 518.7, 609.5, 723.0, 730.7, 771.5

(1-12-2) Al<sub>2</sub>O<sub>2</sub>(3)-2

Al	-0.59618027	-1.13772893	0.00000000
Al	0.22579679	2.17496034	0.00000000
O	0.81276720	-2.20358236	0.00000000
O	-0.21089403	0.51808131	0.00000000

Frequencies -- 64.8, 107.5, 218.6, 507.5, 735.6, 1011.4

(1-12-3) Al<sub>2</sub>O<sub>2</sub>(3)-3

O	0.00000000	0.00000000	1.92376529
O	0.00000000	0.00000000	0.55701729
Al	0.00000000	1.42839700	-0.76331771
Al	0.00000000	-1.42839700	-0.76331771

Frequencies -- 183.0, 191.9, 196.9, 368.0, 460.7, 905.8

(1-12-4) Al<sub>2</sub>O<sub>2</sub>(3)-4

O	-2.77255855	-0.15303488	0.00000000
O	-1.47077544	-0.43195602	0.00000000
Al	-0.03002385	0.60004648	0.00000000

Al 2.64130631 -0.24005207 0.00000000  
Frequencies -- 32.4, 56.1, 157.2, 209.2, 610.5, 1155.8

(1-12-5) Al<sub>2</sub>O<sub>2</sub>(3)-TS1

Al -1.25093940 0.50152736 0.00000000  
Al 1.68540438 -0.27938203 0.00000000  
O -1.12739282 -1.25051616 0.00000000  
O 0.42138724 0.88953000 0.00000000  
Frequencies -- -145.3, 136.1, 228.5, 646.5, 723.6, 861.2

(1-12-6) Al<sub>2</sub>O<sub>2</sub>(3)-TS2

O 0.00000000 0.00000000 1.92117224  
O 0.00000000 0.00000000 0.42761824  
Al 0.00000000 1.49059400 -0.72270476  
Al 0.00000000 -1.49059400 -0.72270476  
Frequencies -- -1019.5, 177.5, 187.4, 204.9, 416.2, 552.6

(1-12-7) Al<sub>2</sub>O<sub>2</sub>(3)-TS3

Al -0.11737660 0.97002250 0.00000000  
Al 2.42574618 -0.39805758 0.00000000  
O -2.54232617 -0.47288046 0.00000000  
O -1.20877439 -0.45656253 0.00000000  
Frequencies -- -48.8, 72.2, 169.2, 215.1, 583.7, 1130.3

(1-13-1) Al<sub>2</sub>O<sub>3</sub>(1)

O 0.00000000 0.00000000 3.27825200  
Al 0.00000000 0.00000000 1.67782300  
Al -0.00000000 0.00000000 -1.67782300  
O -0.00000000 0.00000000 -3.27825200  
O 0.00000000 0.00000000 0.00000000  
Frequencies -- 57.7, 57.7, 177.2, 177.2, 257.7, 257.7, 423.8, 935.3, 1141.3, 1235.6

(1-13-2) Al<sub>2</sub>O<sub>3</sub>(1)-2

Al -0.05511985 -1.62680413 0.00000000  
O -0.03516622 2.41868351 0.00000000  
Al 0.07821765 0.78579189 0.00000000  
O 1.27865106 -0.58922238 0.00000000  
O -1.28101876 -0.46281623 0.00000000  
Frequencies -- 159.4, 200.1, 330.3, 457.4, 495.0, 533.4, 823.8, 853.9, 989.8

(1-13-3) Al<sub>2</sub>O<sub>3</sub>(1)-3

O 0.00000000 0.82290000 -2.16056608  
O 0.00000000 -0.82290000 -2.16056608  
Al 0.00000000 0.00000000 -0.67274908  
O 0.00000000 0.00000000 0.99407492  
Al 0.00000000 0.00000000 2.72016892  
Frequencies -- 65.9, 71.3, 245.9, 249.8, 406.4, 606.0, 767.5, 896.3, 1138.8

(1-13-4) Al<sub>2</sub>O<sub>3</sub>(1)-4

Al 0.00000000 0.00000000 2.27222782  
O 0.00000000 0.00000000 -2.76214518  
Al 0.00000000 0.00000000 -1.16083118  
O 0.00000000 0.79778600 0.47806282  
O 0.00000000 -0.79778600 0.47806282

Frequencies -- 25.5, 134.3, 215.0, 270.1, 369.2, 464.1, 591.4, 784.8, 1130.4

(1-13-5) Al<sub>2</sub>O<sub>3</sub>(1)-5

O	1.77677622	-0.36290222	0.00000000
O	3.08460257	-0.47750311	0.00000000
O	-1.15305308	0.24964162	0.00000000
Al	-2.73767125	-0.41170616	0.00000000
Al	0.45562467	0.77525306	0.00000000

Frequencies -- 49.6, 97.4, 129.2, 170.9, 319.5, 452.6, 610.9, 1009.2, 1137.3

(1-13-6) Al<sub>2</sub>O<sub>3</sub>(1)-TS1

O	-0.40697726	2.52292363	0.00000000
Al	0.11546458	1.00592793	0.00000000
Al	0.19867157	-1.59442955	0.00000000
O	-1.38758755	-1.25930071	0.00000000
O	1.28409356	-0.30730779	0.00000000

Frequencies -- -176.0, 147.7, 169.3, 289.6, 362.4, 632.9, 842.3, 1043.0, 1109.8

(1-13-7) Al<sub>2</sub>O<sub>3</sub>(1)-TS2

Al	0.51253169	-1.71174815	0.00000000
O	0.13869928	2.14790326	0.00000000
Al	-0.59922157	0.62820692	0.00000000
O	-1.12272838	-0.96766505	0.00000000
O	1.12490015	0.58051629	0.00000000

Frequencies -- -390.1, 80.0, 164.9, 263.7, 386.7, 627.9, 691.8, 780.0, 1036.1

(1-13-8) Al<sub>2</sub>O<sub>3</sub>(1)-TS3

Al	-2.13628545	0.04122497	0.00000000
O	2.67803109	0.05837453	0.00000000
Al	1.06414317	0.01059711	0.00000000
O	-0.52091217	0.85545960	0.00000000
O	-0.41488771	-0.99804501	0.00000000

Frequencies -- -488.4, 43.5, 167.1, 235.8, 329.4, 526.5, 579.2, 614.0, 1065.8

(1-13-9) Al<sub>2</sub>O<sub>3</sub>(1)-TS4

O	2.46764816	0.97015787	-0.26590199
O	1.97482410	-0.03664312	0.49046597
O	-1.06629292	-0.30149891	-0.06335903
Al	-2.60885187	0.45220218	0.05768800
Al	0.53120305	-0.84113501	-0.15689105

Frequencies -- -101.9, 49.7, 96.1, 176.6, 190.8, 468.1, 630.6, 996.1, 1015.3

(1-14-1) Al<sub>2</sub>O<sub>3</sub>(3)

Al	0.00000000	0.00000000	-0.72905106
Al	0.00000000	0.00000000	1.68414594
O	0.00000000	1.26543200	0.45811394
O	0.00000000	0.00000000	-2.46825706
O	0.00000000	-1.26543200	0.45811394

Frequencies -- 141.0, 184.4, 347.3, 452.9, 637.5, 682.3, 751.9, 773.1, 928.6

(1-14-2) Al<sub>2</sub>O<sub>3</sub>(3)-2

Al	1.56013328	-0.01363726	0.00000000
O	3.14375799	-0.26069904	0.00000000
O	-0.08486459	0.28207349	0.00000000

Al	-1.76478282	0.56333702	0.00000000
O	-2.72633789	-0.91463657	0.00000000
Frequencies --	47.7, 74.2, 170.8, 228.2, 250.6, 470.8, 744.4, 981.3, 1198.9		

(1-14-3) Al<sub>2</sub>O<sub>3</sub>(3)-3

O	0.00000000	0.74778200	-1.27666504
O	0.00000000	-0.74778200	-1.27666504
Al	0.00000000	-1.38876500	0.36031296
O	0.00000000	0.00000000	1.38231296
Al	-0.00000000	1.38876500	0.36031296
Frequencies --	155.1, 233.4, 347.8, 391.4, 657.3, 697.0, 721.6, 829.8, 834.5		

(1-14-4) Al<sub>2</sub>O<sub>3</sub>(3)-4

O	0.49210528	-1.95260023	0.67775500
O	0.49210528	-1.95260023	-0.67775500
Al	-0.76557391	-0.69846381	0.00000000
O	-0.24306912	0.91762008	0.00000000
Al	0.30948687	2.53697482	0.00000000
Frequencies --	62.6, 82.0, 182.1, 220.9, 391.7, 484.5, 598.6, 1017.5, 1152.3		

(1-14-5) Al<sub>2</sub>O<sub>3</sub>(3)-5

O	2.96919636	-0.25212145	0.00000000
O	1.68769193	-0.64657345	0.00000000
Al	0.52301420	0.73760009	0.00000000
O	-1.09879933	0.24749210	0.00000000
Al	-2.71260741	-0.33685991	0.00000000
Frequencies --	47.9, 55.1, 109.6, 120.6, 227.1, 512.2, 634.3, 1012.3, 1128.1		

(1-14-6) Al<sub>2</sub>O<sub>3</sub>(3)-adduct-1

O	0.40785012	-3.56995426	0.00000000
O	0.71188642	-2.40287481	0.00000000
Al	-1.55353998	0.27445661	0.00000000
O	-0.26628472	1.40891513	0.00000000
Al	1.02833886	2.53410582	0.00000000
Frequencies --	8.55, 9.3, 35.0, 58.9, 109.6, 114.2, 505.9, 983.8, 1630.5		

(1-14-7) Al<sub>2</sub>O<sub>3</sub>(3)-adduct-2

O	-1.89660120	0.04301896	0.00000000
O	4.20281111	0.48337247	0.00000000
Al	-0.18885728	0.20998027	0.00000000
Al	-3.60438615	-0.12053211	0.00000000
O	3.85781066	-0.67174469	0.00000000
Frequencies --	6.21, 10.3, 23.3, 29.1, 111.6, 111.8, 506.1, 984.5, 1640.6		

(1-14-8) Al<sub>2</sub>O<sub>3</sub>(3)-TS1

Al	1.16075516	0.19876586	0.00000000
O	2.66513830	-0.36090758	0.00000000
O	-0.32574766	1.02186878	0.00000000
Al	-1.86189562	0.24263738	0.00000000
O	-1.20003739	-1.37824146	0.00000000
Frequencies --	-150.2, 94.5, 131.8, 229.1, 259.2, 606.3, 738.9, 878.8, 1118.6		

(1-14-9) Al<sub>2</sub>O<sub>3</sub>(3)-TS2

Al	-0.52857412	1.24641326	0.00000000
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Al	-0.16534504	-1.41862364	0.00000000
O	-1.42008161	-0.21918584	0.00000000
O	1.40112767	-0.76216012	0.00000000
O	1.14657259	1.26118782	0.00000000

Frequencies -- -327.9, 115.6, 121.1, 247.4, 366.0, 622.6, 709.0, 805.9, 902.8

(1-14-10) Al<sub>2</sub>O<sub>3</sub>(3)-TS3

O	0.74045407	-1.04772295	-0.49969919
O	1.50434821	-0.60584664	0.58537059
Al	0.79965369	0.91558510	-0.19388245
O	-0.88441526	1.02171976	0.15524491
Al	-1.63681493	-0.52675443	0.04562627

Frequencies -- -250.6, 178.2, 211.8, 291.5, 356.7, 505.3, 710.9, 792.5, 971.0

(1-14-11) Al<sub>2</sub>O<sub>3</sub>(3)-TS4

O	2.90156291	-0.11530451	0.08840708
O	1.70646452	-0.72942529	-0.07445432
Al	0.55493801	0.66012183	-0.02979573
O	-1.08231620	0.22097020	-0.00529237
Al	-2.72460646	-0.27626977	0.02446627

Frequencies -- -90.3, 26.5, 60.4, 112.7, 218.8, 504.5, 677.4, 1010.3, 1135.7

(1-14-12) Al<sub>2</sub>O<sub>3</sub>(3)-TS5

O	-1.86344735	0.09321587	0.00000000
O	3.67383008	-0.73390800	0.00000000
Al	-0.19114746	0.47759670	0.00000000
Al	-3.53705984	-0.28405568	0.00000000
O	4.24795413	0.32618796	0.00000000

Frequencies -- -4.36, 8.08, 29.7, 32.8, 110.7, 110.8, 505.9, 984.1, 1639.6

(1-14-13) Al<sub>2</sub>O<sub>3</sub>(3)-TS6

O	0.63879184	-2.98681109	0.00000000
O	0.62826764	-1.75685871	0.00000000
Al	-1.25215726	-0.30527148	0.00000000
O	-0.32145653	1.13072620	0.00000000
Al	0.67024775	2.52862138	0.00000000

Frequencies -- -137.0, 42.4, 55.7, 114.4, 144.7, 237.8, 512.8, 985.8, 1404.5

(1-15-1) Al<sub>2</sub>O<sub>4</sub>(1)

O	0.00000000	1.26188500	0.00000000
O	0.00000000	-1.26188500	0.00000000
Al	0.00000000	0.00000000	1.19673800
Al	-0.00000000	0.00000000	-1.19673800
O	0.00000000	0.00000000	2.93301700
O	-0.00000000	0.00000000	-2.93301700

Frequencies -- 92.1, 147.6, 207.5, 212.1, 384.1, 405.4, 636.3, 673.4, 730.7, 800.8, 912.1, 953.0

(1-15-2) Al<sub>2</sub>O<sub>4</sub>(1)-2

Al	0.00000000	0.00000000	-0.39425326
O	0.00000000	0.68318300	-2.10933626
O	0.00000000	-0.68318300	-2.10933626
O	1.26470400	-0.00000000	0.79149174
O	-1.26470400	-0.00000000	0.79149174

Frequencies -- 130.3, 136.0, 182.3, 341.3, 389.0, 468.7, 637.7, 643.6, 746.4, 779.0, 869.5,



1135.3

(1-15-3) Al<sub>2</sub>O<sub>4</sub>(1)-3

O	0.00000000	0.82724600	-2.73348391
O	0.00000000	-0.82724600	-2.73348391
Al	0.00000000	0.00000000	-1.25497791
O	0.00000000	0.00000000	0.41437709
Al	0.00000000	0.00000000	2.09211309
O	0.00000000	0.00000000	3.69224609

Frequencies -- 52.0, 56.6, 178.4, 183.8, 271.2, 272.0, 374.3, 590.7, 782.3, 895.5, 1097.6, 1228.6

(1-15-4) Al<sub>2</sub>O<sub>4</sub>(1)-4

O	0.04998492	1.47461215	-0.08689674
O	-1.87805719	-0.94439274	-0.44540684
Al	-1.32799707	0.55774815	0.14531332
Al	1.13344289	0.03144411	-0.04572313
O	-0.52120607	-1.02415692	0.44618095
O	2.66542887	-0.46349992	-0.07571143

Frequencies -- 100.9, 157.0, 182.4, 226.6, 311.7, 399.5, 493.5, 583.2, 596.5, 784.6, 987.8, 1072.9

(1-15-5) Al<sub>2</sub>O<sub>4</sub>(1)-TS1

O	-0.24124857	2.09915052	0.82274600
O	-0.24124857	2.09915052	-0.82274600
Al	0.21040555	0.68253275	0.00000000
O	1.30305087	-0.68112002	0.00000000
Al	0.15582366	-1.91187628	0.00000000
O	-1.41567620	-1.51949777	0.00000000

Frequencies -- -163.4, 75.6, 139.9, 165.2, 295.8, 353.1, 538.2, 673.6, 770.8, 846.5, 1024.2, 1048.2

(1-15-6) Al<sub>2</sub>O<sub>4</sub>(1)-TS2

O	0.74024205	-1.07732179	-0.41105206
O	2.12517608	-0.78638891	0.42577193
Al	1.26641912	0.56590016	-0.13381595
O	-0.14702084	1.44261621	0.03887014
Al	-1.26552889	0.06786426	0.05340607
O	-2.71984392	-0.60877269	0.07707605

Frequencies -- -129.2, 104.5, 166.5, 171.3, 298.3, 379.3, 511.1, 628.6, 676.9, 797.7, 1022.8, 1107.4

(1-15-7) Al<sub>2</sub>O<sub>4</sub>(1)-TS3

O	-0.06713011	1.48904711	0.07620192
O	2.11803901	-0.85067578	0.34790793
Al	1.27391297	0.50974220	-0.17400605
Al	-1.14272403	0.05943905	0.09047175
O	0.39408507	-1.04795284	-0.31782521
O	-2.65817599	-0.51533803	0.02945860

Frequencies -- -200.3, 124.8, 154.9, 172.9, 293.3, 330.6, 434.3, 604.6, 620.8, 769.7, 1007.1, 1058.9

(1-16-1) Al<sub>2</sub>O<sub>4</sub>(3)

O	0.00000000	1.26491500	0.00000000
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O	0.00000000	-1.26491500	0.00000000
Al	0.00000000	0.00000000	1.20151000
Al	-0.00000000	0.00000000	-1.20151000
O	0.00000000	0.00000000	2.92488100
O	-0.00000000	0.00000000	-2.92488100

Frequencies -- 93.5, 119.1, 178.7, 216.0, 379.2, 404.4, 630.4, 664.5, 700.2, 736.8, 779.5, 923.6

(1-16-2) Al<sub>2</sub>O<sub>4</sub>(3)-2

Al	0.00000000	0.00000000	-0.39438586
Al	0.00000000	0.00000000	2.01607414
O	0.00000000	1.26461200	0.79139514
O	-0.68308000	0.00000000	-2.10901686
O	0.68308000	0.00000000	-2.10901686
O	0.00000000	-1.26461200	0.79139514

Frequencies -- 129.9, 137.1, 181.9, 341.0, 389.1, 469.4, 637.8, 643.7, 746.5, 779.0, 869.7, 1135.9

(1-16-3) Al<sub>2</sub>O<sub>4</sub>(3)-3

O	-1.44881388	-2.39908524	0.00000000
O	0.00050543	0.27015134	0.00000000
Al	-0.00588899	-1.41277464	0.00000000
Al	-0.00898095	1.94145002	0.00000000
O	1.49204784	-2.27324626	0.00000000
O	-0.01957574	3.54308266	0.00000000

Frequencies -- 44.4, 63.4, 163.0, 182.3, 204.1, 274.0, 285.9, 439.2, 753.0, 847.0, 1020.1, 1213.7

(1-16-4) Al<sub>2</sub>O<sub>4</sub>(3)-4

Al	0.15077160	0.80760731	0.00000000
Al	0.23897282	-1.64026378	0.00000000
O	-1.04759287	-0.41517396	0.78252300
O	0.03327841	2.54421960	0.00000000
O	1.42857265	-0.36080491	0.00000000
O	-1.04759287	-0.41517396	-0.78252300

Frequencies -- 158.1, 191.6, 300.6, 346.8, 416.8, 464.1, 486.8, 538.1, 698.3, 758.7, 815.8, 910.8

(1-16-5) Al<sub>2</sub>O<sub>4</sub>(3)-5

O	-1.33309929	-0.19592466	0.00000000
O	1.14979538	-1.36587808	0.00000000
Al	-0.58095778	-1.74429543	0.00000000
Al	-0.09980485	0.98568815	0.00000000
O	1.39653677	0.08076965	0.00000000
O	-0.10699360	2.71376991	0.00000000

Frequencies -- 137.2, 186.5, 195.8, 298.0, 340.6, 377.7, 623.8, 664.9, 739.0, 796.9, 830.4, 919.7

(1-16-6) Al<sub>2</sub>O<sub>4</sub>(3)-6

Al	0.57548976	0.27961573	0.00000000
Al	-2.78223874	-0.20474226	0.00000000
O	-1.08535695	0.04258756	0.00000000
O	1.70953777	-1.02259476	0.68254100
O	1.70953777	-1.02259476	-0.68254100
O	1.25224850	1.88093256	0.00000000

Frequencies -- 55.3, 75.1, 143.8, 172.0, 235.1, 269.8, 439.7, 446.9, 652.4, 820.1, 1055.8, 1134.9

(1-16-7) Al<sub>2</sub>O<sub>4</sub>(3)-TS1

O	-2.97267151	0.36418528	0.00000000
O	-0.60636425	-1.62561005	0.00000000
Al	-1.28568536	-0.00766304	0.00000000
O	0.04538934	1.04807655	0.00000000
Al	1.55595002	0.26615954	0.00000000
O	3.09446635	-0.20670860	0.00000000

Frequencies -- -243.5, 45.5, 130.0, 174.8, 194.9, 287.5, 301.4, 627.1, 662.9, 781.1, 943.1, 1065.3

(1-16-8) Al<sub>2</sub>O<sub>4</sub>(3)-TS2

Al	0.86524894	-0.08758096	0.08697701
Al	-1.72944504	-0.45214820	-0.05675477
O	0.05662085	1.39094210	0.58138969
O	2.56572393	-0.24022792	-0.29814904
O	-0.29157695	-1.36008002	0.22421738
O	-0.92644918	1.08642574	-0.55656919

Frequencies -- -176.4, 116.3, 193.5, 223.6, 313.3, 399.7, 631.8, 645.2, 781.2, 791.9, 802.0, 889.3

(1-16-9) Al<sub>2</sub>O<sub>4</sub>(3)-TS3

Al	0.11647354	0.47062961	0.00000000
Al	-0.20258049	-2.46418806	0.00000000
O	1.73752851	-0.11816099	0.00000000
O	-0.35149986	2.12559898	0.68294500
O	-0.35149986	2.12559898	-0.68294500
O	-0.89460500	-0.89350448	0.00000000

Frequencies -- -160.5, 80.2, 143.3, 165.3, 225.7, 272.7, 456.7, 534.7, 726.8, 811.8, 909.6, 1134.7

(1-16-10) Al<sub>2</sub>O<sub>4</sub>(3)-TS4

O	-1.34345542	-0.03472299	0.00000000
O	0.96554352	-1.82916456	0.00000000
Al	-0.68312734	-1.59565369	0.00000000
Al	0.04626086	1.00144016	0.00000000
O	1.51048770	0.09280831	0.00000000
O	-0.09766778	2.73667623	0.00000000

Frequencies -- -480.1, 70.0, 165.6, 168.7, 216.2, 306.9, 323.4, 646.6, 759.5, 783.2, 892.3, 942.0

(1-16-11) Al<sub>2</sub>O<sub>4</sub>(3)-TS5

Al	0.73688328	-0.24696674	0.07937704
Al	-2.06342475	-0.22045106	-0.10532659
O	-0.68658660	-1.15861985	0.32031036
O	-0.09428498	1.32119908	-0.60018407
O	0.62552717	1.47971232	0.61058781
O	2.31097429	-0.88273763	-0.28854609

Frequencies -- -251.3, 116.5, 165.4, 202.8, 278.9, 312.1, 420.4, 533.8, 686.8, 771.0, 904.7, 964.1

(1-17-1) Al<sub>4</sub>O<sub>6</sub>(1)

O	1.43954991	0.83112453	1.17538758
O	-1.43954991	0.83112453	1.17538758
Al	-1.35388887	-0.78166810	0.55272282
Al	-0.00000000	1.56333621	0.55272282
O	-0.00000000	-1.66224905	1.17538758
Al	0.00000000	0.00000000	-1.65816845
O	0.00000000	1.66224905	-1.17538758

Al	1.35388887	-0.78166810	0.55272282
O	1.43954991	-0.83112453	-1.17538758
O	-1.43954991	-0.83112453	-1.17538758

Frequencies -- 190.4, 190.4, 253.0, 253.0, 253.0, 328.0, 328.0, 328.0, 417.1, 417.1, 417.1, 519.5, 626.2, 683.0, 683.0, 683.0, 774.3, 774.3, 778.3, 778.3, 778.3, 778.3, 855.4, 855.4, 855.4

(1-17-2) Al<sub>4</sub>O<sub>6</sub>(1)-2

O	-0.34591635	1.73390529	1.62521800
O	0.34591635	-1.73390529	-1.62521800
Al	0.00000000	0.00000000	1.38112400
O	-1.16682420	-0.52208175	0.00000000
Al	0.18048833	2.01298246	0.00000000
O	1.16682420	0.52208175	0.00000000
Al	-0.18048833	-2.01298246	0.00000000
O	0.34591635	-1.73390529	1.62521800
Al	0.00000000	0.00000000	-1.38112400
O	-0.34591635	1.73390529	-1.62521800

Frequencies -- 151.2, 227.0, 248.7, 292.7, 312.9, 337.1, 362.6, 368.7, 474.1, 481.7, 509.1, 527.0, 530.2, 558.0, 616.0, 650.8, 691.0, 712.9, 718.9, 730.4, 739.4, 807.7, 873.0, 877.0

(1-17-3) Al<sub>4</sub>O<sub>6</sub>(1)-3

Al	-1.46882923	-1.40810277	-0.06044028
O	2.56024491	-0.47583845	0.40000896
Al	-1.06409583	1.04702316	0.01369391
O	-1.49073058	2.68726420	0.43693800
O	-0.61695911	-0.38404799	1.18224583
O	-2.23855498	-0.06822359	-0.75961322
Al	2.36192819	1.05145763	-0.40301495
Al	0.89723684	-0.92910118	0.31434085
O	0.62861117	0.87805493	-0.61336503
O	-0.02275135	-2.24928398	-0.42615628

Frequencies -- 99.1, 118.3, 151.0, 192.9, 204.9, 269.6, 284.3, 299.7, 325.0, 368.5, 422.4, 471.4, 515.9, 538.0, 577.1, 631.9, 661.9, 703.8, 751.6, 764.1, 824.2, 861.7, 885.5, 931.5

(1-17-4) Al<sub>4</sub>O<sub>6</sub>(1)-4

O	-0.07150792	-1.21769488	1.41788700
O	-0.56827922	1.96855911	-1.61116000
Al	0.23094477	0.40575866	1.48044900
O	1.09862018	1.01600775	0.00000000
Al	-0.11327458	-2.32066723	0.00000000
O	-0.17933614	-3.94774325	0.00000000
Al	-0.12689789	2.38915423	0.00000000
O	-0.56827922	1.96855911	1.61116000
Al	0.23094477	0.40575866	-1.48044900
O	-0.07150792	-1.21769488	-1.41788700

Frequencies -- 56.3, 109.5, 185.8, 200.8, 212.9, 215.0, 265.2, 280.7, 320.5, 356.8, 399.3, 462.4, 495.5, 531.2, 566.1, 632.6, 644.6, 669.4, 733.3, 742.9, 876.5, 988.3, 1008.3, 1022.7

(1-17-5) Al<sub>4</sub>O<sub>6</sub>(1)-5

Al	0.00000000	0.00000000	-1.20770581
O	-1.26307965	0.03850014	3.33361819
Al	0.00000000	0.00000000	-3.60831781
O	0.00000000	0.00000000	-5.34615381
O	0.03860237	1.25973466	-2.41638381

O	-0.03860237	-1.25973466	-2.41638381
Al	0.00000000	0.00000000	4.55596119
Al	0.00000000	0.00000000	2.13728019
O	1.26307965	-0.03850014	3.33361819
O	0.00000000	0.00000000	0.46120619

Frequencies -- 24.2, 25.2, 26.2, 88.1, 123.8, 178.2, 195.0, 229.6, 256.1, 262.5, 359.5, 390.8, 462.4, 589.4, 640.4, 668.7, 695.8, 739.6, 771.4, 772.3, 805.0, 882.2, 934.6, 1156.0

(1-17-6) Al<sub>4</sub>O<sub>6</sub>(1)-6

Al	-1.43625166	1.11613397	0.00000000
O	0.31562323	-2.24886926	1.27271000
Al	0.72921786	2.32765840	0.00000000
O	2.18766768	3.17651843	0.00000000
O	0.33834667	0.60590466	0.00000000
O	-0.98148048	2.75743913	0.00000000
Al	0.88177455	-3.25710098	0.00000000
Al	-0.30093503	-1.15602152	0.00000000
O	0.31562323	-2.24886926	-1.27271000
O	-1.97071464	-0.46696224	0.00000000

Frequencies -- 53.8, 81.2, 83.8, 152.0, 164.7, 181.9, 250.4, 285.0, 302.4, 356.6, 400.4, 408.5, 528.8, 586.9, 597.2, 600.2, 669.7, 706.5, 752.6, 785.7, 793.8, 829.0, 920.3, 1025.9

(1-17-7) Al<sub>4</sub>O<sub>6</sub>(1)-7

O	0.00000000	0.00000000	2.87991400
O	-0.00000000	0.00000000	-2.87991400
Al	0.00000000	0.00000000	1.20102700
O	0.00000000	1.25814500	0.00000000
Al	0.00000000	0.00000000	4.55065400
O	0.00000000	0.00000000	6.15232000
Al	-0.00000000	0.00000000	-1.20102700
O	0.00000000	-1.25814500	0.00000000
Al	-0.00000000	0.00000000	-4.55065400
O	-0.00000000	0.00000000	-6.15232000

Frequencies -- 21.1, 22.2, 43.8, 50.8, 109.2, 151.8, 187.4, 188.9, 232.6, 233.1, 257.2, 269.6, 286.9, 396.4, 415.0, 624.5, 671.6, 787.1, 810.7, 814.0, 1023.9, 1051.1, 1210.6, 1228.7

(1-17-8) Al<sub>4</sub>O<sub>6</sub>(1)-8

O	-0.07075878	2.20083719	0.00000000
O	-0.70491766	-3.25378749	0.00000000
Al	-0.55430362	0.60584751	0.00000000
O	-2.11564615	-0.17968876	0.00000000
Al	0.41496295	3.80775221	0.00000000
O	0.84136524	5.35015048	0.00000000
Al	-1.37164552	-1.72502629	0.00000000
O	0.29166409	-0.91584612	0.00000000
Al	1.02206635	-2.69631444	0.00000000
O	2.55278799	-3.18908617	0.00000000

Frequencies -- 31.7, 39.6, 79.0, 109.4, 125.5, 181.3, 188.0, 237.5, 240.9, 279.1, 297.1, 302.9, 374.9, 402.0, 551.0, 583.0, 604.1, 725.3, 760.9, 839.9, 1012.9, 1050.9, 1096.6, 1217.2

(1-17-9) Al<sub>4</sub>O<sub>6</sub>(1)-TS1

O	-0.19862617	1.75234995	1.59836700
O	0.23005288	-1.66138166	1.74028600
Al	0.24749922	-1.72774303	0.00000000

Al	-0.31830137	0.00108413	1.48240900
O	1.09176907	0.16334824	0.00000000
Al	-0.31830137	0.00108413	-1.48240900
O	-1.26958067	-0.49006610	0.00000000
Al	0.45984700	1.81467095	0.00000000
O	-0.19862617	1.75234995	-1.59836700
O	0.23005288	-1.66138166	-1.74028600

Frequencies -- -138.1, 154.7, 215.7, 252.5, 273.6, 316.4, 349.3, 409.5, 437.9, 456.1, 474.8, 487.7, 523.0, 578.7, 601.6, 642.4, 677.2, 679.9, 726.8, 741.6, 757.1, 841.6, 873.6, 899.3

(1-17-10) Al<sub>4</sub>O<sub>6</sub>(1)-TS2

Al	-0.32533586	1.38624107	0.02153100
O	1.94454518	-1.51145686	0.39598828
Al	-2.03316681	-0.38769799	0.07497567
O	-1.35197068	-1.89033696	-0.41810726
O	0.72116134	0.25060713	-0.95982487
O	-2.02470877	1.22059002	-0.51344328
Al	2.33796624	0.03326917	-0.30465761
Al	0.23355421	-1.31192392	0.13814601
O	1.00426003	2.44755910	0.43219624
O	-0.63944100	-0.06178098	1.17694891

Frequencies -- -210.5, 131.6, 179.5, 208.5, 233.7, 278.0, 301.6, 330.5, 346.8, 403.2, 439.4, 481.0, 539.1, 552.4, 589.3, 619.1, 660.9, 701.8, 726.5, 740.7, 745.9, 809.3, 865.9, 904.7

(1-17-11) Al<sub>4</sub>O<sub>6</sub>(1)-TS3

O	0.72103904	-1.40181291	1.46236800
O	-0.68849295	1.56912921	-1.64983900
Al	0.47338878	0.24288159	1.51432600
O	1.10592358	1.03376008	0.00000000
Al	-0.13142207	-2.02747803	0.00000000
O	-1.76195724	-2.09561796	0.00000000
Al	-0.45169919	1.98923809	0.00000000
O	-0.68849295	1.56912921	1.64983900
Al	0.47338878	0.24288159	-1.51432600
O	0.72103904	-1.40181291	-1.46236800

Frequencies -- -103.8, 96.7, 128.2, 206.3, 212.3, 262.9, 296.5, 317.3, 326.5, 389.1, 409.1, 463.7, 517.8, 562.0, 584.8, 624.9, 637.2, 693.0, 728.1, 741.0, 889.6, 961.7, 974.5, 1006.3

(1-17-12) Al<sub>4</sub>O<sub>6</sub>(1)-TS4

Al	-1.22046682	-1.53768417	-0.04949519
O	2.67675396	-0.19123078	0.81094720
Al	-1.80826612	0.85373174	0.11779600
O	-2.29270233	2.48945767	0.22705213
O	-0.59029006	-0.12041219	0.94772199
O	-2.52913490	-0.58346328	-0.59962618
Al	2.72495788	1.11648933	-0.33603268
Al	1.07767605	-0.58184192	0.20209605
O	1.15023396	0.78955320	-0.97988781
O	0.32755027	-2.14128396	-0.29954914

Frequencies -- -104.6, 84.6, 97.1, 142.2, 179.4, 205.4, 264.5, 300.5, 313.8, 352.1, 424.9, 453.0, 521.4, 566.9, 604.0, 618.4, 677.3, 697.6, 738.5, 754.3, 763.7, 817.2, 892.6, 982.5

(1-17-13) Al<sub>4</sub>O<sub>6</sub>(1)-TS5

Al	-1.20474780	1.07893824	0.00000000
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O	0.27311189	-2.49910253	1.26583200
Al	0.61350828	2.65073098	0.00000000
O	1.88899133	3.82392992	0.00000000
O	0.55976874	0.91554547	0.00000000
O	-1.13134309	2.80189320	0.00000000
Al	1.03008057	-3.44848774	0.00000000
Al	-0.46322412	-1.55164446	0.00000000
O	0.27311189	-2.49910253	-1.26583200
O	-1.82401826	-0.47866119	0.00000000

Frequencies -- -106.7, 42.7, 74.0, 79.3, 103.1, 161.6, 174.8, 264.0, 273.9, 333.5, 390.2, 419.4, 480.9, 631.4, 641.9, 661.6, 670.7, 721.5, 755.7, 769.7, 777.7, 867.7, 905.7, 1008.5

(1-17-14) Al<sub>4</sub>O<sub>6</sub>(1)-TS6

O	0.03569409	-2.41092954	0.00000000
O	-0.93291698	3.13641617	0.00000000
Al	-0.44175062	-0.80717960	0.00000000
O	-2.02161058	-0.04073161	0.00000000
Al	0.49711545	-4.02035360	0.00000000
O	0.92368307	-5.56349419	0.00000000
Al	-1.20889679	1.47523396	0.00000000
O	0.38687425	0.72371049	0.00000000
Al	0.77472804	3.39708559	0.00000000
O	2.22383253	4.08225086	0.00000000

Frequencies -- -100.4, 30.7, 36.7, 66.3, 108.3, 149.6, 167.0, 177.9, 234.6, 253.5, 279.6, 291.7, 314.2, 395.6, 546.5, 639.5, 678.7, 751.8, 770.7, 798.5, 990.4, 1045.4, 1134.5, 1218.6

(1-17-15) Al<sub>4</sub>O<sub>6</sub>(1)-TS7

O	-1.70080395	-1.16206419	0.04211385
O	2.84544181	0.86707739	-0.43211001
Al	-0.04617794	-1.28555400	0.19938884
O	1.35507215	-2.04477778	-0.52596322
Al	-2.99516408	-0.06980433	-0.07507007
O	-4.43408317	0.62810450	-0.15731102
Al	2.33657999	-0.70004070	-0.06908112
O	0.96473692	-0.06883993	0.96311092
Al	1.29934272	1.60639717	0.14199704
O	0.00344261	2.51012804	-0.21034689

Frequencies -- -79.2, 43.4, 55.4, 111.7, 158.5, 180.3, 222.5, 231.5, 252.3, 285.7, 322.1, 369.3, 433.6, 449.8, 567.5, 591.7, 633.5, 719.6, 752.0, 795.1, 942.4, 1033.2, 1064.2, 1176.9

(1-18-1) Al<sub>4</sub>O<sub>6</sub>(3)

Al	-0.18213959	-0.24724537	1.42296600
O	-1.10358738	0.26013757	0.00000000
O	0.06141081	-1.92938546	1.45766600
O	0.69212900	1.20203010	1.55139500
Al	0.14136217	-2.86664213	0.00000000
Al	-0.18213959	-0.24724537	-1.42296600
O	0.06141081	-1.92938546	-1.45766600
O	0.69212900	1.20203010	-1.55139500
Al	0.17719596	1.90007485	0.00000000
O	-0.32919550	3.56879244	0.00000000

Frequencies -- 82.5, 107.0, 148.4, 170.1, 210.4, 228.4, 239.2, 287.7, 295.8, 300.7, 367.4, 432.3, 452.1, 589.5, 630.7, 657.6, 691.0, 720.7, 755.3, 815.6, 844.5, 853.1, 948.0, 987.7

(1-18-2) Al<sub>4</sub>O<sub>6</sub>(3)-2

Al	0.50140489	0.37037560	1.33370700
O	1.59302447	0.44674581	0.00000000
O	-0.38675081	1.82672583	1.46769000
O	-0.11838404	-1.22079085	1.46786500
Al	-0.74919257	2.68045622	0.00000000
Al	0.50140489	0.37037560	-1.33370700
O	-0.38675081	1.82672583	-1.46769000
O	-0.11838404	-1.22079085	-1.46786500
Al	-0.25797021	-2.09831696	0.00000000
O	-0.57568116	-3.80831280	0.00000000

Frequencies -- 53.3, 100.4, 122.5, 164.0, 213.4, 235.8, 258.7, 263.0, 269.6, 290.7, 336.8, 421.8, 447.1, 593.4, 636.6, 646.5, 737.6, 761.9, 811.1, 824.8, 884.1, 904.6, 909.9, 956.3

(1-18-3) Al<sub>4</sub>O<sub>6</sub>(3)-3

Al	0.00167497	1.12480104	0.22833404
O	-2.30049418	-1.30036074	-0.58804018
Al	2.22736789	-0.09591407	-0.11843807
O	3.81198885	-0.77188215	-0.32526913
O	0.68654885	-0.83193195	-0.33515913
O	1.68873999	1.45964492	0.36085807
Al	-0.80944320	-1.59364992	0.37309580
Al	-2.29272608	0.36126922	-0.20688203
O	-1.13379809	0.09686303	1.20527795
O	-1.33415499	1.67834421	-0.76634591

Frequencies -- 70.4, 106.6, 136.6, 163.9, 191.4, 235.3, 257.6, 283.8, 335.5, 354.9, 396.9, 467.6, 510.2, 515.6, 570.4, 604.7, 648.2, 668.8, 730.5, 743.5, 832.9, 888.1, 906.5, 953.4

(1-18-4) Al<sub>4</sub>O<sub>6</sub>(3)-4

Al	0.41071350	0.45334709	0.00000000
O	0.01013435	-3.53859965	0.00000000
Al	-0.18996203	2.78045295	0.00000000
O	-0.64372122	4.46326341	0.00000000
O	0.09533642	1.64633748	1.26579100
O	0.09533642	1.64633748	-1.26579100
Al	-1.52628626	-2.66029011	0.00000000
Al	0.88424872	-2.06410821	0.00000000
O	-0.69356211	-1.10856612	0.00000000
O	1.82106601	-0.68655040	0.00000000

Frequencies -- 48.9, 58.5, 96.8, 159.5, 168.3, 181.4, 243.0, 257.1, 283.2, 374.7, 382.9, 466.6, 489.0, 582.1, 590.0, 646.3, 688.4, 713.9, 735.4, 797.1, 813.4, 813.5, 936.7, 1017.8

(1-18-5) Al<sub>4</sub>O<sub>6</sub>(3)-5

O	0.00000000	1.26008400	-2.41634280
O	0.00000000	-1.26008400	-2.41634280
Al	0.00000000	0.00000000	-1.20765680
Al	0.00000000	0.00000000	-3.60821080
O	0.00000000	0.00000000	0.46118520
O	0.00000000	0.00000000	-5.34599880
O	1.26336400	-0.00000000	3.33364420
O	-1.26336400	-0.00000000	3.33364420
Al	0.00000000	0.00000000	4.55573620
Al	0.00000000	0.00000000	2.13718420

Frequencies -- 22.5, 23.4, 25.6, 88.0, 123.6, 178.1, 194.9, 229.7, 256.0, 262.4, 359.4, 390.7,



462.4, 589.5, 641.0, 669.1, 696.0, 740.1, 771.8, 772.8, 805.3, 882.5, 934.9, 1160.2

(1-18-6) Al<sub>4</sub>O<sub>6</sub>(3)-6

Al	-1.45091831	-0.29459715	0.00000000
O	3.08197278	-0.39462222	0.00000000
Al	-3.74881700	0.40144866	0.00000000
O	-5.41362849	0.89928175	0.00000000
O	-2.60767713	0.05581333	-1.26041300
O	-2.60767713	0.05581333	1.26041300
Al	4.46565525	0.54023024	0.00000000
Al	1.71871051	-1.41778187	0.00000000
O	5.80075530	1.42772014	0.00000000
O	0.14623019	-0.79161862	0.00000000

Frequencies -- 13.8, 16.8, 42.6, 45.9, 75.7, 96.5, 167.5, 168.4, 220.6, 228.3, 240.6, 251.2, 338.1, 389.6, 468.2, 564.0, 668.3, 709.4, 804.3, 809.2, 931.8, 978.7, 1117.0, 1199.2

(1-18-7) Al<sub>4</sub>O<sub>6</sub>(3)-TS1

Al	0.29862964	0.28065480	1.38041200
O	1.30570812	-0.06012041	0.00000000
O	-0.15104053	1.92271173	1.46162100
O	-0.55041021	-1.19176831	1.52166600
Al	-0.32283243	2.84225996	0.00000000
Al	0.29862964	0.28065480	-1.38041200
O	-0.15104053	1.92271173	-1.46162100
O	-0.55041021	-1.19176831	-1.52166600
Al	-0.26081917	-1.99063527	0.00000000
O	0.07508086	-3.69778465	0.00000000

Frequencies -- -85.9, 105.7, 113.7, 150.2, 169.0, 230.1, 246.7, 274.8, 289.1, 312.0, 325.1, 427.8, 444.4, 603.6, 636.4, 656.2, 716.9, 775.1, 783.8, 814.9, 861.9, 877.4, 918.8, 963.9

(1-18-8) Al<sub>4</sub>O<sub>6</sub>(3)-TS2

Al	-0.78756908	-1.59663092	0.37621279
O	-1.35918894	1.68328019	-0.76593897
Al	2.21553198	-0.10128602	-0.12144415
O	3.82490395	-0.71989108	-0.31886721
O	0.71617794	-0.90151894	-0.33080618
O	1.66726006	1.45846997	0.34005997
Al	-0.02217395	1.17004105	0.23932797
Al	-2.29719200	0.34418519	-0.21139405
O	-1.11826399	0.09878304	1.19666891
O	-2.28235908	-1.32062578	-0.58050817

Frequencies -- -98.0, 69.3, 134.7, 164.4, 179.1, 227.8, 242.9, 280.9, 335.9, 346.9, 389.4, 469.2, 505.7, 509.6, 570.6, 600.2, 652.3, 670.0, 730.8, 741.4, 847.8, 889.2, 910.2, 961.5

(1-18-9) Al<sub>4</sub>O<sub>6</sub>(3)-TS3

Al	0.31531499	0.76825100	0.16886209
O	-3.01574696	-0.68500484	-0.55737042
Al	2.50415501	-0.21463898	-0.11432489
O	4.08505901	-0.92573397	-0.27723488
O	0.96574206	-0.63195285	-0.77123509
O	1.90943995	1.12315587	0.80366828
Al	-1.81916204	-1.65023701	0.33045152
Al	-2.17071598	0.75642608	-0.17224711
O	-1.10075008	-0.16573113	1.00822982

O                    -0.94183094      1.83809013      -0.55176283  
 Frequencies --    -90.7, 66.6, 102.3, 151.0, 175.9, 230.8, 244.9, 290.5, 305.2, 379.9, 445.9, 467.2,  
 505.3, 582.1, 601.0, 619.6, 678.2, 709.9, 742.1, 745.0, 778.3, 832.1, 933.0, 970.6

(1-18-10) Al<sub>4</sub>O<sub>6</sub>(3)-TS4

Al	-0.70022244	0.74872814	0.00000000
O	-0.28831209	-3.67959799	0.00000000
Al	0.27853259	2.93585312	0.00000000
O	1.00275271	4.51749136	0.00000000
O	-1.70085396	-0.65000228	0.00000000
O	-0.21587708	1.85821531	1.26255100
Al	1.41303682	-3.17119437	0.00000000
Al	-0.71216712	-2.01171075	0.00000000
O	0.96450025	-1.46954543	0.00000000
O	-0.21587708	1.85821531	-1.26255100

Frequencies --    -98.6, 43.5, 49.8, 88.6, 111.4, 174.5, 179.5, 247.7, 259.2, 361.2, 375.5, 433.6,  
 473.2, 607.5, 645.3, 666.9, 697.7, 725.4, 744.8, 764.3, 806.8, 896.7, 943.1, 1000.6

(1-18-11) Al<sub>4</sub>O<sub>6</sub>(3)-TS5

Al	0.65860318	0.71659659	0.00000000
O	0.15591455	-3.42475414	0.00000000
Al	-0.12867215	2.97960704	0.00000000
O	-0.68051807	4.62775198	0.00000000
O	0.27927245	1.85906795	1.26155800
O	0.27927245	1.85906795	-1.26155800
Al	-1.35013038	-2.66324421	0.00000000
Al	1.62175058	-2.51205187	0.00000000
O	-2.61113515	-1.66944636	0.00000000
O	1.27467300	-0.84816215	0.00000000

Frequencies --    -60.1, 29.3, 33.0, 49.1, 107.2, 111.8, 148.2, 169.3, 208.8, 232.1, 268.8, 309.0,  
 353.7, 389.5, 542.2, 628.9, 670.2, 708.0, 805.3, 808.7, 873.2, 930.0, 1090.9, 1153.3

(1-19-X) Al<sub>4</sub>O<sub>7</sub>(1)-X

Al	-4.07111012	0.00000000	-0.00000000
O	2.87647190	-0.90719199	0.87452321
O	2.87647190	0.90719199	-0.87452321
Al	4.07111012	0.00000000	-0.00000000
Al	1.67137688	-0.00000000	0.00000000
O	5.80851988	-0.00000000	-0.00000000
O	0.00000000	0.00000000	0.00000000
Al	-1.67137688	-0.00000000	0.00000000
O	-2.87647190	-0.90719199	-0.87452321
O	-2.87647190	0.90719199	0.87452321
O	-5.80851988	-0.00000000	-0.00000000

Frequencies --    21.8, 21.9, 24.9, 83.5, 84.7, 162.9, 164.0, 206.8, 206.9, 215.4, 268.0, 269.4,  
 390.7, 391.3, 437.1, 554.7, 670.2, 670.2, 677.6, 716.6, 762.0, 804.9, 805.2, 880.6, 928.5, 940.6,  
 1164.6

(1-20-X) Al<sub>4</sub>O<sub>7</sub>(3)-X

O	0.04513924	2.94129747	0.00000000
O	-0.16497038	-2.76230797	1.26019900
O	-0.16497038	-2.76230797	-1.26019900
Al	0.14525677	-1.59877637	0.00000000
O	0.56301418	0.02076738	0.00000000

Al	-0.46804014	-3.91826827	0.00000000
O	-0.90946643	-5.59828016	0.00000000
Al	1.08381377	1.61270777	0.00000000
O	2.78802361	1.94127803	0.00000000
Al	-0.92888000	4.29632270	0.00000000
O	-1.88401426	5.58257623	0.00000000

Frequencies -- 13.8, 17.6, 32.1, 44.0, 63.0, 89.8, 157.8, 161.4, 186.4, 206.1, 236.2, 241.8, 247.6, 319.0, 324.3, 391.1, 457.1, 576.9, 670.9, 708.4, 785.9, 805.1, 854.5, 933.3, 1012.1, 1150.6, 1215.0

(1-21-X) Al<sub>4</sub>O<sub>8</sub>(1)-X

Al	0.00000000	3.99196200	-0.18981690
O	0.00000000	5.70663400	-0.46844090
O	0.00000000	3.01368700	1.24578610
O	0.00000000	2.61007800	-1.24229690
Al	0.00000000	1.63017300	0.19371510
O	-0.80327300	0.00000000	0.45861710
Al	0.00000000	-3.99196200	-0.18981690
O	0.00000000	-5.70663400	-0.46844090
O	0.00000000	-2.61007800	-1.24229690
O	0.00000000	-3.01368700	1.24578610
Al	0.00000000	-1.63017300	0.19371510
O	0.80327300	0.00000000	0.45861710

Frequencies -- 14.5, 42.1, 57.0, 73.1, 118.6, 136.3, 158.3, 173.9, 204.2, 204.5, 205.9, 250.2, 320.1, 381.5, 404.2, 433.4, 531.7, 536.0, 636.9, 676.8, 677.2, 705.6, 725.6, 767.9, 805.5, 813.0, 849.0, 881.6, 940.9, 944.4

(1-22-X) Al<sub>4</sub>O<sub>8</sub>(3)-X

Al	0.00000000	3.99204800	-0.18965305
O	0.00000000	5.70676000	-0.46802605
O	0.00000000	3.01356800	1.24580795
O	0.00000000	2.61031300	-1.24233005
Al	0.00000000	1.63020400	0.19353995
O	-0.80327300	0.00000000	0.45823195
Al	0.00000000	-3.99204800	-0.18965305
O	0.00000000	-5.70676000	-0.46802605
O	0.00000000	-2.61031300	-1.24233005
O	0.00000000	-3.01356800	1.24580795
Al	0.00000000	-1.63020400	0.19353995
O	0.80327300	0.00000000	0.45823195

Frequencies -- 14.5, 42.1, 57.1, 73.1, 118.6, 136.3, 158.3, 173.9, 204.2, 204.5, 205.9, 250.2, 320.1, 381.5, 404.2, 433.4, 531.7, 536.0, 636.9, 676.8, 677.2, 705.6, 725.6, 767.9, 805.5, 813.0, 849.0, 881.6, 940.9, 944.4

(1-23-1) Al<sub>8</sub>O<sub>12</sub>(1)

Al	-2.96066199	0.07431685	0.93584998
O	-2.77907100	1.67595438	0.36106467
O	-3.50973600	-1.09257810	-0.23055107
O	-1.77526297	-0.42724224	2.05352437
Al	-1.22517201	1.73259779	-0.37597139
O	-0.11016302	2.90669225	-1.04938536
O	0.16535301	1.32930283	0.90174692
O	-1.10592702	0.10313412	-1.20514807
Al	-2.22223901	-1.29999397	-1.30962792

O	-0.98447201	-2.32882041	-1.84902810
Al	0.28316999	-1.20386899	-1.34185203
Al	-0.08654998	-0.22051343	1.80780718
O	0.64333401	-1.34979955	0.42937209
Al	1.21227199	2.23149293	-0.21181783
Al	2.13014602	-1.31723375	1.40014404
O	1.33862304	-0.67536365	2.75804753
O	3.47218801	-1.02025956	0.40502579
Al	2.92299499	-0.03509662	-0.90640401
O	1.80090698	-0.70381052	-1.99719845
O	2.75654199	1.64502664	-0.57442837

Frequencies -- 105.1, 108.5, 133.4, 142.1, 152.1, 166.7, 170.1, 185.5, 202.3, 203.6, 214.9, 235.3, 244.6, 266.2, 285.7, 301.3, 304.1, 316.7, 329.4, 341.9, 346.7, 354.1, 365.5, 391.9, 402.3, 405.1, 437.8, 445.3, 478.5, 496.6, 514.0, 552.4, 563.1, 596.1, 643.4, 655.0, 669.1, 698.0, 725.2, 762.8, 770.8, 783.7, 803.5, 809.1, 821.8, 838.0, 846.4, 866.6, 891.1, 913.3, 950.7, 970.0, 988.6, 997.5

(1-23-X) Al<sub>8</sub>O<sub>12</sub>(1)-X

O	1.26795799	1.94038017	1.42630400
O	-1.27563687	3.23763789	1.44659800
Al	-1.65324909	2.40230759	0.00000000
Al	0.44738630	3.43671409	1.34245200
O	-1.04481980	0.76996541	0.00000000
Al	0.44738630	3.43671409	-1.34245200
O	0.91067199	4.42389020	0.00000000
Al	0.98137639	0.98580009	0.00000000
O	1.26795799	1.94038017	-1.42630400
O	-1.27563687	3.23763789	-1.44659800
O	-0.91067199	-4.42389020	0.00000000
O	-1.26795799	-1.94038017	1.42630400
Al	-0.98137639	-0.98580009	0.00000000
Al	-0.44738630	-3.43671409	1.34245200
O	-1.26795799	-1.94038017	-1.42630400
Al	1.65324909	-2.40230759	0.00000000
O	1.27563687	-3.23763789	1.44659800
Al	-0.44738630	-3.43671409	-1.34245200
O	1.27563687	-3.23763789	-1.44659800
O	1.04481980	-0.76996541	0.00000000

Frequencies -- 27.8, 54.3, 107.9, 132.4, 134.3, 153.7, 164.9, 180.4, 214.6, 234.4, 244.6, 250.1, 251.1, 262.5, 271.5, 281.4, 283.9, 314.0, 314.1, 336.7, 349.8, 363.3, 373.7, 384.0, 394.0, 410.2, 412.8, 420.1, 464.4, 466.2, 526.2, 532.4, 621.9, 655.3, 667.6, 677.9, 702.1, 721.1, 747.1, 755.5, 757.0, 766.3, 796.3, 798.6, 831.8, 838.4, 839.6, 841.7, 874.6, 882.0, 885.3, 902.2, 957.1, 958.9

(1-24-1) Al<sub>16</sub>O<sub>24</sub>(1): (b3lyp/6-311g(d,p))

O	0.00000000	0.00000000	4.25805396
Al	0.38014997	-1.31228638	3.17082397
Al	-0.38014997	1.31228638	3.17082397
O	0.00000000	0.00000000	1.73002097
O	-1.93920120	1.90733849	2.68701097
O	1.02427636	2.22309684	2.34494297
O	1.93920120	-1.90733849	2.68701097
O	-1.02427636	-2.22309684	2.34494297
Al	1.43204157	0.88830546	1.08147597
Al	-1.43204157	-0.88830546	1.08147597
Al	0.84648020	3.47250464	0.97112097

Al	-2.19087043	2.19934791	0.98648497
Al	-0.84648020	-3.47250464	0.97112097
Al	2.19087043	-2.19934791	0.98648497
O	-0.91660768	3.40972921	0.60415997
O	0.91660768	-3.40972921	0.60415997
O	1.44266019	2.12533621	-0.12806403
O	-1.44266019	-2.12533621	-0.12806403
O	-2.16112497	0.50762832	0.31903997
O	2.16112497	-0.50762832	0.31903997
O	1.46838339	4.91182379	0.24499997
O	-1.46838339	-4.91182379	0.24499997
Al	1.06061308	4.83933866	-1.44881303
Al	-1.06061308	-4.83933866	-1.44881303
O	-0.64205220	5.02357831	-1.76269403
O	1.77692192	3.63230892	-2.43278503
O	-1.77692192	-3.63230892	-2.43278503
O	0.64205220	-5.02357831	-1.76269403
O	-2.82211743	2.57035597	-0.79493303
Al	-1.36233646	3.57925472	-1.18842603
Al	-2.00752738	0.97655113	-1.48137703
Al	1.36233646	-3.57925472	-1.18842603
Al	-1.28561562	-2.01975656	-1.97760303
O	-1.98987590	-0.47985256	-2.36401203
O	2.82211743	-2.57035597	-0.79493303
O	0.59389263	-2.05094723	-1.89644403
Al	1.28561562	2.01975656	-1.97760303
O	1.98987590	0.47985256	-2.36401203
Al	2.00752738	-0.97655113	-1.48137703
O	-0.59389263	2.05094723	-1.89644403

(2) Al/CO<sub>2</sub> 反应系

(2-1-1) CO

O	0.00000000	0.00000000	0.48298200
C	0.00000000	0.00000000	-0.64397600

Frequencies -- 2220.2

(2-1-2) CO<sub>2</sub>

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16043500
O	-0.00000000	0.00000000	-1.16043500

Frequencies -- 666.5, 666.5, 1375.5, 2435.9

(2-2-1) AlCO<sub>2</sub>

C	0.00000000	0.00000000	-1.14408563
O	0.00000000	1.09655600	-0.52137463
O	0.00000000	-1.09655600	-0.52137463
Al	0.00000000	0.00000000	1.16973137

Frequencies -- 193.1, 317.7, 344.2, 803.0, 1307.1, 1500.6

(2-2-2) AlCO<sub>2</sub>-2

C	-0.11585607	0.73693938	0.00000000
O	0.91480655	-0.04394437	0.00000000
O	-0.33201998	1.89994833	0.00000000
Al	-0.30516585	-1.48228215	0.00000000

Frequencies -- 150.2, 333.4, 411.0, 722.1, 1121.4, 1902.1

(2-2-3) AlCO<sub>2</sub>-3

C	0.40419303	-1.17716904	0.00000000
O	0.01703428	0.08151930	0.00000000
O	-0.23513284	-2.17402162	0.00000000
Al	-0.05233614	1.83100252	0.00000000

Frequencies -- 68.3, 73.0, 466.9, 762.7, 1174.1, 1856.1

(2-2-4) AlCO<sub>2</sub>-adduct-1

C	1.44528514	0.11743992	0.00000000
O	0.51225538	0.81236528	0.00000000
O	2.37719894	-0.56926051	0.00000000
Al	-2.44518042	-0.20380598	0.00000000

Frequencies -- 23.0, 59.4, 650.8, 658.7, 1374.3, 2431.1

(2-2-5) AlCO<sub>2</sub>-TS1

C	0.90074774	-0.24708484	0.00000000
O	-0.05689331	0.65797714	0.00000000
O	2.08033669	-0.15521596	0.00000000
Al	-1.66092565	-0.19535234	0.00000000

Frequencies -- -115.9, 182.9, 481.5, 773.6, 1092.3, 1871.6

(2-2-6) AlCO<sub>2</sub>-TS2

C	-1.12001291	0.39770407	0.00000000
O	0.00895945	1.04138840	0.00000000
O	-1.24535883	-0.80714918	0.00000000
Al	1.27779019	-0.32770294	0.00000000

Frequencies -- -102.6, 264.5, 497.4, 763.2, 1197.4, 1697.4

(2-2-7) AlCO<sub>2</sub>-TS3

C	0.09494667	1.00509041	0.00000000
O	1.08224631	0.34890447	0.00000000
O	-0.69291415	1.86004773	0.00000000
Al	-0.28341056	-1.82324308	0.00000000
Frequencies --	-241.2, 120.0, 382.3, 530.0, 1255.9, 2303.2		

(2-2-8) AlCO<sub>2</sub>-TS4

C	1.25996010	0.19912369	0.00000000
O	0.06872880	0.27396763	0.00000000
O	2.33899716	-0.24541585	0.00000000
Al	-2.06319756	-0.10947356	0.00000000
Frequencies --	-574.7, 70.2, 73.3, 314.4, 1151.8, 2252.8		

(2-2-9) AlCO<sub>2</sub>-TS5

C	-0.52380852	-1.66732586	0.00000000
O	0.44211176	-2.26343785	0.00000000
O	-0.27578525	0.34726373	0.00000000
Al	0.13940300	1.94871909	0.00000000
Frequencies --	-271.5, 52.5, 76.1, 249.2, 843.7, 2131.3		

(2-3-1) Al<sub>2</sub>CO<sub>2</sub>(1)

Al	-0.39651634	2.42878797	0.00000000
Al	-0.11808431	-2.66216772	0.00000000
O	-0.08357342	-0.92170153	0.00000000
C	-0.10483354	0.38890424	0.00000000
O	0.99842462	1.00926545	0.00000000
Frequencies --	37.4, 60.3, 198.0, 324.4, 384.2, 522.2, 839.8, 1321.8, 1456.2		

(2-3-2) Al<sub>2</sub>CO<sub>2</sub>(1)-adduct-1

O	-0.21354336	1.35225967	0.00000000
O	0.42805365	-2.78399494	0.00000000
C	0.61081237	-3.89653041	0.00000000
Al	1.27413572	2.20533631	0.00000000
Al	-1.68805546	0.47413020	0.00000000
Frequencies --	8.2, 14.7, 24.3, 34.8, 110.9, 114.3, 506.1, 984.7, 2215.8		

(2-3-3) Al<sub>2</sub>CO<sub>2</sub>(1)-TS1

C	0.31475741	-0.91361673	0.00000000
O	0.07073876	0.56968610	0.00000000
O	-0.70495655	-1.56072923	0.00000000
Al	-1.78652109	0.69793748	0.00000000
Al	2.03153632	0.33360447	0.00000000
Frequencies --	-211.3, 100.6, 116.5, 287.3, 309.3, 469.6, 519.3, 799.3, 1731.8		

(2-4-1) Al<sub>2</sub>CO<sub>2</sub>(3)

Al	-2.64260349	-0.48319380	0.00000000
O	-1.07145676	0.19018904	0.00000000
Al	0.46969280	0.91448415	0.00000000
C	2.03126249	-0.22186844	0.00000000
O	3.07898976	-0.72463453	0.00000000
Frequencies --	52.5, 107.3, 146.2, 278.9, 340.3, 486.1, 570.3, 1017.4, 1976.5		

(2-4-2) Al<sub>2</sub>CO<sub>2</sub>(3)-2

Al	1.85987887	-0.27809981	-0.14750691
Al	-0.34460322	1.70256425	0.05118648
C	-0.89020057	-0.48191283	0.04284349
O	0.20247699	-1.10424080	0.34164896
O	-1.99714949	-0.84907931	-0.21726088
Frequencies --	70.68, 154.3, 212.8, 228.8, 348.7, 464.6, 727.5, 1124.8, 1807.4		

(2-4-3) Al<sub>2</sub>CO<sub>2</sub>(3)-3

C	0.00000000	0.00000000	0.30932500
O	0.00000000	1.09781000	-0.42825200
O	0.00000000	-1.09781000	-0.42825200
Al	0.00000000	0.00000000	-1.93838500
Al	0.00000000	0.00000000	2.32269900
Frequencies --	124.3, 126.3, 333.6, 387.6871, 444.8, 545.9, 848.9, 1131.0, 1230.1		

(2-4-4) Al<sub>2</sub>CO<sub>2</sub>(3)-4

O	-1.63097211	0.40585741	0.00000000
Al	0.31744443	-2.34455995	0.00000000
Al	0.62410046	2.23108800	0.00000000
C	-0.42296911	0.47346869	0.00000000
O	0.41818849	-0.57656702	0.00000000
Frequencies --	55.8, 92.0, 127.4, 335.7, 524.6, 574.6, 726.3, 1026.6, 1670.0		

(2-4-5) Al<sub>2</sub>CO<sub>2</sub>(3)-5

Al	0.28661530	0.31427676	0.00000000
Al	0.02501350	2.97210979	0.00000000
C	0.09028331	-1.78437930	0.00000000
O	-0.99239182	-1.08292118	0.00000000
O	0.41828254	-2.91917248	0.00000000
Frequencies --	36.9, 44.7, 161.6, 266.7, 391.0, 406.3, 695.7, 1100.2, 1914.0		

(2-4-6) Al<sub>2</sub>CO<sub>2</sub>(3)-adduct-1

Al	0.00000000	1.36869800	-1.87149908
Al	0.00000000	-1.36869800	-1.87149908
C	0.00000000	0.00000000	2.21404292
O	0.00000000	0.00000000	1.05067592
O	0.00000000	0.00000000	3.37116392
Frequencies --	8.7, 15.8, 42.3, 50.3, 262.0, 657.8, 661.4, 1375.4, 2435.4		

(2-4-7) Al<sub>2</sub>CO<sub>2</sub>(3)-TS1

Al	0.23493585	-2.22426593	0.00000000
O	0.72587598	-0.48042614	0.00000000
C	-0.29394246	0.38570506	0.00000000
O	-1.46589182	0.03970239	0.00000000
Al	0.35612426	2.31746283	0.00000000
Frequencies --	-77.1, 92.1, 126.9, 334.9, 543.0, 590.9, 735.7, 1059.2, 1613.6		

(2-4-8) Al<sub>2</sub>CO<sub>2</sub>(3)-TS2

O	0.30105789	-1.86731643	0.00000000
Al	-2.09616536	0.40922170	0.00000000
Al	1.79701223	0.83497478	0.00000000
C	0.65844540	-0.73043292	0.00000000
O	-0.30876810	0.39332184	0.00000000
Frequencies --	-224.8, 83.4, 126.4, 344.5, 427.6, 513.2, 649.3, 689.4, 1760.6		



(2-4-9) Al<sub>2</sub>CO<sub>2</sub>(3)-TS3

O	1.04132699	1.68226902	-0.20859503
Al	-2.16132420	-0.39236069	-0.16350874
Al	1.67956274	-1.15075005	-0.02469023
C	0.56890592	0.61278505	0.06675498
O	-0.68514406	0.36569715	0.46435212
Frequencies --	-101.6, 80.6, 146.9, 314.4, 479.3, 508.3, 754.7, 1003.0, 1723.1		

(2-4-10) Al<sub>2</sub>CO<sub>2</sub>(3)-TS4

Al	-0.28969853	1.09954782	-0.34008802
Al	-2.43446686	-0.62233304	0.12501174
C	1.37339529	-0.32802000	-0.06391505
O	1.35491956	0.76491164	0.59864797
O	2.04180273	-1.29437066	-0.20121273
Frequencies --	-33.0, 61.2, 168.9, 192.4, 358.9, 378.0, 700.6, 1123.4, 1915.0		

(2-4-11) Al<sub>2</sub>CO<sub>2</sub>(3)-TS5

Al	1.53971188	-1.07900644	-0.30093972
Al	0.85769745	1.58727978	0.07888574
C	-1.31309494	-0.18241974	0.06450897
O	-0.64505411	-0.77349973	0.87271012
O	-2.26591485	0.08437036	-0.56025413
Frequencies --	-306.5, 65.3, 80.6, 130.9, 242.7, 362.6, 421.9, 1186.5, 2174.9		

(2-4-12) Al<sub>2</sub>CO<sub>2</sub>(3)-TS6

Al	0.36114846	0.96260509	0.00000000
Al	2.71805375	-0.30901049	0.00000000
C	-1.74575688	-0.22092693	0.00000000
O	-0.82626059	-1.00903404	0.00000000
O	-2.86812533	0.11263802	0.00000000
Frequencies --	-257.9, 29.9, 39.0, 135.1, 281.3, 473.7, 493.5, 1191.0, 2155.9		

(2-5-1) Al<sub>2</sub>CO<sub>3</sub>(1)

Al	0.00000000	0.00000000	3.01206205
Al	0.00000000	0.00000000	-0.38615695
O	0.00000000	0.00000000	1.28366805
O	0.00000000	1.08404900	-1.80551495
O	0.00000000	-1.08404900	-1.80551495
C	0.00000000	0.00000000	-2.58631195
Frequencies --	59.0, 60.7, 154.0, 211.2, 348.6, 407.5, 554.8, 652.1, 916.0, 1050.9, 1121.7, 1125.1		

(2-5-2) Al<sub>2</sub>CO<sub>3</sub>(1)-adduct-1

C	3.09416231	-0.39199505	0.00000000
O	-2.01988704	0.26988923	0.00000000
O	1.98348828	-0.73207500	0.00000000
O	4.20300398	-0.05355189	0.00000000
Al	-3.13794087	-1.03032860	0.00000000
Al	-0.85419879	1.52862641	0.00000000
Frequencies --	5.2, 11.5, 18.0, 46.0, 110.7, 118.5, 506.9, 664.4, 665.2, 985.5, 1375.2, 2433.1		

(2-5-3) Al<sub>2</sub>CO<sub>3</sub>(1)-adduct-2

C	2.71431199	0.39323324	-0.39272905
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O	3.45311911	-0.41530161	-0.13006491
Al	-0.62373309	1.14198595	0.32129588
Al	-1.46988980	-1.09833426	-0.15963466
O	-1.84696303	0.51054257	-0.76641897
O	-0.23975286	-0.46109988	0.92833119

Frequencies -- 13.0 26.7, 45.7, 55.7, 118.9, 307.9, 512.7, 551.7, 614.0, 749.3, 785.8, 2223.6

(2-5-4) Al<sub>2</sub>CO<sub>3</sub>(1)-TS1

Al	-2.87505884	0.12866233	-0.41733722
Al	0.27246416	-0.16053741	0.88597526
O	-1.29785684	-0.02059652	0.24958503
O	2.15067211	1.10671806	-0.11516278
O	1.68545321	-1.04938548	-0.43850629
C	2.25459716	0.02008127	-0.60993702

Frequencies -- -302.6, 27.3, 59.4, 86.3, 132.9, 170.6, 482.0, 536.0, 698.8, 997.0, 1289.6, 1910.8

(2-5-5) Al<sub>2</sub>CO<sub>3</sub>(1)-TS2

Al	1.58605409	-0.72266297	-0.19141265
Al	-0.30680500	0.92005314	0.35741469
O	1.24684804	1.05822998	-0.31226022
O	-0.14498797	-0.81476476	0.66819624
O	-1.93802192	0.18192384	-0.43062721
C	-1.65682389	-0.99486410	-0.26008283

Frequencies -- -416.9, 118.0, 199.9, 229.3, 326.6, 395.2, 471.5, 538.6, 645.8, 758.0, 841.0, 1579.1

(2-6-1) Al<sub>2</sub>CO<sub>4</sub>(1)

C	0.00000000	0.00000000	-2.11549592
O	0.00000000	0.00000000	-3.30149792
O	0.00000000	1.10870700	-1.28374392
O	0.00000000	-1.10870700	-1.28374392
Al	0.00000000	0.00000000	0.06629608
O	0.00000000	0.00000000	1.72851108
Al	0.00000000	0.00000000	3.45807108

Frequencies -- 53.4, 54.4, 142.6, 220.6, 290.9, 351.4, 525.3, 657.1, 683.0, 801.6, 889.0, 912.0, 1070.6, 1100.6, 1904.5

(2-6-2) Al<sub>2</sub>CO<sub>4</sub>(1)-2

Al	3.24665126	0.31400966	0.00000000
O	1.61907105	-0.44525316	0.00000000
O	-0.49816789	-1.22467580	0.00000000
C	0.34836652	-0.25888512	0.00000000
O	-0.18249804	0.91999681	0.00000000
Al	-1.86403898	0.07188711	0.00000000
O	-3.44642497	0.31701373	0.00000000

Frequencies -- 37.5, 51.3, 126.2, 187.0, 268.9, 343.8, 383.3, 504.7, 660.3, 833.1, 853.8, 1110.2, 1122.0, 1465.0, 1574.6

(2-6-3) Al<sub>2</sub>CO<sub>4</sub>(1)-3

O	0.19047411	0.76421447	0.00000000
C	-0.84513742	-2.30190263	0.00000000
O	-1.37932931	-3.29965186	0.00000000
Al	-0.10432685	2.41091154	0.00000000
O	-0.41612671	3.98159112	0.00000000

Al	0.57282181	-0.87343974	0.00000000
O	1.47753066	-2.21811844	0.00000000

Frequencies -- 38.7, 54.9, 87.3, 168.7, 187.9, 244.4, 267.8, 317.8, 344.6, 365.8, 502.6, 935.8, 1118.0, 1225.4, 2181.9

(2-6-4) Al<sub>2</sub>CO<sub>4</sub>(1)-4

O	-0.08694975	-0.89348621	0.00000000
C	-0.20573192	2.70453075	0.00000000
O	-0.48515357	3.84787337	0.00000000
Al	-0.03886947	-2.57039020	0.00000000
O	-0.01537453	-4.17122931	0.00000000
Al	-0.14111022	0.78568873	0.00000000
O	1.03424378	2.08858399	0.00000000

Frequencies -- 39.5, 42.7, 132.3 136.9, 235.2, 238.2, 310.8, 414.3, 430.0, 631.8, 714.2, 958.9, 1037.8, 1206.9, 1921.5

(2-6-5) Al<sub>2</sub>CO<sub>4</sub>(1)-5

O	0.00000000	1.08126500	-0.42437402
C	0.00000000	0.00000000	0.25621998
O	0.00000000	-1.08126500	-0.42437402
Al	0.00000000	0.00000000	-2.01365402
O	0.00000000	0.00000000	-3.61195402
Al	0.00000000	0.00000000	2.26426698
O	0.00000000	0.00000000	3.86129098

Frequencies -- 57.0, 70.9, 132.3, 168.1, 226.4, 235.9, 287.6, 359.6, 476.3, 571.0, 910.3, 1112.3, 1119.3, 1406.2, 1457.2

(2-6-6) Al<sub>2</sub>CO<sub>4</sub>(1)-adduct-1

Al	0.00000000	-1.22202500	1.39403850
Al	-0.00000000	1.22202500	1.39403850
O	0.00000000	0.00000000	0.12829350
O	0.00000000	0.00000000	2.65452050
C	0.00000000	0.00000000	-2.63519750
O	0.00000000	-1.16034000	-2.66852050
O	-0.00000000	1.16034000	-2.66852050

Frequencies -- 13.4, 20.4, 27.9, 76.8, 127.5, 298.2, 516.4, 615.6, 630.9, 641.7, 672.4, 747.4, 787.6, 1373.7, 2430.8

(2-6-7) Al<sub>2</sub>CO<sub>4</sub>(1)-TS1

Al	-1.38707389	-1.17803707	-0.16643712
Al	-0.54954494	1.12070597	0.40088480
O	0.00994315	-0.57124700	0.78710779
O	-1.87864297	0.46492490	-0.52491911
C	1.68051507	-0.02683595	-0.13779532
O	2.46117111	-0.87895992	-0.11896435
O	1.29414801	1.09857203	-0.42085531

Frequencies -- -285.6, 92.3, 129.7, 190.5, 331.6, 348.2, 485.3, 522.5, 634.0, 656.5, 675.8, 725.7, 770.2, 1237.0, 2211.9

(2-6-8) Al<sub>2</sub>CO<sub>4</sub>(1)-TS2

Al	-0.62855032	-1.07492278	0.00000000
Al	-1.04700162	1.99712750	0.00000000
O	-2.23346033	-1.17355730	0.00000000
O	1.15151781	-1.35852292	0.00000000

O	2.51253136	0.48745050	0.00000000
C	1.48108255	-0.08263795	0.00000000
O	0.18137115	0.60802552	0.00000000

Frequencies -- -92.1, 72.8, 114.6, 191.5, 261.7, 337.4, 397.5, 483.0, 613.4, 775.9, 798.3, 828.8, 1106.0, 1136.2, 1952.7

(2-6-9) Al<sub>2</sub>CO<sub>4</sub>(1)-TS3

O	0.14731914	0.82374101	0.00000000
C	-0.65750610	-2.45256880	0.00000000
O	-1.10639066	-3.50426632	0.00000000
Al	-0.09621019	2.48090028	0.00000000
O	-0.34586720	4.06233054	0.00000000
Al	0.40998894	-0.83301765	0.00000000
O	1.28817783	-2.22018790	0.00000000

Frequencies -- -122.5, 44.7, 53.6, 164.2, 184.2, 246.1, 275.1, 345.3, 351.0, 404.7, 579.8, 928.6, 1100.1, 1221.9, 2110.7

(2-6-10) Al<sub>2</sub>CO<sub>4</sub>(1)-TS4

O	-0.09306049	0.46293002	0.00000000
C	-0.28560108	-1.16891382	0.00000000
O	0.80422622	-1.65227727	0.00000000
Al	1.69164173	0.30073531	0.00000000
O	3.20698422	0.80119114	0.00000000
Al	-1.86719022	0.15024656	0.00000000
O	-3.41868285	0.53199593	0.00000000

Frequencies -- -334.5, 71.1, 114.0, 145.3, 165.6, 207.3, 242.6, 316.1, 371.8, 483.9, 585.3, 850.4, 1127.4, 1133.9, 1806.5

(2-6-11) Al<sub>2</sub>CO<sub>4</sub>(1)-TS5

Al	-0.47231840	2.49489253	0.00000000
O	1.13127137	2.15420192	0.00000000
O	-0.17387520	-0.19112903	1.08616800
C	-0.23867480	0.47187871	0.00000000
O	-0.17387520	-0.19112903	-1.08616800
Al	0.01569836	-1.74621043	0.00000000
O	0.13749270	-3.34246129	0.00000000

Frequencies -- -322.1, 69.6, 127.7, 158.3, 210.3, 222.8, 299.5, 393.9, 494.6, 558.1, 886.8, 980.0, 1101.0, 1317.7, 1452.0

(3) Al/H<sub>2</sub>O 反应系

(3-1-1) H<sub>2</sub>

H	0.00000000	0.00000000	0.37208700
H	-0.00000000	0.00000000	-0.37208700
Frequencies --	4419.2		

(3-1-2) OH

O	0.00000000	0.00000000	0.10835644
H	0.00000000	0.00000000	-0.86685156
Frequencies --	3702.9		

(3-1-3) H<sub>2</sub>O

O	0.00000000	0.00000000	0.11869660
H	0.00000000	0.75707300	-0.47478640
H	0.00000000	-0.75707300	-0.47478640
Frequencies --	1638.5, 3810.0, 3907.0		

(3-2-1) AlOH(1)

Al	0.00000000	0.00000000	0.73095886
O	0.00000000	0.00000000	-0.94989614
H	0.00000000	0.00000000	-1.90329614
Frequencies --	150.2, 150.2, 844.4, 3990.7		

(3-2-2) AlOH(3)

Al	-0.01549394	-0.72673805	0.00000000
O	0.11465538	0.99587533	0.00000000
H	-0.71582191	1.48059197	0.00000000
Frequencies --	718.0, 808.9, 3863.5		

(3-2-3) AlOH(3)-2

Al	0.14061968	-0.60445403	0.00000000
O	-0.06504660	1.14480603	0.00000000
H	-1.30768307	-1.30054579	0.00000000
Frequencies --	480.5, 754.2, 1786.0		

(3-2-4) AlOH(3)-adduct1

H	6.21600663	-0.78999720	0.00000000
Al	-0.56556290	-0.52163385	0.00000000
O	0.14203888	0.94640466	0.00000000
Frequencies --	4.0, 8.5, 952.5		

(3-2-5) AlOH(3)-TS1

Al	0.02727696	-0.67459491	0.00000000
O	0.10500980	1.03065330	0.00000000
H	-1.19467890	0.52450742	0.00000000
Frequencies --	-1613.9, 804.2, 1512.9		

(3-2-6) AlOH(3)-TS2

H	4.72015807	0.87981117	0.00000000
Al	-0.00524159	-0.62264299	0.00000000
O	-0.58150217	0.90181847	0.00000000
Frequencies --	-15.9, 10.7, 952.3		

(3-3-1) AlO<sub>2</sub>H(1)

Al	0.00048536	0.09689962	0.00000000
O	0.01466517	1.69890469	0.00000000
O	-0.08504452	-1.57142793	0.00000000
H	0.55672511	-2.27950911	0.00000000
Frequencies --	200.4, 207.3, 445.4, 778.8, 1177.3, 3968.0		

(3-3-2) AlO<sub>2</sub>H(3)

Al	0.05525590	0.53310604	0.00000000
O	1.54202795	-0.42625862	0.00000000
O	-1.34891739	-0.42269326	0.00000000
H	-2.26321110	-0.13876349	0.00000000
Frequencies --	196.3, 208.1, 515.8, 710.6, 867.1, 3938.5		

(3-3-3) AlO<sub>2</sub>H(3)-2

Al	0.06290894	0.55360913	0.00000000
O	1.50789550	-0.46298572	0.00000000
O	-1.41364057	-0.28301780	0.00000000
H	-1.57185565	-1.22889050	0.00000000
Frequencies --	191.8, 215.8, 509.3, 723.4, 859.6, 3906.1		

(3-3-4) AlO<sub>2</sub>H(3)-3

H	0.00000000	0.00000000	1.98064413
O	0.00000000	1.50091900	-0.46160187
Al	0.00000000	0.00000000	0.41576813
O	0.00000000	-1.50091900	-0.46160187
Frequencies --	200.0, 443.0, 529.6, 718.4, 855.8, 1991.9		

(3-3-5) AlO<sub>2</sub>H(3)-TS1

Al	0.06591690	0.53968342	0.01785597
O	1.52317420	-0.45594279	-0.00049932
O	-1.38049799	-0.33133637	-0.09409961
H	-1.99832935	-0.71765119	0.52466389
Frequencies --	-252.1, 200.9, 390.2, 713.5, 867.4, 3956.8		

(3-3-6) AlO<sub>2</sub>H(3)-TS2

H	-1.27804452	1.23453612	0.00000000
O	1.71338273	-0.17900200	0.00000000
Al	0.01201126	0.21070706	0.00000000
O	-1.57314546	-0.31771399	0.00000000
Frequencies --	-1169.9, 215.5, 270.8, 680.5, 939.7, 1718.7		

(3-4-1) AlO<sub>3</sub>H(1)

O	0.83257512	-1.26807311	0.00000000
O	-0.81654337	-1.27318925	0.00000000
Al	0.00116153	0.21282783	0.00000000
O	-0.08955198	1.87493770	0.00000000
H	0.57306191	2.56383540	0.00000000
Frequencies --	179.7, 215.1, 224.6, 471.9, 545.8, 762.6, 776.6, 1109.0, 3967.2		

(3-4-2) AlO<sub>3</sub>H(1)-2

Al	0.43849621	0.10775810	-0.02424902
H	-1.82644779	-0.95239402	0.69266981
O	-1.17778976	0.80511214	0.02253125
O	2.01829021	-0.14561697	0.03278683
O	-1.32475082	-0.71555282	-0.10249715
Frequencies --	186.1, 197.6, 327.0, 584.9, 647.4, 815.7, 1141.2, 1184.5, 3758.2		

(3-4-3) AlO<sub>3</sub>H(1)-TS1

O	1.34997179	-0.38522146	0.31917293
O	0.72396411	0.97709092	-0.19895545
Al	-0.25709821	-0.58944086	-0.23746628
O	-1.60247107	0.23566019	0.23184404
H	-0.42944191	1.04249393	0.27056951
Frequencies --	-1587.6, 224.3, 372.8, 567.6, 643.7, 835.1, 1024.1, 1254.7, 1946.1		

(3-4-4) AlO<sub>3</sub>H(3)

O	1.64653187	0.52398524	0.00000000
O	-1.18071289	1.32573282	0.00000000
Al	-0.01137201	0.02518781	0.00000000
O	-0.46112624	-1.59522548	0.00000000
H	0.11029421	-2.36338222	0.00000000
Frequencies --	172.1, 221.4, 257.7, 339.2, 561.6, 666.2, 842.0, 941.8, 3940.5		

(3-4-5) AlO<sub>3</sub>H(3)-2

O	0.22155412	-1.24852808	0.67864100
O	0.47981064	1.65295145	0.00000000
Al	-0.58357262	0.32174933	0.00000000
O	0.22155412	-1.24852808	-0.67864100
H	0.20309295	2.57009644	0.00000000
Frequencies --	139.4, 204.0, 255.6, 405.7, 546.6, 597.8, 845.5, 1149.2, 3928.7		

(3-4-6) AlO<sub>3</sub>H(3)-adduct1

O	2.25009413	0.49872291	0.00000000
O	-0.93002886	0.27122574	0.00000000
Al	-2.55008329	-0.17219376	0.00000000
O	2.82626735	-0.55978895	0.00000000
H	-0.01957815	0.55724126	0.00000000
Frequencies --	17.7, 28.0, 51.6, 85.9, 225.8, 255.0, 849.7, 1639.6, 3972.5		

(3-4-7) AlO<sub>3</sub>H(3)-adduct2

Al	-0.99280983	0.07889388	0.00000000
O	0.56824488	0.65868463	0.00000000
H	1.45221854	0.28159684	0.00000000
O	-2.51576102	-0.42068248	0.00000000
O	3.37930481	-0.40140431	0.00000000
Frequencies --	33.8, 129.3, 205.1, 215.6, 290.5, 497.5, 790.1, 1180.8, 3852.3		

(3-4-8) AlO<sub>3</sub>H(3)-TS1

O	1.82519729	0.58481134	-0.21453466
O	-1.39650379	0.86787411	0.11213579
Al	-0.90329064	-0.73973485	-0.12035618
O	1.31274027	-0.42546771	0.29236121

H	-2.18869181	1.39881106	0.04493167
Frequencies --	-180.7, 46.9, 116.6, 222.2, 268.0, 316.3, 826.2, 1343.7, 3954.6		

(3-4-9) AlO<sub>3</sub>H(3)-TS2

O	1.35117721	-0.68918953	-0.24552632
O	-1.78687298	0.18502177	-0.25046387
Al	-0.24654890	-0.23896221	0.31074691
O	1.16140784	0.92691929	-0.00389039
H	-2.60056088	-0.27550353	-0.04066515
Frequencies --	-1257.1, 130.3, 221.8, 265.0, 485.1, 581.2, 697.9, 948.4, 3926.4		

(3-4-10) AlO<sub>3</sub>H(3)-TS3

Al	0.19532713	0.75530282	0.00000000
O	1.35849169	-0.45651364	0.00000000
H	1.12545965	-1.38901713	0.00000000
O	-0.90079105	1.92741054	0.00000000
O	-0.91578969	-2.52463685	0.00000000
Frequencies --	-73.6, 100.7, 180.2, 207.8, 311.3, 604.2, 771.1, 1150.7, 3869.4		

(3-5-1) Al<sub>2</sub>OH

Al	0.11545754	-1.63414714	0.00000000
O	0.01866988	0.06988540	0.00000000
H	-1.27100200	-2.45272913	0.00000000
Al	-0.02917731	1.77981221	0.00000000
Frequencies --	101.9, 111.9, 504.6, 597.0, 1011.0, 1765.4		

(3-5-2) Al<sub>2</sub>OH-2

O	0.00000000	0.00000000	0.89344891
Al	0.00000000	1.45406600	-0.34637009
H	0.00000000	0.00000000	1.85803091
Al	0.00000000	-1.45406600	-0.34637009
Frequencies --	192.6, 374.4, 418.9, 509.7, 773.5, 3794.0		

(3-5-3) Al<sub>2</sub>OH-3

H	0.82842084	2.83471291	0.00000000
Al	-0.18729792	0.57045887	0.00000000
Al	0.07954611	-2.17218801	0.00000000
O	0.07154408	2.24847074	0.00000000
Frequencies --	43.7, 88.9, 210.0, 386.5, 841.5, 3930.9		

(3-5-4) Al<sub>2</sub>OH-TS1

Al	1.86271287	0.15580654	0.00436891
Al	-0.84045523	-0.78073417	0.00349157
O	-1.38801405	0.85450691	-0.04561883
H	-2.18523700	1.28800388	0.26276434
Frequencies --	-174.9, 121.3, 268.7, 398.9, 768.2, 3909.3		

(3-5-5) Al<sub>2</sub>OH-TS2

O	0.07123288	0.15393426	0.00000000
Al	1.82188244	-0.08226954	0.00000000
H	-0.54029530	1.21923592	0.00000000
Al	-1.82415688	-0.10624662	0.00000000



Frequencies -- -1315.0, 149.6, 177.9, 422.3, 686.1, 1294.3

(3-6-1) Al<sub>2</sub>O<sub>2</sub>H

O	0.00000000	1.26365200	0.05889116
Al	0.00000000	0.00000000	-1.14525284
H	0.00000000	0.00000000	-2.70610284
O	0.00000000	-1.26365200	0.05889116
Al	0.00000000	0.00000000	1.28093316

Frequencies -- 268.4, 493.5, 521.7, 559.8, 647.9, 736.9, 774.6, 795.6, 2018.2

(3-6-2) Al<sub>2</sub>O<sub>2</sub>H-2

O	0.70375833	-2.17881594	0.00000000
Al	-0.58336745	-1.05040060	0.00000000
H	0.56391713	-3.12755670	0.00000000
O	-0.22298408	0.61223752	0.00000000
Al	0.24412813	2.25503015	0.00000000

Frequencies -- 65.0, 106.7, 246.6, 328.3, 501.0, 605.7, 817.1, 1024.2, 3910.7

(3-6-3) Al<sub>2</sub>O<sub>2</sub>H-3

Al	-0.20563123	2.27673346	0.00000000
Al	0.58267023	-1.04338527	0.00000000
O	0.11741077	0.59931319	0.00000000
O	-0.54295966	-2.32605814	0.00000000
H	-1.49711591	-2.21956689	0.00000000

Frequencies -- 75.5, 99.9, 225.6, 312.2, 482.7, 593.1, 834.4, 1013.8, 3885.2

(3-6-4) Al<sub>2</sub>O<sub>2</sub>H-4

O	0.00000000	0.00000000	1.24773874
Al	0.00000000	1.35599000	-0.10092726
H	0.00000000	0.00000000	2.21021674
O	0.00000000	0.00000000	-1.19600226
Al	0.00000000	-1.35599000	-0.10092726

Frequencies -- 201.2, 240.9, 370.3, 417.2, 543.1, 674.5, 735.0, 802.3, 3855.5

(3-6-5) Al<sub>2</sub>O<sub>2</sub>H-5

O	-0.86597638	-2.19757524	0.00000000
Al	0.48095237	-1.09638214	0.00000000
H	1.90188666	-1.75538472	0.00000000
O	0.17124736	0.56531585	0.00000000
Al	-0.19972580	2.23587905	0.00000000

Frequencies -- 67.1, 104.4, 221.3, 477.0, 504.6, 607.3, 803.0, 1035.8, 1989.5

(3-6-6) Al<sub>2</sub>O<sub>2</sub>H-TS1

Al	-2.27608420	0.23094601	-0.00812848
Al	1.04067877	-0.57296211	0.01085551
O	-0.61623222	-0.16894306	0.02477052
O	2.27662082	0.58665988	-0.09577809
H	2.77716179	1.10447469	0.53260908

Frequencies -- -322.5, 69.6, 105.4, 247.9, 387.3, 502.7, 839.1, 1017.3, 3954.6

(3-6-7) Al<sub>2</sub>O<sub>2</sub>H-TS2

O	-0.72900313	-1.20321951	0.00000000
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Al	-1.20728550	0.49223632	0.00000000
H	-1.21621680	-2.03054798	0.00000000
O	0.39764916	1.09205303	0.00000000
Al	1.50475078	-0.26763019	0.00000000

Frequencies -- -149.8, 179.7, 338.7, 374.5, 675.2, 685.7, 709.5, 796.1, 3890.8

(3-6-8) Al<sub>2</sub>O<sub>2</sub>H-TS3

O	-1.11069139	-1.31814748	0.00000000
Al	-1.16353853	0.41131589	0.00000000
H	-2.45548497	1.28944820	0.00000000
O	0.47542905	0.90095799	0.00000000
Al	1.74335266	-0.25377221	0.00000000

Frequencies -- -153.6, 142.5, 249.5, 484.0, 562.6, 687.9, 785.2, 883.9, 2010.2

(3-6-9) Al<sub>2</sub>O<sub>2</sub>H-TS4

O	-0.43498083	-2.54548435	0.00000000
Al	0.24290051	-1.01673143	0.00000000
H	1.12647563	-2.41013001	0.00000000
O	0.07527146	0.65518354	0.00000000
Al	-0.10819288	2.36538808	0.00000000

Frequencies -- -1176.9, 71.8, 92.8, 242.5, 288.0, 468.5, 868.3, 1076.2, 1712.8

(3-6-10) Al<sub>2</sub>O<sub>2</sub>H-TS5

O	-0.08621525	1.26449796	-0.07691328
Al	-1.20530791	-0.18436228	-0.02001988
H	-1.44726222	1.35640178	0.53743181
O	0.14117234	-1.26887997	0.00248523
Al	1.28281603	0.08272030	0.02448085

Frequencies -- -1529.8, 222.0, 280.7, 459.4, 483.7, 653.4, 663.4, 779.8, 1686.8

(3-7-1) Al<sub>2</sub>O<sub>3</sub>H

O	1.26238306	-0.53877197	0.00000000
O	0.08833296	2.36628164	0.00000000
Al	-0.02482358	-1.73319989	0.00000000
Al	0.02414873	0.68367268	0.00000000
O	-1.26589301	-0.49093481	0.00000000
H	-0.66981095	2.95125476	0.00000000

Frequencies -- 148.6, 200.4, 297.5, 352.0, 457.3, 582.2, 641.8, 698.2, 764.4, 774.7, 982.3, 3937.7

(3-7-2) Al<sub>2</sub>O<sub>3</sub>H-2

Al	0.00000000	0.00000000	1.61414776
Al	0.00000000	0.00000000	-0.79220024
O	0.00000000	1.25997900	0.39915876
O	0.00000000	-1.25997900	0.39915876
O	0.00000000	0.00000000	-2.53035524
H	0.00000000	0.00000000	3.17098376

Frequencies -- 136.7, 183.4, 335.0, 455.8, 494.0, 571.0, 665.9, 693.3, 780.5, 812.2, 934.6, 2038.0

(3-7-3) Al<sub>2</sub>O<sub>3</sub>H-3

Al	0.06173670	-2.57459784	0.00000000
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O	-1.56182350	1.65991784	0.00000000
O	-0.03556186	-0.86695967	0.00000000
Al	-0.03998761	0.81577163	0.00000000
O	1.38266307	1.72947644	0.00000000
H	1.43504013	2.68526399	0.00000000
Frequencies --	56.3, 81.5, 180.9, 257.0, 291.8, 294.1, 479.1, 589.1, 781.7, 895.1, 1062.4, 3940.5		

(3-7-4) Al<sub>2</sub>O<sub>3</sub>H-4

Al	-0.06445066	-2.56257590	0.00000000
O	1.64068894	1.50707522	0.00000000
O	-0.09032644	-0.85187540	0.00000000
Al	0.03682425	0.83102764	0.00000000
O	-1.23428202	1.94105338	0.00000000
H	-2.16950059	1.74010180	0.00000000
Frequencies --	60.6, 82.3, 196.5, 244.4, 264.7, 292.6, 469.8, 580.6, 767.8, 921.4, 1053.3, 3949.8		

(3-7-5) Al<sub>2</sub>O<sub>3</sub>H-5

Al	1.75935992	-0.03433020	0.00000000
Al	-0.88584109	-0.18646105	0.00000000
O	0.47040899	1.22976388	0.00000000
O	0.54011985	-1.21971613	0.00000000
O	-2.47457207	0.07570004	0.00000000
H	0.35660104	2.18430388	0.00000000
Frequencies --	128.6, 188.4, 305.1, 333.4, 412.7, 419.1, 649.7, 670.6, 810.4, 840.6, 1083.0, 3883.3		

(3-7-6) Al<sub>2</sub>O<sub>3</sub>H-6

Al	1.63411171	-0.01461615	0.00000000
Al	-1.68548396	0.56467153	0.00000000
O	0.00283296	0.33050778	0.00000000
O	3.21133417	-0.30400770	0.00000000
O	-2.67631217	-0.81851955	0.00000000
H	-3.63500048	-0.81456416	0.00000000
Frequencies --	41.5, 72.4, 184.9, 228.8, 264.1, 325.6, 464.4, 578.3, 832.1, 986.6, 1202.3, 3919.0		

(3-7-7) Al<sub>2</sub>O<sub>3</sub>H-7

Al	1.65867290	-0.03310811	0.00000000
Al	-1.66098487	0.55996998	0.00000000
O	0.00017180	0.14859582	0.00000000
O	3.25236603	-0.21043114	0.00000000
O	-2.89701316	-0.59985526	0.00000000
H	-2.81414180	-1.55567968	0.00000000
Frequencies --	49.3, 65.4, 184.8, 222.8, 241.5, 298.0, 445.3, 554.9, 851.0, 978.8, 1198.9, 3899.4		

(3-7-8) Al<sub>2</sub>O<sub>3</sub>H-8

Al	1.61092613	-0.00597854	0.00000000
O	-2.68051517	-0.98873778	0.00000000
O	-0.03527198	0.26559003	0.00000000

O	3.19549542	-0.24415995	0.00000000
Al	-1.71847331	0.45948406	0.00000000
H	-2.43955285	1.84288970	0.00000000
Frequencies --	50.5, 78.1, 176.0, 228.9, 256.2, 470.0, 475.2, 605.0, 811.2, 1001.5, 1211.6, 2018.6		

(3-7-9) Al<sub>2</sub>O<sub>3</sub>H-9

Al	-1.09322459	0.12117922	0.00000000
O	-0.16849550	-0.82795804	1.15696000
O	-0.02873969	1.46250051	0.00000000
O	-0.16849550	-0.82795804	-1.15696000
Al	1.11330431	0.00491049	0.00000000
H	2.66480902	-0.09184176	0.00000000
Frequencies --	273.0, 281.0, 337.4, 388.1, 514.7, 532.9, 564.0, 618.1, 636.9, 776.7, 821.2, 2041.2		

(3-7-10) Al<sub>2</sub>O<sub>3</sub>H-10

Al	-1.29263253	0.20116492	0.00000000
O	-0.03945446	-1.04686422	0.78191000
O	-0.05494681	1.43229323	0.00000000
O	-0.03945446	-1.04686422	-0.78191000
Al	1.16586337	0.19453315	0.00000000
H	2.71884481	0.14740685	0.00000000
Frequencies --	259.7, 307.1, 442.0, 473.5, 473.5, 523.1, 541.0, 603.0, 738.3, 789.3, 820.7, 2048.0		

(3-7-11) Al<sub>2</sub>O<sub>3</sub>H-11

Al	-1.41263594	0.46600763	0.00000000
O	0.58125885	-1.33388732	0.00000000
O	0.05878013	1.36271476	0.00000000
O	-0.89761778	-1.22071177	0.00000000
Al	1.34863480	0.23434289	0.00000000
H	2.89264524	0.43051781	0.00000000
Frequencies --	171.1, 227.9, 354.0, 397.0, 477.8, 570.7, 667.7, 712.9, 759.4, 853.4, 901.3, 2037.0		

(3-7-12) Al<sub>2</sub>O<sub>3</sub>H-12

Al	-1.00488091	-0.69247544	0.00000000
O	1.50956101	-1.45727306	0.00000000
O	-0.56220742	0.92670833	0.00000000
O	0.25767566	-1.95020412	0.00000000
Al	0.45177059	2.31740390	0.00000000
H	-2.44979977	-1.27791929	0.00000000
Frequencies --	34.1, 88.1, 125.1, 192.9, 303.7, 470.5, 515.0, 617.5, 729.9, 1035.0, 1154.9, 2023.5		

(3-7-13) Al<sub>2</sub>O<sub>3</sub>H-TS1

Al	2.56925619	-0.08037823	-0.00576526
O	-1.54795071	1.61688801	0.00353469
O	0.85993220	-0.03322412	0.02072189
Al	-0.82412080	0.03724497	0.00673503
O	-1.86323889	-1.27957899	-0.09207854

H                    -2.27670087   -1.87194681   0.52996865  
 Frequencies -- -290.8, 58.6, 83.4, 191.4, 261.5, 284.0, 423.8, 485.9, 775.0, 916.7,  
 1059.7, 4000.1

(3-7-14) Al<sub>2</sub>O<sub>3</sub>H-TS2

Al                    -0.14195125   -2.19192339   0.00000000  
 O                    1.67186687   0.21451017   0.00000000  
 O                    -0.89809704   -0.65057878   0.00000000  
 Al                    0.03546008   0.77699138   0.00000000  
 O                    -0.43404335   2.39504763   0.00000000  
 H                    -1.33342669   2.72228408   0.00000000  
 Frequencies -- -158.4, 87.5, 187.7, 238.4, 283.4, 292.5, 558.6, 648.0, 770.3, 833.0,  
 985.6, 3944.0

(3-7-15) Al<sub>2</sub>O<sub>3</sub>H-TS3

Al                    -0.10590940   -2.19886805   0.00000000  
 O                    1.65937974   0.25853812   0.00000000  
 O                    -0.89379715   -0.67579035   0.00000000  
 Al                    0.00470821   0.76957075   0.00000000  
 O                    -0.59261869   2.34647264   0.00000000  
 H                    -0.06809572   3.14710165   0.00000000  
 Frequencies -- -157.1, 86.6, 191.4, 233.5, 288.0, 292.1, 575.4, 630.1, 780.8, 835.1,  
 979.6, 3942.8

(3-7-16) Al<sub>2</sub>O<sub>3</sub>H-TS4

Al                    1.65715032   0.02659301   0.00137128  
 Al                    -1.66881972   -0.55229877   0.00670286  
 O                    0.01063229   -0.23752188   0.02827207  
 O                    3.24347533   0.26218890   -0.01200752  
 O                    -2.82152263   0.67270431   -0.09047925  
 H                    -3.30897766   1.25520433   0.48875370  
 Frequencies -- -307.8, 43.7, 69.0, 189.6, 228.3, 256.4, 350.3, 464.6, 857.5, 983.3,  
 1199.4, 3967.6

(3-7-17) Al<sub>2</sub>O<sub>3</sub>H-TS5

Al                    -0.33075147   -1.74852503   0.00000000  
 Al                    -0.20442909   1.16296822   0.00000000  
 O                    -1.15643796   -0.24662158   0.00000000  
 O                    0.45535081   2.62549648   0.00000000  
 O                    1.30141514   -1.22038248   0.00000000  
 H                    2.15472328   -1.65570076   0.00000000  
 Frequencies -- -116.3, 113.7, 164.0, 254.2, 346.4, 351.4, 601.6, 648.5, 804.0, 876.8,  
 1147.9, 3931.2

(3-7-18) Al<sub>2</sub>O<sub>3</sub>H-TS6

Al                    -0.11956763   -1.94681641   0.00000000  
 O                    -0.27831297   2.49637913   0.00000000  
 O                    -1.12141333   -0.51875491   0.00000000  
 Al                    -0.05848091   0.81582886   0.00000000  
 O                    1.39748153   -0.14792822   0.00000000  
 H                    2.33258924   0.06527012   0.00000000  
 Frequencies -- -203.9, 108.4, 194.3, 297.8, 354.4, 366.0, 640.5, 691.2, 744.0, 794.6,

853.9, 3906.5

(3-7-19) Al<sub>2</sub>O<sub>3</sub>H-TS7

Al	0.36756235	-1.58849187	0.00000000
Al	-0.56834725	0.72803863	0.00000000
O	1.19910882	-0.05353013	0.00000000
O	-1.23611558	-0.85919787	0.00000000
O	0.21037512	2.17557849	0.00000000
H	1.22325684	1.08308827	0.00000000

Frequencies -- -1165.2, 89.9, 298.0, 325.0, 442.5, 568.3, 694.5, 730.2, 805.3, 999.1, 1057.6, 1924.0

(3-7-20) Al<sub>2</sub>O<sub>3</sub>H-TS8

Al	1.61568208	-0.35925897	-0.13015391
Al	-1.02212396	0.07079296	0.34299692
O	1.86998501	1.23925005	0.00111800
O	0.12253810	-1.17512001	0.00268506
O	-2.56101093	0.27897287	-0.32747417
H	-3.16835297	1.00523485	-0.17759025

Frequencies -- -238.9, 36.0, 141.6, 213.1, 256.3, 277.3, 524.8, 652.5, 756.2, 907.7, 1037.9, 3923.3

(3-7-21) Al<sub>2</sub>O<sub>3</sub>H-TS9

Al	1.00163884	0.32390111	0.23937359
O	0.83736131	-0.79176864	-1.07996255
O	-0.28061255	1.41481296	-0.12283047
O	-0.01023846	-0.78766027	1.14560692
Al	-1.14251229	-0.17353819	-0.15450133
H	-2.54072748	-0.63779033	-0.64585065

Frequencies -- -221.0, 244.1, 364.7, 483.1, 495.8, 547.5, 576.8, 634.5, 679.3, 791.5, 812.1, 2049.1

(3-7-22) Al<sub>2</sub>O<sub>3</sub>H-TS10

Al	-1.76714904	0.17380644	0.00000000
Al	1.20188666	0.22219753	0.00000000
O	-1.09945206	-1.42565619	0.00000000
O	2.70678081	-0.34248439	0.00000000
O	-0.28473592	1.03810681	0.00000000
H	-3.23233171	0.69221857	0.00000000

Frequencies -- -178.6, 99.6, 131.4, 230.8, 250.2, 484.4, 555.8, 646.3, 782.3, 889.8, 1098.1, 2048.2

(3-7-23) Al<sub>2</sub>O<sub>3</sub>H-TS11

Al	-1.44621984	-0.07212928	-0.06013156
O	0.80183506	1.14380269	-0.55253809
O	-0.31532186	-1.36794129	-0.12683078
O	-0.30508270	1.20501572	0.51048016
Al	1.14154420	-0.45749930	0.11316187
H	2.50933931	-0.96184530	0.66171558

Frequencies -- -177.3, 134.2, 283.1, 421.0, 489.7, 600.3, 647.0, 724.8, 778.4, 793.3, 807.2, 2030.7

(3-7-24) Al<sub>2</sub>O<sub>3</sub>H-TS12

Al	1.71888990	-0.01924820	0.00000000
Al	-1.62962870	0.24194073	0.00000000
O	0.04879272	0.10607173	0.00000000
O	3.31695287	-0.12256415	0.00000000
O	-3.13206173	-0.48298068	0.00000000
H	-3.02986648	1.10078202	0.00000000

Frequencies -- -1180.9, 53.3, 69.2, 183.4, 210.4, 261.2, 288.5, 433.1, 868.4, 1043.7, 1210.4, 1740.6

(3-7-25) Al<sub>2</sub>O<sub>3</sub>H-TS13

Al	1.68906303	-0.08077839	0.00297545
Al	-0.78744087	-0.04483672	-0.01480395
O	0.39802583	1.26210822	-0.09822938
O	0.42962988	-1.27873204	-0.00655405
O	-2.50389020	0.03850173	0.04641756
H	1.68878783	1.45797314	0.62069755

Frequencies -- -1474.6, 128.4, 168.6, 286.3, 337.7, 425.5, 458.4, 678.1, 706.5, 720.5, 865.2, 1681.2

(3-7-26) Al<sub>2</sub>O<sub>3</sub>H-TS14

Al	1.20635292	0.20630313	0.01692613
O	0.19313307	-0.94382900	-0.93333302
O	-0.00485512	1.44741706	0.03178019
O	0.05025097	-0.98546407	0.94161197
Al	-1.14581916	0.09119995	-0.03264198
H	-2.69517024	-0.01253185	-0.11616705

Frequencies -- -924.1, 314.4, 327.2, 448.5, 479.9, 516.7, 548.7, 559.3, 667.5, 726.2, 790.5, 2040.3

(3-7-27) Al<sub>2</sub>O<sub>3</sub>H-TS15

Al	-0.64271969	1.22079134	0.00000000
O	1.44070534	-0.47361891	0.00000000
O	-1.36862733	-0.31060873	0.00000000
O	1.00458983	1.45831210	0.00000000
Al	-0.01120169	-1.40763136	0.00000000
H	-0.11236477	-2.96375552	0.00000000

Frequencies -- -507.2, 122.3, 202.1, 237.0, 369.4, 474.7, 572.1, 708.3, 743.6, 811.5, 950.2, 2021.4

(3-7-28) Al<sub>2</sub>O<sub>3</sub>H-TS16

Al	1.10513305	-0.80293354	0.00846799
O	0.10320141	1.60482498	0.11624897
O	-0.53354348	-1.15444149	0.06721051
O	1.28371582	0.99330171	-0.10473461
Al	-1.81621550	0.04055239	-0.05329901
H	2.41708181	-1.63852664	-0.04699568

Frequencies -- -226.4, 158.3, 173.7, 301.3, 348.4, 463.4, 545.8, 593.9, 695.8, 902.8, 1059.6, 2036.2

(3-8-1) Al<sub>2</sub>O<sub>4</sub>H

O	1.26683481	-0.06805048	0.00000000
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O	0.07249025	2.82905428	0.00000000
Al	-0.00460278	-1.24755086	0.00000000
Al	0.01920896	1.15078078	0.00000000
O	-1.25562739	-0.04635233	0.00000000
O	-0.02270077	-2.98535785	0.00000000
H	-0.67785544	3.42366214	0.00000000

Frequencies -- 93.1, 154.2, 215.9, 223.0, 291.8, 387.0, 406.7, 570.4, 650.8, 669.5, 738.1, 808.1, 926.6, 996.8, 3942.4

(3-8-2) Al<sub>2</sub>O<sub>4</sub>H-2

O	0.06211683	0.30501192	0.00000000
O	1.56036443	-2.21759233	0.00000000
Al	-0.00546842	1.97036587	0.00000000
Al	0.03786241	-1.38097472	0.00000000
O	-0.06228950	3.57178170	0.00000000
O	-1.41830060	-2.22097185	0.00000000
H	-1.55625122	-3.16792059	0.00000000

Frequencies -- 42.1, 61.0, 172.0, 188.1, 209.6, 280.4, 288.3, 300.8, 448.1, 561.1, 780.6, 918.5, 1022.2, 1218.5, 3948.1

(3-8-3) Al<sub>2</sub>O<sub>4</sub>H-3

O	0.08488341	0.29694190	0.00000000
O	-1.64802785	-2.03513995	0.00000000
Al	-0.03522409	-1.39053609	0.00000000
Al	0.03882993	1.96377717	0.00000000
O	1.24704384	-2.47080211	0.00000000
O	0.03657583	3.56611731	0.00000000
H	2.18932227	-2.30907135	0.00000000

Frequencies -- 44.7, 61.0, 176.9, 196.8, 208.3, 254.4, 270.1, 298.7, 436.3, 543.0, 768.3, 942.7, 1015.2, 1214.5, 3960.6

(3-8-4) Al<sub>2</sub>O<sub>4</sub>H-4

Al	-0.58460850	-1.77997843	0.00000000
O	1.40699236	0.03039120	0.00000000
O	-1.33788876	-0.23127537	0.00000000
O	1.14373321	-1.43210302	0.00000000
Al	-0.08761514	0.93125864	0.00000000
H	0.55022279	3.21791175	0.00000000
O	-0.18925124	2.60991789	0.00000000

Frequencies -- 115.3, 168.4, 189.1, 287.7, 307.4, 335.6, 376.1, 574.8, 646.7, 688.8, 752.4, 830.6, 901.7, 982.7, 3941.9

(3-8-5) Al<sub>2</sub>O<sub>4</sub>H-5

Al	-0.62777755	-1.76215002	0.00000000
O	1.42536290	-0.01050881	0.00000000
O	-1.33245155	-0.19053844	0.00000000
O	1.10804657	-1.46163080	0.00000000
Al	-0.04098218	0.93191828	0.00000000
H	-0.77637960	3.19486258	0.00000000
O	-0.01717591	2.61244681	0.00000000

Frequencies -- 113.2, 167.0, 189.4, 270.1, 308.1, 333.2, 378.1, 561.1, 638.9, 690.2, 758.2, 828.8, 902.2, 982.0, 3948.5



(3-8-6) Al<sub>2</sub>O<sub>4</sub>H-6

O	0.35032875	0.40545918	0.00000000
O	-0.19307930	-2.69306381	0.82338700
Al	0.56125478	2.09762218	0.00000000
Al	0.04459872	-1.22528381	0.00000000
O	-0.84157720	3.06070820	0.00000000
O	-0.19307930	-2.69306381	-0.82338700
H	-0.85683918	4.01928320	0.00000000

Frequencies -- 20.6, 41.3, 67.1, 191.5, 242.4, 274.6, 327.6, 412.7, 578.0, 606.9, 769.0, 827.2, 932.9, 1168.9, 3919.2

(3-8-7) Al<sub>2</sub>O<sub>4</sub>H-7

O	-0.62551408	-0.94537484	0.00000000
O	1.24103007	1.41314519	0.00000000
Al	-0.39450751	0.71565101	0.00000000
Al	-0.17044615	-2.60400869	0.00000000
O	-1.55982770	1.93120449	0.00000000
H	-2.50753921	1.79725698	0.00000000
O	2.17580380	0.44494927	0.00000000

Frequencies -- 35.6, 58.5, 88.0, 180.2, 220.6, 270.4, 278.0, 341.0, 485.9, 590.8, 722.0, 897.3, 1053.0, 1159.7, 3943.3

(3-8-8) Al<sub>2</sub>O<sub>4</sub>H-8

O	-0.42516003	-1.02487193	0.00000000
O	1.06000642	1.60141397	0.00000000
Al	-0.44153585	0.64766785	0.00000000
Al	-0.00699706	-2.68890965	0.00000000
O	-1.84079810	1.58613483	0.00000000
H	-1.86365709	2.54344517	0.00000000
O	2.16777482	0.83641042	0.00000000

Frequencies -- 30.9, 55.1, 83.2, 159.4, 223.4, 278.6, 280.1, 346.9, 475.8, 595.1, 718.7, 893.3, 1074.6, 1157.2, 3936.1

(3-8-9) Al<sub>2</sub>O<sub>4</sub>H-TS1

O	-0.30190291	-0.01085808	0.02007015
O	2.09872403	1.61605800	0.00081935
Al	-1.96820091	-0.02746913	-0.00051778
Al	1.38711108	0.03440298	0.00919408
O	-3.57035691	-0.06244419	-0.00678771
O	2.37073812	-1.30980797	-0.08877523
H	2.77654917	-1.95372207	0.48459563

Frequencies -- -279.8, 43.1, 61.7, 175.8, 198.5, 211.2, 280.3, 292.2, 385.4, 453.2, 775.2, 939.4, 1019.7, 1216.8, 4009.4

(3-8-10) Al<sub>2</sub>O<sub>4</sub>H-TS2

Al	1.63935107	0.27649034	0.00000000
O	-0.48110745	-1.58546858	0.00000000
O	0.08442036	0.95298315	0.00000000
O	3.19343048	-0.13370561	0.00000000
Al	-1.29514456	-0.05997743	0.00000000
H	-3.39303273	1.11322345	0.00000000

O                    -2.93194989      0.27520463      0.00000000  
 Frequencies -- -178.8, 61.8, 128.9, 182.4, 200.2, 249.5, 263.1, 294.4, 509.9, 621.3,  
 733.4, 860.2, 1005.9, 1102.9, 3956.7

(3-8-11) Al<sub>2</sub>O<sub>4</sub>H-TS3

O                    0.09186623      0.96369212      0.00000000  
 O                    -0.49606167     -1.58380580      0.00000000  
 Al                   1.64059167      0.27815249      0.00000000  
 Al                   -1.28768325     -0.04442595      0.00000000  
 O                    3.18531330     -0.16850512      0.00000000  
 O                    -2.89364476      0.42266939      0.00000000  
 H                    -3.68759431     -0.11084969      0.00000000  
 Frequencies -- -181.6, 61.9, 126.0, 186.8, 199.0, 242.6, 260.4, 296.0, 520.6, 608.8,  
 739.3, 859.1, 1002.4, 1098.4, 3956.1

(3-8-12) Al<sub>2</sub>O<sub>4</sub>H-TS4

O                    -0.49707359     -1.64285592      0.00000000  
 O                    -2.89590869      0.25961600      0.00000000  
 Al                   1.60441264      0.26802112      0.00000000  
 Al                   -1.24958996     -0.04146766      0.00000000  
 O                    0.07816410      1.02408339      0.00000000  
 O                    3.15588541     -0.14743001      0.00000000  
 H                    -3.34123253      1.10749720      0.00000000  
 Frequencies -- -209.8, 54.8, 146.6, 194.8, 204.3, 296.3, 311.8, 354.3, 555.1, 642.4,  
 685.1, 820.7, 991.1, 1092.1, 3938.1

(3-8-13) Al<sub>2</sub>O<sub>4</sub>H-TS5

Al                   -1.77360283     -0.60618776      0.00215673  
 O                    0.00561844      1.41056900      0.00017708  
 O                    -0.21266892     -1.33259897      0.00243956  
 O                    -1.45138560      1.12586019      0.00579705  
 Al                   0.93588825     -0.06542812      0.00100779  
 H                    3.32012824     -0.13364855      0.54708174  
 O                    2.60470624     -0.09574833     -0.08194124  
 Frequencies -- -278.9, 122.0, 170.5, 202.9, 300.6, 339.3, 375.4, 434.5, 641.0, 692.0,  
 748.3, 832.2, 902.9, 991.5, 4000.4

(3-8-14) Al<sub>2</sub>O<sub>4</sub>H-TS6

Al                   -0.65591885     -1.64796328      0.00000000  
 O                    1.47042890      0.04316320      0.00000000  
 O                    -1.35410541     -0.10541655      0.00000000  
 O                    0.99127340     -1.88742781      0.00000000  
 Al                   0.01002373      0.96778596      0.00000000  
 H                    0.60545916      3.25685390      0.00000000  
 O                    -0.13369971      2.64786258      0.00000000  
 Frequencies -- -495.5, 85.5, 165.2, 176.2, 225.5, 307.8, 313.6, 326.9, 602.2, 658.6,  
 750.6, 794.2, 942.7, 960.2, 3935.6

(3-8-15) Al<sub>2</sub>O<sub>4</sub>H-TS7

Al                   -0.69638586     -1.63056114      0.00000000  
 O                    1.49628235      0.00418794      0.00000000  
 O                    -1.34105624     -0.06438819      0.00000000

O	0.94361809	-1.91210587	0.00000000
Al	0.06174049	0.96715340	0.00000000
H	-0.76309326	3.19077668	0.00000000
O	0.02784118	2.65149661	0.00000000

Frequencies -- -487.5, 82.4, 167.2, 176.7, 223.4, 282.3, 316.6, 324.3, 577.8, 662.3, 747.7, 787.1, 939.5, 965.1, 3940.5

(3-8-16) Al<sub>2</sub>O<sub>4</sub>H-TS8

O	-0.92628179	-0.64245767	0.00985868
O	1.35020879	1.27650935	-0.00696181
Al	0.73044012	-0.39310762	0.00686559
Al	-2.59486720	-0.23341859	-0.00253695
O	1.93165388	-1.54682127	-0.08026223
H	2.48546123	-2.07389242	0.48694274
O	0.36343047	2.19011123	0.00946348

Frequencies -- -341.1, 30.9, 72.8, 89.1, 184.6, 234.9, 273.5, 289.7, 369.9, 497.5, 706.2, 914.3, 1062.5, 1157.1, 4022.6

(3-8-17) Al<sub>2</sub>O<sub>4</sub>H-TS9

Al	2.07444099	-0.64245620	-0.05515957
O	-0.33495581	1.51209601	-0.13539208
O	0.41788792	-1.21379005	0.05831215
O	0.98384815	1.55655090	0.14471316
Al	-0.90769499	-0.19006194	0.01187988
H	-3.08219607	-1.16867274	0.02663752
O	-2.57746800	-0.35593079	-0.00063342

Frequencies -- -217.3, 92.7, 157.7, 183.6, 276.1, 292.5, 314.9, 331.5, 545.7, 582.3, 697.6, 812.8, 1006.8, 1061.6, 3945.9

(3-8-18) Al<sub>2</sub>O<sub>4</sub>H-TS10

O	-0.44728278	-1.20865426	0.06427089
O	0.36614045	1.49363414	-0.12941782
Al	0.90419775	-0.22377336	0.01564023
Al	-2.09044557	-0.60674930	-0.05877690
O	2.55374120	-0.53091161	0.00158123
H	3.26534709	0.10758034	-0.04390961
O	-0.95311455	1.58208351	0.13915150

Frequencies -- -220.4, 92.5, 158.6, 183.2, 276.4, 292.7, 304.2, 330.8, 549.9, 571.2, 685.6, 817.9, 1006.1, 1062.7, 3944.7

(3-8-19) Al<sub>2</sub>O<sub>4</sub>H-TS11

Al	1.25356095	0.11663781	0.53644603
O	-0.88531807	-1.17074105	-0.20805015
O	0.20215288	1.39989193	-0.03994757
O	-2.27222004	-0.58686225	0.38861709
Al	-1.20944712	0.53435498	-0.35829169
H	3.04033894	-1.30296795	-0.19597547
O	2.50365790	-0.53728091	-0.40562323

Frequencies -- -241.2, 70.9, 132.1, 168.0, 222.7, 242.1, 354.4, 528.3, 557.1, 619.5, 674.3, 773.1, 879.0, 984.8, 3926.0

(3-9-1) AlOH<sub>2</sub>

Al	0.15375813	-0.65106256	0.00000000
H	-1.16316834	-1.56915632	0.00000000
O	-0.16713681	1.03852847	0.00000000
H	0.50140716	1.72474180	0.00000000
Frequencies --	419.6, 521.9, 630.7, 825.9, 1802.9, 3927.1		

(3-9-2) AlOH<sub>2</sub>-2

Al	0.12537126	-0.65660686	0.00000000
H	-1.24133830	-1.51823082	0.00000000
O	0.04487076	1.05709645	0.00000000
H	-0.74745413	1.59734839	0.00000000
Frequencies --	371.6, 468.3, 622.7, 844.1, 1764.9, 3902.4		

(3-9-3) AlOH<sub>2</sub>-adduct1

O	0.28096992	0.76852087	0.00000000
H	0.58884775	1.67128182	0.00000000
Al	-0.12528885	-0.86378454	0.00000000
H	-1.20785205	3.40975032	0.00000000
Frequencies --	19.6, 94.9, 141.9, 145.3, 840.5, 3981.9		

(3-9-4) AlOH<sub>2</sub>-adduct2

O	0.00000000	0.00000000	1.20620998
H	0.00000000	-0.78403552	1.76736080
H	-0.00000000	0.78403552	1.76736080
Al	0.00000000	-0.00000000	-1.01419101
Frequencies --	89.2, 227.3, 292.4, 1596.9, 3769.1, 3878.3		

(3-9-5) AlOH<sub>2</sub>-adduct3

Al	0.00000000	0.00000000	-0.94201432
H	0.00000000	0.00000000	3.75160033
O	-0.00000000	-0.00000000	0.68637929
H	-0.00000000	0.00000000	3.00355145
Frequencies --	10.6, 10.6, 177.1, 407.4, 407.4, 957.5, 4343.4		

(3-9-6) AlOH<sub>2</sub>-TS1

Al	-0.65519889	-0.13403284	0.01647526
H	-1.57283968	1.19706029	-0.02273713
O	1.02887712	0.04107484	-0.06931332
H	1.85940827	0.21676792	0.36306535
Frequencies --	-393.6, 209.6, 585.0, 865.5, 1747.5, 4015.7		

(3-9-7) AlOH<sub>2</sub>-TS2

O	0.34787858	0.83767870	0.00000000
H	0.62233871	1.75085302	0.00000000
Al	-0.08054250	-0.78869403	0.00000000
H	-2.35831483	1.80073983	0.00000000
Frequencies --	-85.5, 92.5, 142.5, 161.3, 839.7, 3989.3		

(3-9-8) AlOH<sub>2</sub>-TS3

Al	-0.85153609	-0.02745071	0.01306351
H	0.61940119	1.10898680	0.10088206
O	1.09060191	-0.06045805	-0.10810439

H 1.72575280 -0.26846310 0.59412739  
Frequencies -- -1355.0, 360.4, 487.5, 744.7, 1227.4, 3721.4,

(3-9-9) AlOH<sub>2</sub>-TS4

O 0.00000000 0.00000000 -0.78528170  
H 0.00000000 0.00000000 -2.08982870  
Al 0.00000000 0.00000000 0.87122830  
H 0.00000000 0.00000000 -2.95388570  
Frequencies -- -1095.1, 107.9, 107.9, 856.1, 886.1, 886.1, 2253.7

(3-9-10) AlOH<sub>2</sub>-TS5

Al 0.11751771 -0.66605107 0.00000000  
H -1.77525057 -0.11667627 0.00000000  
O 0.18374339 1.02562512 0.00000000  
H -1.22242677 0.57033921 0.00000000  
Frequencies -- -1030.4, 525.9, 833.1, 1046.6, 1512.7, 2308.0

(3-10-1) AlO<sub>2</sub>H<sub>2</sub>

Al 0.00000000 0.00000000 0.49560026  
O 0.00000000 1.45064500 -0.40243974  
H 0.00000000 2.32115000 -0.00188374  
O 0.00000000 -1.45064500 -0.40243974  
H 0.00000000 -2.32115000 -0.00188374  
Frequencies -- 227.7, 266.6, 317.8, 548.6, 621.0, 745.0, 902.2, 3923.2, 3923.6

(3-10-2) AlO<sub>2</sub>H<sub>2</sub>-2

O -1.51291475 -0.25494640 0.00000000  
H 2.31285465 -0.07183331 0.00000000  
H -1.63205621 -1.20764024 0.00000000  
O 1.42399036 -0.43069245 0.00000000  
Al 0.00235359 0.52035265 0.00000000  
Frequencies -- 215.3, 298.9, 322.6, 582.2, 596.6, 762.9, 900.0, 3887.3, 3917.6

(3-10-3) AlO<sub>2</sub>H<sub>2</sub>-3

Al 0.06014199 0.42873852 0.00000000  
O 1.54237778 -0.48401030 0.00000000  
H 0.22032491 1.98825034 0.00000000  
O -1.38304525 -0.44781907 0.00000000  
H -2.27683095 -0.10721611 0.00000000  
Frequencies -- 212.4, 282.2, 472.2, 510.9, 619.4, 751.5, 928.4, 1986.1, 3951.3

(3-10-4) AlO<sub>2</sub>H<sub>2</sub>-4

Al 0.06828072 0.45003139 0.00000000  
O 1.51182198 -0.52542326 0.00000000  
H 0.22019884 2.00352656 0.00000000  
O -1.44574582 -0.30139761 0.00000000  
H -1.63645744 -1.23936769 0.00000000  
Frequencies -- 198.1, 337.8, 483.0, 559.2, 616.4, 769.0, 899.9, 2016.1, 3941.3

(3-10-5) AlO<sub>2</sub>H<sub>2</sub>-5

Al 0.45261288 -0.69210984 0.00435652  
O 1.08647721 0.82193403 0.01542559

H	-0.91819375	0.99656944	-0.03213143
O	-1.44428994	0.15957752	-0.09490090
H	-2.10327191	0.14876609	0.61129913
Frequencies --	170.2, 277.0, 353.8, 531.1, 749.9, 943.2, 1560.4, 3376.4, 3811.0		

(3-10-6) AlO<sub>2</sub>H<sub>2</sub>-adduct1

O	0.00000000	1.64947700	0.21686465
Al	0.00000000	0.00000000	0.06837065
O	0.00000000	-1.64947700	0.21686465
H	0.00000000	-0.37731300	-2.17932635
H	-0.00000000	0.37731300	-2.17932635
Frequencies --	183.8, 192.0, 195.2, 296.5, 423.6, 685.7, 775.3, 840.8, 4261.7		

(3-10-7) AlO<sub>2</sub>H<sub>2</sub>-TS1

Al	-0.00603526	0.49202771	0.01677995
O	1.48745773	-0.30028728	-0.09622517
H	2.12179182	-0.61612521	0.54495978
O	-1.45269925	-0.42050331	0.00081024
H	-2.32140126	-0.01391032	0.00022031
Frequencies --	-305.0, 233.5, 330.0, 411.9, 603.7, 748.2, 909.2, 3908.4, 3958.6		

(3-10-7) AlO<sub>2</sub>H<sub>2</sub>-TS2

Al	0.06846584	0.43525410	0.00966898
O	1.52499990	-0.51803082	0.00558048
H	0.28011876	1.98598812	0.01377867
O	-1.40399409	-0.35881400	-0.08073713
H	-2.13822118	-0.62953292	0.46177779
Frequencies --	-323.4, 211.0, 338.8, 478.6, 612.7, 762.0, 930.0, 1995.9, 4018.4		

(3-10-8) AlO<sub>2</sub>H<sub>2</sub>-TS3

Al	0.04716349	0.20573128	0.00000000
O	1.63247576	-0.32650668	0.00000000
H	1.34657545	1.21310068	0.00000000
O	-1.60982886	-0.05328140	0.00000000
H	-2.14087595	-0.84930271	0.00000000
Frequencies --	-1205.7, 187.6, 213.7, 266.0, 466.9, 740.6, 1018.3, 1736.2, 3945.6		

(3-10-9) AlO<sub>2</sub>H<sub>2</sub>-TS4

Al	-0.04462599	0.20510843	0.00000000
O	-1.63645944	-0.29930952	0.00000000
H	-1.32271884	1.24525533	0.00000000
O	1.57762788	-0.22753272	0.00000000
H	2.37350918	0.30307295	0.00000000
Frequencies --	-1179.7, 197.1, 220.6, 277.7, 481.8, 737.7, 1019.2, 1723.2, 3954.0		

(3-10-10) AlO<sub>2</sub>H<sub>2</sub>-TS5

Al	0.17958820	0.23292319	0.00348084
O	1.72284619	-0.22169685	0.00720287
H	-2.07825875	-0.63025448	0.61351749
O	-1.58155683	-0.21582181	-0.11176576
H	-1.38670276	1.10240231	0.17773463
Frequencies --	-1129.0, 195.1, 217.9, 481.1, 605.9, 817.4, 1059.2, 1325.1, 3720.9		

(3-10-11) AlO<sub>2</sub>H<sub>2</sub>-TS6

O	1.70036783	0.02026313	0.00000000
Al	0.04966163	0.11517199	0.00000000
O	-1.61613017	0.16856933	0.00000000
H	-1.03810049	-1.29908926	0.00000000
H	-0.28140188	-1.70880627	0.00000000

Frequencies -- -678.9, 199.8, 213.6, 545.2, 757.5, 868.6, 979.8, 1528.3, 2552.7

(3-11-1) AlO<sub>3</sub>H<sub>2</sub>

Al	0.00956271	0.03081829	0.00000000
O	1.64771920	-0.35859347	0.00000000
H	2.01596891	-1.24188927	0.00000000
O	-0.42847212	1.71629735	0.00000000
O	-1.21671989	-1.13099400	0.00000000
H	-2.16050172	-0.97242744	0.00000000

Frequencies -- 198.8, 2201.0, 255.4, 276.9, 296.3, 577.4, 586.4, 691.1, 891.9, 967.7, 3943.8, 3945.4

(3-11-2) AlO<sub>3</sub>H<sub>2</sub>-2

Al	0.00000000	0.00000000	0.02330605
O	0.00000000	1.52235900	-0.69849795
H	0.00000000	1.76120700	-1.62368995
O	0.00000000	0.00000000	1.76504605
O	0.00000000	-1.52235900	-0.69849795
H	0.00000000	-1.76120700	-1.62368995

Frequencies -- 123.0, 213.0, 229.9, 257.6, 280.8, 492.3, 547.3, 692.0, 912.9, 958.4, 3963.7, 3966.5

(3-11-3) AlO<sub>3</sub>H<sub>2</sub>-3

Al	0.52331031	0.31475732	0.00000000
O	-0.26207807	-1.25024847	0.67894600
H	2.07439252	0.37376810	0.00000000
O	-0.26207807	-1.25024847	-0.67894600
O	-0.41460782	1.71702622	0.00000000
H	-1.36731488	1.80215249	0.00000000

Frequencies -- 179.5, 219.5, 314.2, 425.0, 521.6, 543.1, 598.5, 671.5, 890.7, 1150.0, 2053.2, 3950.0

(3-11-4) AlO<sub>3</sub>H<sub>2</sub>-4

Al	-0.51351070	0.31206840	0.00000000
O	0.25382816	-1.25042344	0.67925000
H	-2.07113340	0.36693581	0.00000000
O	0.25382816	-1.25042344	-0.67925000
O	0.54637371	1.62836022	0.00000000
H	0.31453235	2.55606833	0.00000000

Frequencies -- 169.3, 220.4, 272.4, 442.2, 516.9, 529.5, 592.6, 668.1, 891.4, 1149.1, 2024.5, 3955.2

(3-11-5) AlO<sub>3</sub>H<sub>2</sub>-5

Al	-0.03121326	-0.34571225	0.00000000
O	-0.04070445	1.58507852	0.00000000

H	0.16446427	2.08817848	0.79943700
O	0.02515496	-0.77267037	1.60659400
O	0.02515496	-0.77267037	-1.60659400
H	0.16446427	2.08817848	-0.79943700

Frequencies -- 116.1, 161.9, 210.3, 311.5, 319.4, 440.2, 526.5, 794.1, 829.1, 1592.7, 3752.2, 3864.3

(3-11-6) AlO<sub>3</sub>H<sub>2</sub>-6

Al	0.59975203	0.60646018	0.00000000
O	-1.58385178	-0.74976817	0.00000000
H	1.23179152	2.02720105	0.00000000
O	-1.18192302	0.53768186	0.00000000
O	1.50022962	-0.81604981	0.00000000
H	1.09579353	-1.68609442	0.00000000

Frequencies -- 97.1, 147.5, 253.7, 431.1, 497.6, 601.5, 620.7, 725.1, 903.6, 1149.7, 2044.3, 3910.8

(3-11-7) AlO<sub>3</sub>H<sub>2</sub>-7

Al	-0.58307950	0.58456107	0.00000000
O	0.74676654	-1.70017064	0.00000000
H	-2.04523827	1.13182849	0.00000000
O	-0.49662856	-1.18171255	0.00000000
O	0.83746365	1.48568192	0.00000000
H	0.92445872	2.43848780	0.00000000

Frequencies -- 69.2, 142.9, 267.0, 328.4, 469.5, 511.5, 629.5, 689.8, 916.8, 1154.0, 2016.1, 3949.1

(3-11-8) AlO<sub>3</sub>H<sub>2</sub>-adduct1

Al	-1.05684998	0.07114057	0.00000000
O	0.51703911	0.61479363	0.00000000
H	1.38590940	0.18967618	0.00000000
O	-2.59852755	-0.36936550	0.00000000
H	3.76060026	0.33993480	0.00000000
O	3.15555596	-0.42723293	0.00000000

Frequencies -- 37.7, 61.7, 167.5, 211.2, 212.8, 286.5, 397.6, 703.7, 827.1, 1183.1, 3690.0, 3729.1

(3-11-9) AlO<sub>3</sub>H<sub>2</sub>-adduct2

Al	-0.04647172	0.38217362	0.00000000
O	-0.11690192	-1.33906203	0.68392200
H	2.27253518	-0.01962103	0.00000000
O	-0.11690192	-1.33906203	-0.68392200
O	-0.23670187	1.96999762	0.00000000
H	2.09564289	0.71637544	0.00000000

Frequencies -- 92.5, 178.6, 201.3, 211.8, 294.2, 414.3, 442.0, 539.8, 747.1, 1104.5, 1151.6, 4212.4

(3-11-10) AlO<sub>3</sub>H<sub>2</sub>-TS1

Al	0.00395683	0.02304511	0.00375907
O	1.53830128	-0.67568991	0.01764913
H	1.74966687	-1.60291280	-0.08519869
O	-0.03309128	1.76137608	0.00626170



O	-1.47651367	-0.76823086	-0.08601466
H	-2.03067633	-1.23631608	0.53316147

Frequencies -- -255.4, 207.6, 232.6, 269.8, 276.5, 435.2, 565.2, 690.9, 903.2, 962.6, 3950.2, 3993.4

(3-11-11) AlO<sub>3</sub>H<sub>2</sub>-TS2

Al	0.31004595	0.51847922	0.01298014
O	-1.24265741	-0.26234253	-0.67902935
H	0.31151868	2.07405320	0.03448560
O	-1.25816646	-0.27356382	0.67748874
O	1.66848955	-0.46093133	-0.08639476
H	2.31655852	-0.83958171	0.50025560

Frequencies -- -298.2, 193.9, 232.0, 386.7, 438.9, 518.7, 584.8, 672.5, 904.1, 1151.9, 2035.3, 4010.3

(3-11-12) AlO<sub>3</sub>H<sub>2</sub>-TS3

O	1.02211050	1.15736510	-0.08683614
Al	-0.27254922	-0.21503116	-0.03210396
H	1.23812145	1.84592315	0.55377483
O	1.01183200	-1.24747690	0.03595587
O	-1.94197829	0.17922351	0.02866025
H	1.56930470	0.23658821	0.04133679

Frequencies -- -831.2, 152.6, 196.2, 411.0, 416.9, 611.9, 706.7, 785.6, 933.6, 1300.2, 2296.6, 3818.0

(3-11-13) AlO<sub>3</sub>H<sub>2</sub>-TS4

O	-1.55877996	-0.72809381	0.06853110
H	-1.08021253	2.02661004	-0.38188739
O	1.22106222	0.47886081	0.23362698
H	-1.25769409	-1.63168283	0.17731628
Al	-0.53824675	0.60345502	-0.06447011
O	1.50460704	-0.78074731	-0.17182277

Frequencies -- -136.6, 154.4, 217.0, 416.1, 491.6, 600.6, 629.1, 7223.0, 906.2, 1144.5, 2040.6, 3922.6

(3-11-14) AlO<sub>3</sub>H<sub>2</sub>-TS5

Al	-0.80775414	0.17862986	-0.00874386
O	0.47311658	1.26659330	0.02769911
H	1.38551514	0.97821543	-0.09756376
O	-2.08351711	-0.79410814	0.01122530
H	3.06797078	-1.07697057	0.51683143
O	2.36631526	-0.75041429	-0.07712411

Frequencies -- -78.2, 55.5, 155.9, 191.4, 223.1, 249.3, 327.7, 691.9, 778.1, 1137.2, 3705.3, 3797.6

(3-11-15) AlO<sub>3</sub>H<sub>2</sub>-TS6

O	-1.49749422	-0.80260173	0.08552596
H	-1.06631472	2.02417616	-0.36880127
O	1.19371404	0.46630376	0.22312658
H	-2.44534625	-0.87199855	-0.02560492
Al	-0.55227197	0.58119208	-0.06459223
O	1.64017976	-0.75216136	-0.15438939

Frequencies -- -107.5, 133.9, 234.1, 327.2, 476.5, 516.2, 638.0, 695.1, 916.8, 1147.1, 2013.3, 3947.5

(3-11-16) AlO<sub>3</sub>H<sub>2</sub>-TS7

Al	0.58318910	0.58829684	0.02585201
O	-1.69479926	-0.75710954	0.03869958
H	1.08802149	2.06122370	0.09328512
O	-1.18492391	0.48555532	-0.05346031
O	1.52703975	-0.77077441	-0.07806683
H	2.15198752	-1.37045359	0.31325927

Frequencies -- -364.2, 73.2, 149.6, 243.4, 292.4, 467.6, 628.2, 696.2, 944.5, 1155.4, 2026.0, 4049.8

(3-11-17) AlO<sub>3</sub>H<sub>2</sub>-TS8

Al	0.27972683	-0.10383296	0.22504301
O	-1.15011006	0.87356409	0.02270545
H	-0.86188031	-1.22939150	0.86552958
O	-1.41546521	-0.60578005	-0.28861177
O	1.88854286	0.10927663	-0.20974005
H	2.64169080	-0.43726533	0.01408226

Frequencies -- -1198.0, 180.0, 222.1, 242.8, 415.6, 543.6, 623.2, 784.4, 792.3, 981.6, 1522.8, 3945.7

(3-11-18) AlO<sub>3</sub>H<sub>2</sub>-TS9

Al	0.14201205	-0.11476124	0.26264568
O	-0.97801610	1.29892575	-0.07576287
H	-0.40015180	-0.71658967	1.68398855
O	-1.26038390	-1.00632821	-0.32784747
O	1.77776702	-0.06433598	-0.12909341
H	2.23905894	0.38239325	-0.83675232

Frequencies -- -187.1, 140.8, 192.1, 212.9, 350.9, 466.2, 508.7, 572.3, 638.6, 928.8, 1638.7, 3965.2

(3-11-19) AlO<sub>3</sub>H<sub>2</sub>-TS10

Al	0.02753079	0.33603907	0.00000000
O	-0.05759888	-1.37929179	0.68372400
H	1.81912605	0.83684841	0.00000000
O	-0.05759888	-1.37929179	-0.68372400
O	-0.31695740	1.91763872	0.00000000
H	1.28021503	1.52220246	0.00000000

Frequencies -- -739.0, 119.9, 205.1, 246.2, 450.5, 545.6, 738.4, 1042.1, 1086.1, 1142.2, 1686.3, 2572.3

(3-12-1) Al<sub>2</sub>OH<sub>2</sub>(1)

Al	0.00000000	0.00000000	-1.56610183
O	0.00000000	0.00000000	0.13367617
H	0.00000000	1.38130800	-2.32762783
H	0.00000000	-1.38130800	-2.32762783
Al	0.00000000	0.00000000	1.84193617

Frequencies -- 98.1, 112.6, 512.5, 569.2, 626.1, 812.8, 1033.6, 1948.0, 1951.1

(3-12-2) Al<sub>2</sub>OH<sub>2</sub>(1)-2

Al	0.00000000	1.48763400	-0.29326572
O	0.00000000	0.00000000	0.89421228
H	0.00000000	0.00000000	-1.38361772
H	0.00000000	0.00000000	1.85482828
Al	0.00000000	-1.48763400	-0.29326572

Frequencies -- 333.1, 346.7, 422.0, 517.3, 620.7, 804.6, 1081.9, 1233.3, 3885.1

(3-12-3) Al<sub>2</sub>OH<sub>2</sub>(1)-3

Al	-1.46599965	-0.32900484	0.00000000
O	-0.05565720	0.92722293	0.00000000
H	2.59629552	0.54630190	0.00000000
H	-0.00927391	1.89080939	0.00000000
Al	1.30124857	-0.42906399	0.00000000

Frequencies -- 201.8, 249.4, 362.2, 493.5, 523.9, 604.1, 823.7, 1756.3, 3793.3

(3-12-4) Al<sub>2</sub>OH<sub>2</sub>(1)-4

Al	-0.58954832	0.66579811	0.00000000
O	0.80712933	1.67689373	0.00000000
H	-1.99018604	1.46290302	0.00000000
H	0.77922338	2.63607424	0.00000000
Al	0.18600432	-2.01303866	0.00000000

Frequencies -- 73.9, 259.9, 276.9, 474.7, 544.1, 701.1, 811.6, 1795.4, 3889.0

(3-12-5) Al<sub>2</sub>OH<sub>2</sub>(1)-5

Al	-0.52487681	0.64192447	0.00000000
O	0.59376430	1.95258707	0.00000000
H	-2.02302006	1.20915962	0.00000000
H	1.54552516	1.84605687	0.00000000
Al	0.19621377	-2.07853317	0.00000000

Frequencies -- 102.6, 243.4, 257.4, 467.0, 572.5, 674.9, 801.1, 1834.0, 3923.5

(3-12-6) Al<sub>2</sub>OH<sub>2</sub>(1)-adduct1

Al	0.00000000	1.71583900	0.24141772
O	0.00000000	0.00000000	0.20470772
H	0.00000000	0.00000000	-4.32932128
H	0.00000000	0.00000000	-3.58520128
Al	0.00000000	-1.71583900	0.24141772

Frequencies -- 23.6, 29.4, 99.8, 100.6, 108.2, 115.7, 505.1, 982.4, 4419.0

(3-12-7) Al<sub>2</sub>OH<sub>2</sub>(1)-TS1

Al	-1.80480341	-0.23244570	0.00000000
O	0.15536867	0.21844053	0.00000000
H	-1.55684807	1.57901475	0.00000000
H	-0.48185637	1.14925801	0.00000000
Al	1.86601534	-0.11184637	0.00000000

Frequencies -- -1079.1, 130.8, 140.9, 395.4, 717.6, 1024.2, 1185.1, 1503.4, 1874.4

(3-12-8) Al<sub>2</sub>OH<sub>2</sub>(1)-TS2

Al	-1.82878975	-0.28512715	-0.00569212
O	-0.30811875	0.60064786	-0.00927920
H	1.80453709	-0.30729870	1.54410328
H	-0.20073978	1.54796490	0.14284355

Al 1.89503226 -0.17993816 -0.11836275  
Frequencies -- -318.3, 93.4, 154.6, 168.9, 556.7, 683.3, 711.6, 1592.3, 3811.1

(3-12-9) Al<sub>2</sub>OH<sub>2</sub>(1)-TS3

Al -0.68260733 0.80228098 0.00000000  
O 1.01911700 1.13707399 0.00000000  
H -1.64163197 2.09354846 0.00000000  
H 1.46644044 1.98643592 0.00000000  
Al 0.06893468 -1.81586378 0.00000000  
Frequencies -- -84.8, 265.7, 302.0, 480.7, 541.0, 682.1, 780.7, 1807.5, 3878.4

(3-12-10) Al<sub>2</sub>OH<sub>2</sub>(1)-TS4

Al 0.64855993 0.56442701 0.01522192  
O 1.80852684 -0.66870107 -0.06015320  
H 1.28044704 2.04431196 -0.01061501  
H 2.36323980 -1.34722414 0.30777473  
Al -2.04178313 -0.20654079 -0.00106301  
Frequencies -- -466.3, 87.1, 187.8, 269.8, 294.8, 662.1, 833.6, 1799.4, 4039.2

(3-12-11) Al<sub>2</sub>OH<sub>2</sub>(1)-TS5

Al -1.74472221 0.02419028 0.00000000  
O 0.13537315 0.14867122 0.00000000  
H -2.22214835 -1.51589607 0.00000000  
H -0.55024441 1.23858892 0.00000000  
Al 1.87467664 -0.09434894 0.00000000  
Frequencies -- -1512.9, 113.6, 142.2, 405.5, 430.0, 609.5, 749.0, 1694.8, 1797.2

(3-12-12) Al<sub>2</sub>OH<sub>2</sub>(1)-TS6

Al -0.16781428 -1.55114205 0.00000000  
O -0.13890575 0.14544856 0.00000000  
H 0.59120026 -2.91717424 0.00000000  
H 1.66720341 -2.04188754 0.00000000  
Al 0.07957139 1.84310153 0.00000000  
Frequencies -- -1558.6, 74.9, 113.9, 485.1, 489.8, 537.0, 1010.8, 1106.5, 2035.3

(3-12-13) Al<sub>2</sub>OH<sub>2</sub>(3)

O 0.00000000 0.00000000 0.00722678  
Al 0.08768998 1.69651023 -0.07946022  
H -0.76620518 2.52408921 1.00407578  
Al -0.08768998 -1.69651023 -0.07946022  
H 0.76620518 -2.52408921 1.00407578  
Frequencies -- 105.0, 106.4, 126.9, 506.1, 580.3, 608.0, 1043.8, 1767.8, 1771.9

(3-12-14) Al<sub>2</sub>OH<sub>2</sub>(3)-2

Al 0.22388374 -1.92503509 0.00000000  
Al -0.51575287 0.55292325 0.00000000  
H -2.06808138 0.84724927 0.00000000  
O 0.54508278 1.88842746 0.00000000  
H 1.50171779 1.88278498 0.00000000  
Frequencies -- 119.1, 260.6, 292.7, 370.8, 530.8, 623.4, 835.1, 1917.0, 3945.5

(3-12-15) Al<sub>2</sub>OH<sub>2</sub>(3)-3

Al	-0.52848121	0.55304410	0.00000000
Al	0.22147136	-1.90501638	0.00000000
H	-2.07951131	0.89183362	0.00000000
O	0.68962044	1.74841241	0.00000000
H	0.55367573	2.69650677	0.00000000
Frequencies --	108.4, 221.5, 304.4, 366.1, 505.8, 627.3, 842.2, 1885.6, 3923.9		

(3-12-16) Al<sub>2</sub>OH<sub>2</sub>(3)-4

O	-0.07600353	0.93124027	0.04434989
Al	-1.44894096	-0.37705351	0.00525815
Al	1.34868580	-0.28592268	-0.13526159
H	1.96340008	-0.72546844	1.27368055
H	-0.05205480	1.89423670	0.06156517
Frequencies --	192.8, 277.8, 352.0, 427.7, 518.1, 555.4, 809.4, 1813.1, 3811.1		

(3-12-17) Al<sub>2</sub>OH<sub>2</sub>(3)-5

Al	-1.86783319	-0.18553794	-0.00427612
H	-3.03793019	0.88266911	0.11181844
Al	0.53732081	0.23045806	0.00111171
O	2.18722281	-0.13990598	-0.08247713
H	2.83680880	-0.34738270	0.58913595
Frequencies --	99.0, 114.7, 253.1, 324.8, 393.0, 454.3, 872.6, 1882.0, 3937.6		

(3-12-18) Al<sub>2</sub>OH<sub>2</sub>(3)-adduct1

Al	-0.65176044	-1.34925795	0.00000000
Al	-0.66676868	1.34086683	0.00000000
O	1.59979634	0.01013514	0.00000000
H	2.17125392	0.01400168	0.77619500
H	2.17125392	0.01400168	-0.77619500
Frequencies --	24.7, 161.2, 204.3, 251.2, 274.7, 293.9, 1607.2, 3788.5, 3895.1		

(3-12-19) Al<sub>2</sub>OH<sub>2</sub>(3)-TS1

Al	-1.90345853	-0.23329967	0.00302480
Al	0.55600801	0.53918800	0.00793424
H	0.85077946	2.09708301	0.03822263
O	1.79092822	-0.62751889	-0.09301024
H	2.33865151	-1.05348020	0.56339190
Frequencies --	-262.0, 106.4, 301.2, 332.1, 443.8, 593.4, 841.2, 1888.1, 3965.8		

(3-12-20) Al<sub>2</sub>OH<sub>2</sub>(3)-TS2

Al	-0.91459830	-0.59311146	0.00544745
Al	1.53149227	-0.14905729	0.00868840
H	-2.33598918	-1.28092102	0.03572247
O	-0.59883799	1.14011587	-0.09382825
H	-0.89292844	1.80818782	0.53113757
Frequencies --	-118.6, 256.5, 315.4, 334.9, 538.6, 622.4, 731.0, 1917.5, 3865.2		

(3-12-21) Al<sub>2</sub>OH<sub>2</sub>(3)-TS3

Al	1.53166408	0.02187619	-0.10075166
H	2.55595309	0.78721208	0.85390543
Al	-0.88343692	-0.77661780	0.04048925
O	-1.14239691	0.93959220	0.02827142

H                    -1.84373090      1.50769124     -0.29666552  
 Frequencies -- -141.8, 158.8, 285.8, 322.3, 347.9, 561.1, 759.4, 1845.8, 3894.7

(3-12-22) Al<sub>2</sub>OH<sub>2</sub>(3)-TS4

Al                    -1.74377280     -0.03015126     -0.03811475  
 Al                    1.87285417      0.13638603     -0.01409259  
 H                    0.62789489     -1.16237804      0.43406837  
 O                    -0.00139281     -0.20581019     -0.01264969  
 H                    -2.29481025      1.42780745      0.34582449  
 Frequencies -- -1376.6, 68.9, 126.6, 192.9, 426.5, 565.4, 742.3, 1271.2, 1785.6

(3-12-23) Al<sub>2</sub>OH<sub>2</sub>(3)-TS5

Al                    1.86787254     -0.07854449      0.00000000  
 Al                    -1.19055368     -0.79281113      0.00000000  
 O                    -0.96017804      1.04477535      0.00000000  
 H                    0.39324359      1.13423106      0.00000000  
 H                    -1.51696442      1.83518916      0.00000000  
 Frequencies -- -888.9, 130.3, 196.0, 293.9, 357.5, 583.1, 638.5, 1013.4, 3762.7

(3-13-1) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)

Al                    0.51576897     -1.02630203      0.00000000  
 Al                    -0.20202348      2.30094244      0.00000000  
 O                    -0.66850891     -2.24267831      0.00000000  
 O                    0.11021823      0.62277616      0.00000000  
 H                    -1.61582905     -2.10425596      0.00000000  
 H                    2.00346319     -1.50685209      0.00000000  
 Frequencies -- 77.0, 101.9, 252.7, 383.2, 494.0, 506.4, 606.5, 701.3, 862.0, 1041.3, 2003.9, 3934.4

(3-13-2) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-2

Al                    0.51492280     -1.03135294      0.00000000  
 Al                    -0.23536065      2.28032904      0.00000000  
 O                    -0.81930219     -2.08441381      0.00000000  
 O                    0.21137871      0.63303878      0.00000000  
 H                    -0.75507145     -3.03970564      0.00000000  
 H                    1.98415140     -1.58598349      0.00000000  
 Frequencies -- 66.9, 106.0, 271.3, 359.0, 499.2, 507.0, 572.4, 702.4, 866.2, 1052.6, 1972.7, 3934.0

(3-13-3) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-3

O                    0.00000000      0.00000000      1.16251500  
 O                    -0.00000000      0.00000000     -1.16251500  
 H                    0.00000000      0.00000000      2.12310800  
 Al                    0.00000000      1.52617800      0.00000000  
 H                    -0.00000000      0.00000000     -2.12310800  
 Al                    0.00000000     -1.52617800      0.00000000  
 Frequencies -- 140.4, 352.6, 372.7, 375.4, 456.2, 464.7, 476.9, 566.1, 807.8, 868.2, 3885.0, 3892.5

(3-13-4) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-adduct1

O                    1.90543198     -1.01180017     -0.09478661  
 O                    -0.48473885      0.09141328      0.02854012

H	1.09575147	-1.50454237	0.10824973
H	2.60775850	-1.32119155	0.49022141
Al	0.99657911	1.04529277	0.00026577
Al	-2.15573718	-0.26153669	-0.00553494
Frequencies --	94.9, 109.0, 146.1, 180.3, 255.2, 364.7, 455.9, 588.1, 938.7, 1574.0, 3716.3, 3855.2		

(3-13-5) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-adduct2

O	0.83911491	-1.84381954	0.00000000
H	1.14468832	-2.75238292	0.00000000
Al	-0.84918626	-1.30791675	0.00000000
O	0.27184199	0.57085579	0.00000000
H	1.08534649	0.02582117	0.00000000
Al	-0.00602067	2.30101457	0.00000000
Frequencies --	75.8, 86.9, 182.6, 260.3, 327.2, 598.8, 615.1, 680.0, 737.1, 898.2, 3560.9, 3910.2		

(3-13-6) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-adduct3

Al	-0.14547247	-0.83463412	0.00000000
Al	0.14071976	2.55322018	0.00000000
O	-0.25090158	-2.43538423	0.00000000
O	-0.02544311	0.83526958	0.00000000
H	0.93627242	-4.45370926	0.00000000
H	1.33627033	-5.08699219	0.00000000
Frequencies --	20.9, 73.4, 74.4, 202.6, 232.1, 233.7, 460.0, 482.1, 483.7, 944.2, 1183.9, 4329.4		

(3-13-7) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-adduct4

O	0.00000000	0.00000000	-1.07722498
O	0.00000000	0.00000000	1.45295102
Al	0.00000000	1.21957600	0.18984402
Al	0.00000000	-1.21957600	0.18984402
H	0.00000000	0.00000000	-3.59735098
H	0.00000000	0.00000000	-4.34440198
Frequencies --	19.5, 43.8, 169.7, 298.1, 404.1, 428.5, 516.6, 614.5, 628.4, 745.7, 785.3, 4367.4		

(3-13-8) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS1

Al	1.02605518	0.51483511	0.00939787
Al	-2.29157982	-0.23267489	-0.00505641
O	2.15957519	-0.72162489	-0.07878796
O	-0.63432082	0.17049011	0.01842973
H	2.74814114	-1.26680786	0.43191512
H	1.50164418	2.00780311	-0.00548816
Frequencies --	-384.8, 71.7, 106.4, 281.2, 305.8, 498.9, 509.4, 708.0, 885.5, 1047.6, 1985.6, 4035.1		

(3-13-9) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS2

O	-1.05105865	-1.35762735	0.19042379
H	-1.63556822	-2.11379839	0.08904490
Al	0.63258314	-1.41985485	-0.30896589
O	0.60725276	0.68172340	0.57645050

H	0.35506925	0.44065387	1.47898779
Al	-0.26097190	1.96449917	-0.28357465

Frequencies -- -151.9, 68.2, 132.4, 160.9, 363.1, 427.1, 601.0, 668.7, 720.4, 748.0, 3779.2, 3871.6

(3-13-10) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS3

O	-1.62220290	0.98665225	-0.08818215
H	-2.19831387	1.53826343	0.44728571
Al	-1.26035809	-0.89620076	0.00327729
O	0.44738801	0.07062908	0.03516214
H	-0.39101191	0.91734816	0.03489991
Al	2.18250001	0.05667290	-0.00774079

Frequencies -- -1058.0, 105.2, 119.6, 336.9, 397.2, 491.4, 562.4, 656.2, 888.6, 1202.6, 1789.8, 3878.9

(3-13-11) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS4

Al	0.04140471	-0.97652610	0.00000000
Al	-0.04910850	2.41846018	0.00000000
O	-0.37685491	-2.54883151	0.00000000
O	0.01473359	0.69697038	0.00000000
H	1.19388262	-2.28160788	0.00000000
H	1.80323719	-1.64864603	0.00000000

Frequencies -- -811.5, 75.0, 77.7, 240.4, 294.4, 459.4, 699.5, 942.8, 1073.0, 1156.3, 1674.6, 2493.1

(3-13-12) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS5

Al	-0.96447607	-0.63580711	-0.00667206
Al	2.33587993	0.24346587	0.00301984
O	-2.25921807	0.67398391	-0.08300081
O	0.67377293	-0.15839812	0.00573989
H	-2.48425304	1.51017085	0.36476231
H	-2.66043605	-0.53442114	0.30080406

Frequencies -- -1483.6, 71.8, 100.5, 199.9, 274.5, 323.5, 501.9, 592.5, 811.0, 1009.0, 1672.3, 3638.2

(3-13-13) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS6

O	-0.37272147	0.63170031	0.00000000
O	0.89126218	-2.00078715	0.00000000
H	-1.62199883	0.18892597	0.00000000
Al	0.34209810	2.24157859	0.00000000
H	1.01302873	-2.95133498	0.00000000
Al	-0.61435622	-1.18657060	0.00000000

Frequencies -- -1493.6, 84.2, 103.6, 247.1, 288.6, 323.1, 437.0, 560.6, 764.5, 813.6, 1662.6, 3920.3

(3-13-14) Al<sub>2</sub>O<sub>2</sub>H<sub>2</sub>(1)-TS7

Al	0.45467878	-1.00994794	0.00000000
Al	-1.21298996	1.05319527	0.00000000
O	1.46701394	0.26289993	0.00000000
O	-1.21393118	-0.72637173	0.00000000
H	3.58821109	1.39378466	0.00000000
H	4.24517213	1.75177457	0.00000000



Frequencies -- -206.7, 15.6, 34.8, 196.5, 244.0, 347.5, 462.6, 480.4, 625.8, 804.2, 1033.0, 4346.3

(3-14-1) AlO<sub>2</sub>H<sub>3</sub>(1)

Al	0.00274634	0.45911379	0.00000000
H	0.02042349	2.02437205	0.00000000
O	-1.50019649	-0.32209811	0.00000000
H	-1.62287051	-1.27197431	0.00000000
O	1.40756305	-0.49654544	0.00000000
H	2.30781210	-0.17172860	0.00000000

Frequencies -- 240.1, 334.9, 385.7, 509.0, 558.5, 617.1, 690.1, 799.5, 933.7, 1998.6, 3930.4, 3939.8

(3-14-2) AlO<sub>2</sub>H<sub>3</sub>(1)-2

Al	0.00000000	0.00000000	0.43484294
H	0.00000000	0.00000000	2.00744094
O	0.00000000	1.43475000	-0.46730906
H	0.00000000	2.31477400	-0.09172706
O	0.00000000	-1.43475000	-0.46730906
H	0.00000000	-2.31477400	-0.09172706

Frequencies -- 248.7, 300.7, 349.3, 498.9, 514.8, 608.2, 692.5, 781.0, 952.0, 1965.7, 3944.5, 3944.8

(3-14-3) AlO<sub>2</sub>H<sub>3</sub>(1)-adduct1

Al	-0.50328368	-0.83051614	0.00277711
O	-0.86348116	0.89973376	0.01966313
H	-1.73456826	1.29913452	-0.01597195
O	1.49609806	0.15347542	-0.09880466
H	1.07429481	1.02844330	0.00393232
H	2.14202602	0.04345858	0.60906940

Frequencies -- 186.0, 264.2, 312.1, 348.9, 459.1, 586.6, 684.7, 747.3, 1584.0, 3606.0, 3841.2, 3905.7

(3-14-4) AlO<sub>2</sub>H<sub>3</sub>(1)-adduct2

O	0.09634977	-2.56068556	0.00000000
H	-0.42771706	-2.82531751	0.76336400
H	-0.42771706	-2.82531751	-0.76336400
Al	-0.01426652	1.91582277	0.00000000
O	0.01370430	0.24293179	0.00000000
H	0.16046639	-0.71303082	0.00000000

Frequencies -- 48.4, 51.6, 179.2, 211.5, 221.5, 679.4, 770.1, 879.8, 1630.7, 3720.6, 3806.9, 3903.5

(3-14-5) AlO<sub>2</sub>H<sub>3</sub>(1)-adduct3

Al	-0.08908518	0.15617688	0.00000000
O	-0.36184044	-1.42314934	0.00000000
O	0.13322814	1.81034266	0.00000000
H	0.89248754	2.39080511	0.00000000
H	1.25116770	-4.07331639	0.00000000
H	0.84335051	-3.44533469	0.00000000

Frequencies -- 27.4, 33.6, 196.3, 208.1, 210.9, 444.9, 474.4, 480.6, 781.1, 1176.8, 3967.6, 4334.0

(3-14-6) AlO<sub>2</sub>H<sub>3</sub>(1)-adduct-4

Al	-0.06122041	0.10607835	0.00000000
O	-0.20443753	1.70226359	0.00000000
O	-0.11678259	-1.57620264	0.00000000
H	-0.87340499	-2.16226412	0.00000000
H	2.13968583	-0.49030832	0.00000000
H	2.09934547	0.26506631	0.00000000

Frequencies -- 182.6, 218.1, 226.3, 233.5, 323.7, 449.5, 540.2, 768.0, 786.5, 1167.8, 3946.3, 4227.3

(3-14-7) AlO<sub>2</sub>H<sub>3</sub>(1)-TS1

Al	-0.00644236	0.43796609	0.00964181
H	-0.07801186	2.00611607	0.01339572
O	1.46009789	-0.37199145	-0.08146830
H	2.19425804	-0.63729418	0.46248363
O	-1.42555406	-0.49506036	0.00782704
H	-2.30884618	-0.12596664	-0.01209288

Frequencies -- -363.4, 261.7, 339.4, 361.6, 499.8, 572.3, 704.0, 793.3, 954.7, 1975.8, 3932.8, 4028.2

(3-14-8) AlO<sub>2</sub>H<sub>3</sub>(1)-TS2

O	2.52539792	-0.22096973	-0.10210291
H	1.56180491	-0.13808978	-0.14542691
H	2.69681393	-0.36469472	0.83312309
Al	-1.72855908	-0.29993798	-0.00459191
O	-0.26188813	0.58727111	0.02721210
H	0.10457082	1.47156713	-0.02887490

Frequencies -- -54.1, 111.2, 163.3, 199.6, 291.0, 331.6, 673.5, 789.2, 1656.1, 3727.8, 3873.8, 3911.6

(3-14-9) AlO<sub>2</sub>H<sub>3</sub>(1)-TS3

Al	-0.01956261	0.03812278	0.00000000
O	0.32426958	1.62620229	0.00000000
O	-0.00118464	-1.63425246	0.00000000
H	0.70866482	-2.27520288	0.00000000
H	-1.80002791	0.58344866	0.00000000
H	-1.23900253	1.26055943	0.00000000

Frequencies -- -806.4, 167.9, 213.5, 264.8, 473.5, 732.1, 786.3, 1058.5, 1140.4, 1703.1, 2494.7, 3956.7

(3-14-10) AlO<sub>2</sub>H<sub>3</sub>(1)-TS4

Al	-0.01890635	0.03674534	0.00000000
O	0.29900715	1.62868242	0.00000000
O	0.17258490	-1.62141758	0.00000000
H	-0.42467300	-2.36726119	0.00000000
H	-1.83036965	0.58030990	0.00000000
H	-1.27191119	1.25114309	0.00000000

Frequencies -- -765.0, 108.2, 217.5, 260.6, 453.0, 677.5, 781.7, 1055.5, 1148.1, 1656.5, 2549.1, 3970.1

(3-14-11) AlO<sub>2</sub>H<sub>3</sub>(1)-TS5

Al	0.09154240	0.54794042	-0.01538481
O	-1.49066447	-0.37381403	-0.08659169
H	2.38817692	-0.19683689	0.07552022
O	1.46944714	-0.45902056	0.00783718
H	-1.55322707	0.88383915	0.37419155
H	-1.85526243	-1.14755100	0.38032697

Frequencies -- -1464.4, 184.6, 263.8, 299.3, 380.0, 510.5, 608.9, 789.8, 861.5, 1661.4, 3650.5, 3928.9

(3-14-12) AlO<sub>2</sub>H<sub>3</sub>(1)-TS6

Al	0.09571891	-0.53953945	-0.01166258
O	-1.50393311	0.38787853	-0.08256451
H	1.76649600	1.23921064	-0.09345096
O	1.56745516	0.30997966	0.03042745
H	-1.55941349	-0.90420158	0.25549223
H	-1.95960479	1.09613835	0.40666881

Frequencies -- -1471.2, 187.8, 233.0, 258.7, 329.0, 460.5, 585.4, 784.4, 861.4, 1691.4, 3654.7, 3912.6

●結合/解離過程において律速となる分子構造およびその振動状態@2000 K

(4) Al/O<sub>2</sub> 反応系

(4-1-1) Al + O (Doublet reaction surface)

Al	0.00000000	0.00000000	1.90476200
O	0.00000000	0.00000000	-3.09523800
Frequencies --	-71.5		

(4-2-1) Al + O<sub>2</sub> (Doublet reaction surface)

O	-0.30772608	1.28902036	0.00000000
O	0.23508723	2.38612346	0.00000000
Al	0.04470083	-2.26162697	0.00000000
Frequencies --	-74.1, 69.9, 1456.4		

(4-2-2) AlO + O (Doublet reaction surface)

O	0.00000000	0.00000000	2.89984483
Al	0.00000000	0.00000000	-0.47925517
O	0.00000000	0.00000000	-2.12105517
Frequencies --	-150.5, 82.6, 83.1		

(4-3-1) AlO + O<sub>2</sub> (Doublet reaction surface)

Al	0.04719341	0.80613696	0.00000000
O	0.04255621	2.44038527	0.00000000
O	0.32831852	-2.37690728	0.00000000
O	-0.44756402	-1.37345055	0.00000000
Frequencies --	-336.8, 124.8, 136.7, 340.7, 989.4, 1164.0		

(4-3-2) AlO<sub>2</sub> + O (Doublet reaction surface)

O	-0.51380712	-2.60369312	0.00000000
O	0.69678788	-0.86290818	0.00000000
Al	0.12623311	0.72850445	0.00000000
O	-0.38810956	2.28278157	0.00000000
Frequencies --	-279.3, 100.1, 215.0, 218.0, 681.0, 884.7		

(4-4-1) Al + Al (Singlet reaction surface)

Al	0.00000000	0.00000000	2.75000000
Al	-0.00000000	0.00000000	-2.75000000
Frequencies --	-42.2		

(4-5-1) Al + Al (Triplet reaction surface)

Al	0.00000000	0.00000000	2.80000000
Al	-0.00000000	0.00000000	-2.80000000
Frequencies --	-44.9		

(4-6-1) Al + AlO (Singlet reaction surface)

Al	4.44257699	0.00639232	0.00000000
O	-1.74776222	-0.05009823	0.00000000
Al	-3.36703101	0.02443736	0.00000000
Frequencies --	-14.4, 25.3, 997.2		

(4-6-2) Al<sub>2</sub>(3) + O (Singlet reaction surface)

O	0.00000000	0.00000000	3.90000000
Al	0.00000000	0.00000000	0.17885800
Al	0.00000000	0.00000000	-2.57885800
Frequencies --	-128.5, 52.0, 60.8, 250.4		

(4-7-1) Al + AlO (Triplet reaction surface)  
 Al 0.00000000 0.00000000 -2.46828647  
 O 0.00000000 0.00000000 0.50736553  
 Al 0.00000000 0.00000000 2.15606153  
 Frequencies -- -142.0, 94.8, 96.9, 912.6

(4-8-1) Al + AlO<sub>2</sub> (Singlet reaction surface)  
 Al 0.00000000 0.00000000 -2.48754286  
 Al 0.00000000 0.00000000 5.51245714  
 O 0.00000000 0.00000000 -0.81134286  
 O 0.00000000 0.00000000 -4.10414286  
 Frequencies -- -34.3, 22.3, 27.7, 227.9, 242.6, 688.2, 944.7

(4-8-2) Al<sub>2</sub>(3) + O<sub>2</sub> (Singlet reaction surface)  
 Al -0.00000000 -0.00000000 -0.16998762  
 Al 0.00000000 0.00000000 -3.04058762  
 O -0.00000000 -0.00000000 3.29471238  
 O 0.00000000 -0.00000000 1.92247238  
 Frequencies -- -134.7, 109.9, 110.0, 148.8, 185.4, 240.0, 874.8

(4-8-3) AlO + AlO (Singlet reaction surface)  
 Al 0.00000000 0.00000000 -1.77427812  
 O 0.00000000 0.00000000 -3.41963012  
 Al 0.00000000 0.00000000 3.03478288  
 O 0.00000000 0.00000000 1.37130988  
 Frequencies -- -165.5, 87.6, 87.6, 133.7, 133.7, 863.5, 935.0

(4-9-1) Al + AlO<sub>2</sub> (Triplet reaction surface)  
 Al 1.66905738 -0.03329646 0.00000000  
 Al -3.73006263 0.06418764 0.00000000  
 O 3.33263771 0.14480659 0.00000000  
 O 0.01649582 -0.19500476 0.00000000  
 Frequencies -- -65.4, 38.3, 154.6, 183.0 714.9, 803.1

(4-9-2) Al<sub>2</sub>O(1) + O (Triplet reaction surface)  
 O 0.00000000 0.00000000 -0.95364876  
 O 0.00000000 0.00000000 4.04635124  
 Al 0.00000000 0.00000000 -2.68190476  
 Al 0.00000000 0.00000000 0.77870324  
 Frequencies -- -105.3, 44.0, 45.8, 131.4, 131.8, 497.6, 962.7

(4-9-3) AlO + AlO (Triplet reaction surface)  
 O 3.10153405 -0.36671277 0.00000000  
 Al 1.57677645 0.32275204 0.00000000  
 O -1.13327301 -0.07822260 0.00000000  
 Al -2.78801401 -0.04894565 0.00000000  
 Frequencies -- -214.6, 77.8, 97.2, 119.4, 728.1, 908.2

(4-10-1) Al + AlO<sub>3</sub> (Singlet reaction surface)  
 O 0.00000000 -0.75108700 3.66849676  
 O -0.00000000 0.75108700 3.66849676  
 Al 0.00000000 -0.00000000 2.05263476  
 O 0.00000000 -0.00000000 0.42866776

Al 0.00000000 0.00000000 -6.83150324  
 Frequencies -- -21.8, 25.4, 28.6, 237.5, 255.9, 504.1, 599.5, 806.8, 1090.4

(4-10-2) Al<sub>2</sub>O<sub>2</sub>(3) + O (Singlet reaction surface)

Al 0.00000000 0.00000000 -2.02815666  
 O 0.00000000 0.00000000 4.17184334  
 Al 0.00000000 0.00000000 0.43206434  
 O 0.00000000 1.27672300 -0.78909666  
 O 0.00000000 -1.27672300 -0.78909666  
 Frequencies -- -122.9, 68.2, 75.4, 284.3, 502.0, 597.2, 709.1, 715.8, 766.8

(4-10-3) AlO + AlO<sub>2</sub> (Singlet reaction surface)

Al 0.00000000 0.00000000 -2.17348598  
 Al 0.00000000 0.00000000 2.29724102  
 O 0.00000000 0.00000000 3.95578702  
 O 0.00000000 0.00000000 -0.37013298  
 O 0.00000000 0.00000000 -3.78675598  
 Frequencies -- -208.5, 116.8, 116.8, 208.3, 208.3, 239.2, 239.2, 517.1, 911.7, 1084.0

(4-11-1) Al + AlO<sub>3</sub> (Triplet reaction surface)

O -0.04168486 2.86622165 0.68283700  
 O -0.04168486 2.86622165 -0.68283700  
 Al 0.04584572 1.11508307 0.00000000  
 O 0.05071562 -0.50209211 0.00000000  
 Al -0.02575089 -4.33376072 0.00000000  
 Frequencies -- -77.0, 44.7, 49.6, 141.5, 164.6, 401.7, 481.6, 1084.8, 1145.4

(4-11-2) Al<sub>2</sub>O<sub>2</sub>(1) + O (Triplet reaction surface)

O 0.00000000 0.00000000 -4.11400486  
 Al 0.00000000 0.00000000 -0.43880686  
 Al 0.00000000 0.00000000 2.01079614  
 O 0.00000000 1.27550400 0.77976114  
 O 0.00000000 -1.27550400 0.77976114  
 Frequencies -- -119.6, 58.1, 62.6, 300.0, 503.8, 610.1, 625.2, 745.0, 782.7

(4-11-3) AlO + AlO<sub>2</sub> (Triplet reaction surface)

Al 0.01949523 -2.26751822 0.00000000  
 O 0.02890726 -3.94257015 0.00000000  
 O 0.00389185 -0.61932273 0.00000000  
 Al -0.17451665 2.53063536 0.00000000  
 O 0.21911070 4.13432753 0.00000000  
 Frequencies -- -99.8, 29.5, 41.8, 53.5, 216.3, 232.8, 741.3, 876.9, 891.2

(4-12-1) Al<sub>2</sub>O<sub>2</sub>(3) + O<sub>2</sub> (Singlet reaction surface)

O 1.24800138 1.10289750 0.00000000  
 O -1.28926678 1.25792748 0.00000000  
 Al -0.09441976 -0.06410205 0.00000000  
 Al 0.05388171 2.39993816 0.00000000  
 O -0.27881305 -3.61263885 0.00000000  
 O 0.38595278 -2.54391981 0.00000000  
 Frequencies -- -233.9, 34.8, 96.0, 98.9, 306.1, 324.0, 493.3, 600.4, 641.3, 742.1, 778.5, 1225.4

(4-12-2) Al<sub>2</sub>O<sub>3</sub>(3) + O (Singlet reaction surface)

Al 0.00000000 0.00000000 -1.46822410

O	0.00000000	0.00000000	4.53177590
O	0.00000000	1.27147600	-0.25769210
O	0.00000000	-1.27147600	-0.25769210
Al	0.00000000	0.00000000	0.97344590
O	0.00000000	0.00000000	-3.21237710

Frequencies -- -139.0, 60.3, 65.3, 151.7, 175.0, 349.3, 437.8, 629.3, 668.8, 751.0, 756.4, 922.1

(4-12-3) AlO + AlO<sub>3</sub> (Singlet reaction surface)

Al	0.00000000	0.00000000	1.65126339
O	0.00000000	-0.82554986	3.14920426
O	-0.00000000	0.82554986	3.14920426
O	0.00000000	0.00000000	-0.18483663
Al	0.00000000	0.00000000	-2.71643686
O	0.00000000	0.00000000	-4.38103628

Frequencies -- -193.4, 120.7, 130.8, 228.3, 231.5, 250.4, 279.9, 434.9, 598.0, 759.7, 896.0, 981.7

(4-12-4) AlO<sub>2</sub> + AlO<sub>2</sub> (Singlet reaction surface)

Al	0.00000000	0.00000000	-2.41219697
Al	0.00000000	0.00000000	2.48780303
O	0.00000000	1.65387000	-2.56067997
O	0.00000000	-1.65387000	-2.56067997
O	0.00000000	0.00000000	0.83553803
O	0.00000000	0.00000000	4.16296203

Frequencies -- -83.3, 31.4, 55.4, 80.3, 183.4, 213.3, 216.9, 238.7, 745.5, 775.1, 825.2, 845.1

(4-13-1) Al<sub>2</sub>O<sub>2</sub>(1) + O<sub>2</sub> (Triplet reaction surface)

O	1.24751647	1.06641906	0.00000000
O	-1.29148483	1.23811488	0.00000000
Al	-0.10281150	-0.07958462	0.00000000
Al	0.06078713	2.37627153	0.00000000
O	-0.28825523	-3.54018436	0.00000000
O	0.40051317	-2.49646580	0.00000000

Frequencies -- -214.6, 24.3, 85.1, 88.5, 301.1, 313.2, 496.0, 606.1, 639.4, 743.7, 779.6, 1277.3

(4-13-2) Al<sub>2</sub>O<sub>3</sub>(1) + O (Triplet reaction surface)

O	4.89054897	0.47644596	0.00000000
O	-0.78255313	-0.07664765	0.00000000
Al	0.89476016	-0.21609533	0.00000000
Al	-2.45978838	0.07074911	0.00000000
O	2.49449946	-0.37492881	0.00000000
O	-4.05932444	0.21131812	0.00000000

Frequencies -- -6.15, 50.9, 61.1, 79.9, 192.7, 193.2, 285.7, 286.3, 427.4, 938.2, 1146.4, 1244.7

(4-13-3) AlO + AlO<sub>3</sub> (Triplet reaction surface)

O	0.00000000	-0.68267112	3.31652855
O	-0.00000000	0.68267112	3.31652855
O	0.00000000	0.00000000	-4.48347140
Al	0.00000000	0.00000000	-2.82313240
Al	0.00000000	0.00000000	1.55199060
O	0.00000000	0.00000000	-0.08398040

Frequencies -- -152.1, 86.2, 89.7, 97.7, 98.5, 223.4, 230.3, 385.6, 471.4, 895.9, 1017.6, 1141.5

(4-13-4) AlO<sub>2</sub> + AlO<sub>2</sub> (Triplet reaction surface)

Al	0.00000000	0.00000000	-2.24845048
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Al	0.00000000	0.00000000	2.35154952
O	0.00000000	1.65227346	-2.44476416
O	0.00000000	-1.65227346	-2.44476416
O	0.00000000	0.00000000	0.69514952
O	0.00000000	0.00000000	4.02674952

Frequencies -- -128.6, 33.1, 71.3, 104.9, 189.4, 216.5, 220.7, 242.6, 746.1, 769.1, 809.2, 834.6

(4-14-1) Al<sub>2</sub>O<sub>3</sub>(1) + Al<sub>2</sub>O<sub>3</sub>(1) (Singlet reaction surface)

O	3.68216246	0.34207952	0.00000000
O	-3.59860869	-0.18742155	0.00000000
Al	1.96774541	0.34665838	0.00000000
O	0.34208998	0.48953279	0.00000000
Al	5.36564929	0.22637744	0.00000000
O	6.96833957	0.13544609	0.00000000
Al	-1.99378428	-0.85183972	0.00000000
O	-1.12098868	-2.21882679	0.00000000
Al	-5.13637648	0.46993794	0.00000000
O	-6.60324980	1.12859714	0.00000000

Frequencies -- -129.1, 20.1, 24.7, 51.2, 66.3, 77.2, 121.7, 163.8, 183.6, 201.6, 217.8, 218.5, 277.6, 291.4, 299.7, 309.3, 399.1, 419.7, 898.2, 919.1, 1083.4, 1093.0, 1204.4, 1212.9

(4-14-2) Al<sub>2</sub>O<sub>3</sub>(3) + Al<sub>2</sub>O<sub>3</sub>(3) (Singlet reaction surface)

Al	0.00000000	0.00000000	2.86405621
Al	0.00000000	-0.00000000	5.28855620
O	0.00000000	1.28017900	4.10928021
O	0.00000000	-1.28017900	4.10928021
O	0.00000000	0.00000000	1.11785621
Al	0.00000000	0.00000000	-4.43594378
Al	0.00000000	0.00000000	-1.86054379
O	1.24758187	-0.00000000	-3.10328514
O	-1.24758187	-0.00000000	-3.10328514

Frequencies -- -144.2, 14.5, 52.1, 62.8, 83.7, 111.9, 149.7, 174.2, 203.5, 216.2, 340.7, 373.5, 388.4, 428.2, 528.8, 556.7, 608.3, 631.4, 706.7, 716.1, 764.8, 769.0, 834.8, 862.3

(4-15-1) Al<sub>2</sub>O<sub>2</sub>(1) + Al<sub>2</sub>O<sub>4</sub>(3) (Triplet reaction surface)

O	0.00000000	-1.26570000	3.05904000
O	-0.00000000	1.26570000	3.05904000
Al	0.00000000	-0.00000000	1.67204000
Al	0.00000000	-0.00000000	4.20864000
O	0.00000000	0.00000000	-0.11646000
O	0.00000000	-0.00000000	5.95774000
O	-1.26120000	0.00000000	-4.14096000
O	1.26120000	0.00000000	-4.14096000
Al	0.00000000	0.00000000	-5.33886000
Al	0.00000000	0.00000000	-2.80486000

Frequencies -- -151.2, 14.9, 59.0, 76.6, 121.5, 122.5, 171.1, 180.6, 237.2, 243.4, 330.4, 344.3, 386.0, 457.8, 471.0, 506.5, 532.0, 572.7, 688.6, 719.4, 761.5, 798.1, 843.1, 958.2

(4-15-2) Al<sub>2</sub>O<sub>3</sub>(1) + Al<sub>2</sub>O<sub>3</sub>(3) (Triplet reaction surface)

O	0.00000000	0.00000000	-3.98329272
O	0.00000000	0.00000000	-0.62169272
O	0.00000000	0.00000000	-7.27459272
Al	0.00000000	0.00000000	-5.66809272
Al	0.00000000	0.00000000	-2.26529272



Al	0.00000000	0.00000000	4.71670728
Al	0.00000000	0.00000000	2.23890728
O	1.26704100	-0.00000000	3.50207428
O	-1.26704100	-0.00000000	3.50207428
O	0.00000000	0.00000000	6.46430728

Frequencies -- -129.6, 30.2, 30.6, 50.7, 57.4, 111.3, 114.4, 141.5, 177.7, 208.8, 209.5, 285.3, 285.6, 343.1, 369.9, 426.0, 601.3, 653.6, 722.8, 745.7, 855.0, 912.9, 1057.8, 1202.2

(4-16-1) Al<sub>2</sub>O<sub>3</sub>(3) + Al<sub>2</sub>O<sub>4</sub>(3) (Singlet reaction surface)

Al	0.00000000	0.00000000	4.95561822
O	0.00000000	1.26600000	-3.64438178
O	0.00000000	-1.26600000	-3.64438178
Al	0.00000000	0.00000000	-4.79598178
Al	0.00000000	0.00000000	-2.27008178
O	0.00000000	0.00000000	-6.54498178
O	0.00000000	0.00000000	-0.49598178
Al	0.00000000	0.00000000	2.34971822
O	1.23858200	-0.00000000	3.62399522
O	-1.23858200	-0.00000000	3.62399522
O	0.00000000	0.00000000	6.69291822

Frequencies -- -135.4, 13.2, 55.1, 67.8, 94.4, 100.7, 152.3, 153.0, 203.1, 210.6, 228.6, 232.4, 336.8, 377.7, 382.8, 402.8, 471.6, 532.2, 542.0, 616.8, 685.1, 705.4, 724.0, 750.6, 838.2, 888.4, 956.7

(4-17-1) Al<sub>2</sub>O<sub>3</sub>(1) + Al<sub>2</sub>O<sub>4</sub>(3) (Triplet reaction surface)

O	-4.13177324	-0.24067036	0.00000000
O	3.88204564	1.38088156	0.00000000
O	3.23455872	-1.08058276	0.00000000
Al	2.36739003	0.45171438	0.00000000
O	0.78225221	1.16402151	0.00000000
Al	4.70403784	-0.14762766	0.00000000
O	6.38779733	-0.60913692	0.00000000
Al	-2.45631791	-0.46343939	0.00000000
O	-0.87204096	-0.78519484	0.00000000
Al	-5.79125845	0.05603054	0.00000000
O	-7.37159841	0.33858028	0.00000000

Frequencies -- -44.0, 16.9, 19.5, 21.8, 52.4, 68.3, 92.5, 102.1, 161.7, 194.6, 197.1, 213.1, 222.2, 291.9, 292.8, 382.0, 394.1, 421.0, 629.6, 647.6, 720.5, 799.3, 899.1, 926.4, 951.3, 1129.3, 1228.1

(4-18-1) Al<sub>2</sub>O<sub>4</sub>(3) + Al<sub>2</sub>O<sub>4</sub>(3) (Singlet reaction surface)

Al	2.57611914	0.35156336	0.00000000
Al	-2.57611914	-0.35156336	0.00000000
O	0.87619018	0.79936080	0.00000000
O	-0.87619018	-0.79936080	0.00000000
O	3.50979546	-1.12639210	0.00000000
O	3.99541702	1.37669698	0.00000000
Al	4.92670337	-0.10257474	0.00000000
O	6.63740427	-0.43659462	0.00000000
O	-3.99541702	-1.37669698	0.00000000
O	-3.50979546	1.12639210	0.00000000
Al	-4.92670337	0.10257474	0.00000000
O	-6.63740427	0.43659462	0.00000000

Frequencies -- -88.9, 17.7, 20.4, 22.6, 39.1, 63.3, 89.6, 97.7, 150.0, 167.1, 199.8, 204.3, 208.5, 250.6, 377.4, 382.5, 387.3, 395.9, 623.6, 627.1, 667.9, 667.9, 719.3, 719.3, 801.6, 803.3, 880.4, 899.5, 947.9, 948.6

(4-19-1) Al<sub>2</sub>O<sub>4</sub>(1) + Al<sub>2</sub>O<sub>4</sub>(3) (Triplet reaction surface)

Al	2.57611961	0.35158048	0.00000000
Al	-2.57611961	-0.35158048	0.00000000
O	0.87621213	0.79938149	0.00000000
O	-0.87621213	-0.79938149	0.00000000
O	3.50980032	-1.12640526	0.00000000
O	3.99542319	1.37670389	0.00000000
Al	4.92674785	-0.10258038	0.00000000
O	6.63744266	-0.43661577	0.00000000
O	-3.99542319	-1.37670389	0.00000000
O	-3.50980032	1.12640526	0.00000000
Al	-4.92674785	0.10258038	0.00000000
O	-6.63744266	0.43661577	0.00000000

Frequencies -- -88.9, 17.7, 20.4, 23.1, 39.1, 63.4, 89.3, 97.4, 150.0, 167.0, 199.8, 204.3, 208.5, 250.7, 377.4, 382.5, 387.3, 396.0, 623.7, 627.2, 667.8, 667.8, 719.1, 719.3, 801.6, 803.3, 880.4, 899.7, 948.0, 949.0

(4-20-1) Al<sub>4</sub>O<sub>6</sub>(1) + Al<sub>4</sub>O<sub>6</sub>(1) (Singlet reaction surface)

O	5.44085468	-0.80414116	0.00000000
Al	1.91501300	-0.82434797	0.00000000
Al	4.33311743	-0.38796536	1.31261833
Al	4.33311743	-0.38796536	-1.31261833
O	2.84290228	-1.28748876	1.40646980
O	2.84290228	-1.28748876	-1.40646980
O	1.43960049	0.87801471	0.00000000
Al	3.03652441	1.61837673	0.00000000
O	3.97834625	1.31696138	1.42865604
O	3.97834625	1.31696138	-1.42865604
O	-5.44085468	0.80414116	0.00000000
Al	-1.91501300	0.82434797	0.00000000
Al	-4.33311743	0.38796536	1.31261833
Al	-4.33311743	0.38796536	-1.31261833
O	-2.84290228	1.28748876	1.40646980
O	-2.84290228	1.28748876	-1.40646980
O	-1.43960049	-0.87801471	0.00000000
Al	-3.03652441	-1.61837673	0.00000000
O	-3.97834625	-1.31696138	1.42865604
O	-3.97834625	-1.31696138	-1.42865604

Frequencies -- -68.0, 21.9, 25.6, 47.3, 64.9, 100.3, 140.9, 141.7, 222.4, 226.8, 236.7, 237.0, 256.0, 260.9, 261.5, 266.7, 305.7, 309.7, 310.4, 315.5, 340.2, 346.0, 404.7, 407.9, 408.9, 411.3, 426.8, 428.6, 509.4, 515.7, 614.3, 616.4, 650.3, 651.9, 653.9, 658.1, 669.3, 669.8, 741.6, 742.6, 747.1, 747.3, 755.4, 755.9, 763.6, 768.1, 768.1, 771.6, 825.3, 829.5, 833.0, 834.0, 847.2, 868.0

(5) Al/CO<sub>2</sub> 反応系

(5-1) AlO + CO (Doublet reaction surface)

O	1.08390993	-0.53778291	0.00000000
Al	-0.46715348	-1.22804538	0.00000000
C	-0.33017912	0.81086959	0.00000000
O	-0.07715119	1.92520447	0.00000000

Frequencies -- -249.3, 266.4, 310.6, 436.3, 854.1, 2074.1

(5-2-1) Al + AlCO<sub>2</sub> (Singlet reaction surface)

O	0.00000000	-1.09119000	1.11966773
O	-0.00000000	1.09119000	1.11966773
Al	0.00000000	0.00000000	-4.38033227
C	0.00000000	-0.00000000	0.46431873
Al	0.00000000	-0.00000000	2.78797873

Frequencies -- -55.7, 38.2, 38.3, 255.9, 315.6, 387.7, 785.4, 1238.9, 1421.2

(5-2-2) Al + AlCO<sub>2</sub> (Triplet reaction surface)

C	0.00000000	0.00000000	-0.00629360
Al	0.00000000	0.00000000	-2.34508760
O	0.00000000	-1.09672000	-0.63075760
O	-0.00000000	1.09672000	-0.63075760
Al	0.00000000	-0.00000000	3.12430940

Frequencies -- -108.9, 77.5, 77.9, 207.7, 326.2, 397.8, 788.9, 1262.8, 1501.2

(5-3) AlO + AlCO<sub>2</sub> (Singlet reaction surface)

O	0.00000000	0.00000000	-2.42514189
Al	0.00000000	0.00000000	-4.08384189
Al	0.00000000	-0.00000000	0.86529211
C	0.00000000	-0.00000000	3.22572411
O	-1.09700000	0.00000000	2.61799611
O	1.09700000	0.00000000	2.61799611

Frequencies -- -111.3, 43.7, 54.9, 104.9, 108.1, 179.7, 267.9, 372.1, 794.5, 890.9, 1284.8, 1552.0

(6) Al/H<sub>2</sub>O 反応系

(6-1-1) AlO + H (Singlet reaction surface)

O	0.00000000	0.00000000	-0.86961427
Al	0.00000000	0.00000000	0.77896373
H	0.00000000	0.00000000	-3.16961427
Frequencies --	-715.0, 269.6, 269.6, 908.3		

(6-1-2) Al + OH (Singlet reaction surface)

O	0.00447630	0.00000000	-3.53994666
H	-0.03087530	0.00000000	-4.50941433
Al	-0.00037962	0.00000000	2.52530674
Frequencies --	-15.3, 32.8, 3790.6		

(6-1-3) Al + OH (Triplet reaction surface)

Al	1.23982073	0.01074582	0.00000000
O	-1.71663346	-0.09474929	0.00000000
H	-2.38460178	0.61829866	0.00000000
Frequencies --	-180.3, 312.3, 3681.1		

(6-2-1) AlO<sub>2</sub> + H (Singlet reaction surface)

H	3.46998989	0.80907220	0.00000000
Al	-0.13637320	-0.01805855	0.00000000
O	1.55869666	-0.14478370	0.00000000
O	-1.77083895	0.07299482	0.00000000
Frequencies --	-967.6, 219.0, 219.3, 371.1, 682.9, 900.4		

(6-2-2) AlO + OH (Singlet reaction surface)

H	3.32810739	-0.46276409	0.00000000
O	-2.14178597	0.11192421	0.00000000
O	2.54156842	0.13309409	0.00000000
Al	-0.50202823	-0.11518325	0.00000000
Frequencies --	-232.4, 124.2, 290.0, 551.1, 903.1, 3549.3		

(6-2-3) AlO<sub>2</sub> + H (Triplet reaction surface)

Al	0.00000000	0.00000000	-0.04027413
H	0.00000000	0.00000000	2.75972587
O	0.00000000	1.66150614	-0.13976288
O	0.00000000	-1.66150614	-0.13976288
Frequencies --	-553.3, 194.9, 218.3, 224.8, 760.2, 866.5		

(6-2-4) AlOH(1) + O (Triplet reaction surface)

O	2.73489179	0.03788401	0.00000000
O	-1.96488708	-0.00770824	0.00000000
Al	-0.25603716	-0.04879051	0.00000000
H	-2.83155466	0.39287051	0.00000000
Frequencies --	-137.6, 67.3, 103.5, 172.2, 810.4, 3971.1		

(6-2-5) AlO + OH (Triplet reaction surface)

O	-2.29505499	-0.11099182	0.00000000
Al	0.59783117	0.58662330	0.00000000
O	1.61128738	-0.70617988	0.00000000
H	-2.30166428	-1.08872929	0.00000000

Frequencies -- -98.5, 64.0, 117.0, 326.3, 936.5, 3677.8

(6-3-1)  $\text{AlO}_3 + \text{H}$  (Singlet reaction surface)

Al	0.00000000	0.00000000	0.26539537
H	0.00000000	0.00000000	3.76539537
O	0.00000000	0.71587300	-1.38806863
O	0.00000000	-0.71587300	-1.38806863
O	0.00000000	0.00000000	1.87419537

Frequencies -- -1279.0, 168.0, 212.8, 357.0, 370.6, 542.3, 552.1, 906.1, 1137.5

(6-3-2)  $\text{AlO}_2 + \text{OH}$  (Singlet reaction surface)

Al	0.00000000	0.00000000	-0.83175137
H	0.00000000	0.00000000	3.66824863
O	0.00000000	1.65834403	-0.89863615
O	0.00000000	-1.65834403	-0.89863615
O	0.00000000	0.00000000	2.69032963

Frequencies -- -63.5, 41.1, 104.0, 206.3, 216.8, 264.6, 773.8, 837.4, 3675.7

(6-3-3)  $\text{AlO}_3 + \text{H}$  (Triplet reaction surface)

Al	0.00000000	-0.00000000	0.29615368
H	0.00000000	-0.00000000	3.79615368
O	0.00000000	-0.00000000	1.92303168
O	0.00000000	-0.68369800	-1.43940032
O	-0.00000000	0.68369800	-1.43940032

Frequencies -- -856.6, 168.6, 178.1, 260.3, 265.1, 434.2, 530.5, 1049.1, 1139.9

(6-3-4)  $\text{AlO}_2 + \text{OH}$  (Triplet reaction surface)

Al	0.56260495	0.23907990	0.00000000
H	-2.85268282	-0.89925637	0.00000000
O	-0.56507121	1.46365529	0.00000000
O	1.87379884	-0.79119287	0.00000000
O	-1.86637532	-0.94856021	0.00000000

Frequencies -- -233.7, 104.7, 208.7, 212.8, 333.0, 527.4, 759.3, 831.4, 3553.1

(6-4-1)  $\text{Al}_2\text{O}(1) + \text{H}$  (Doublet reaction surface)

H	4.33054526	0.57491328	0.00000000
O	-0.12947023	-0.02363645	0.00000000
Al	1.60237509	-0.07185129	0.00000000
Al	-1.85581997	0.04217270	0.00000000

Frequencies -- -399.9, 118.3, 125.6, 149.1, 498.1, 965.7

(6-4-2)  $\text{Al}_2(3) + \text{OH}$  (Doublet reaction surface)

O	0.10331202	4.08410881	0.00000000
H	-0.86808852	4.11585050	0.00000000
Al	0.00858413	-0.00371610	0.00000000
Al	-0.00538472	-2.82618551	0.00000000

Frequencies -- -92.8, 37.8, 45.2, 216.1, 243.3, 3728.3

(6-4-3)  $\text{Al} + \text{AlOH}(1)$  (Doublet reaction surface)

Al	2.65551804	0.04260882	0.00000000
O	-2.54446745	0.03032537	0.00000000
Al	-0.83591922	-0.10872308	0.00000000

H                    -3.29904512    0.61688254    0.00000000  
 Frequencies --   -73.8, 64.8, 123.5, 261.1, 807.8, 3955.3

(6-5-1) Al<sub>2</sub>O<sub>2</sub>(1) + H (Doublet reaction surface)

O                    0.00000000   -1.27507800   -0.11226442  
 O                    -0.00000000   1.27507800   -0.11226442  
 Al                   0.00000000   0.00000000   -1.33023942  
 Al                   0.00000000   -0.00000000   1.12320058  
 H                    0.00000000   -0.00000000   4.48773558  
 Frequencies --   -517.2, 184.1, 195.1, 300.6, 502.7, 607.4, 628.1, 744.4, 782.0

(6-5-2) Al<sub>2</sub>OH + O (Doublet reaction surface)

O                    -1.06892471   0.07239117   0.00000000  
 Al                   0.61078218   0.43245357   0.00000000  
 H                    1.10020598   1.95418263   0.00000000  
 Al                   -2.74741185   -0.33289408   0.00000000  
 O                    4.40342216   -0.47844818   0.00000000  
 Frequencies --   -105.1, 53.0, 91.9, 139.4, 166.5, 498.9, 592.5, 989.5, 1821.7

(6-5-3) Al<sub>2</sub>O(1) + OH (Doublet reaction surface)

H                    4.17420039   -0.11619162   0.00000000  
 O                    -0.92567908   -0.08112890   0.00000000  
 O                    3.28074691   0.33771664   0.00000000  
 Al                   0.86063015   -0.31007027   0.00000000  
 Al                   -2.63099500   0.16110794   0.00000000  
 Frequencies --   -309.0, 102.5, 150.0, 171.0, 425.6, 429.3, 783.8, 881.9, 3337.9

(6-5-4) Al + AlO<sub>2</sub>H(1) (Doublet reaction surface)

Al                   -1.56746734   0.06894740   0.00000000  
 O                    0.04683786   0.16606683   0.00000000  
 O                    -3.24886616   -0.06101749   0.00000000  
 H                    -3.80670557   -0.83925109   0.00000000  
 Al                    3.83076981   -0.06903538   0.00000000  
 Frequencies --   -78.1, 40.6, 53.8, 175.9, 191.2, 479.5, 737.4, 1150.4, 3929.6

(6-5-5) AlO + AlOH(1) (Doublet reaction surface)

Al                    3.02572087   0.02717560   0.00000000  
 O                    -3.27427605   0.02094677   0.00000000  
 O                    1.33630549   0.01660827   0.00000000  
 Al                   -1.52937541   -0.10426110   0.00000000  
 H                    -3.94872642   0.70167127   0.00000000  
 Frequencies --   -157.4, 87.6, 125.8, 146.3, 148.5, 328.6, 730.0, 803.9, 3914.1

(6-6-1) Al<sub>2</sub>O<sub>3</sub>(3) + H (Doublet reaction surface)

Al                   -0.06819333   0.65211406   0.00000000  
 O                    1.28776899   -0.45075663   0.00000000  
 O                    -1.26308285   -0.62498906   0.00000000  
 Al                   0.09617697   -1.75992167   0.00000000  
 O                    -0.26182136   2.37938816   0.00000000  
 H                    1.53329437   3.97235911   0.00000000  
 Frequencies --   -670.2, 131.9, 176.5, 253.6, 295.8, 341.6, 445.6, 635.2, 677.3, 746.8,  
 768.6, 923.1

(6-6-2) Al<sub>2</sub>O<sub>2</sub>H + O (Doublet reaction surface)

Al	0.00000000	0.00000000	0.49602675
O	0.00000000	1.27550199	-0.71634528
O	0.00000000	-1.27550199	-0.71634528
Al	0.00000000	0.00000000	-1.92856425
O	0.00000000	0.00000000	4.19602675
H	0.00000000	0.00000000	-3.48899825

Frequencies -- -125.0, 51.7, 54.5, 262.5, 474.8, 510.6, 537.2, 645.6, 733.2, 776.1, 795.2, 2027.9

(6-6-3) Al<sub>2</sub>OH + O<sub>2</sub> (Doublet reaction surface)

Al	0.12268912	1.11855807	-0.14765103
O	-1.32372501	0.22980026	-0.03593919
H	0.45344332	2.42503686	0.69122022
Al	-2.74044615	-0.75729355	0.04238363
O	2.33414394	-0.16473234	0.29659668
O	3.18675582	-0.95525237	-0.17600049

Frequencies -- -233.9, 49.9, 83.7, 115.4, 136.1, 180.4, 346.7, 501.8, 573.2, 1009.8, 1281.7, 1882.1

(6-6-4) Al<sub>2</sub>O<sub>2</sub>(1) + OH (Doublet reaction surface)

Al	-0.39351499	-0.11368217	0.00000000
O	0.69506217	1.26771670	0.00000000
O	0.92132387	-1.27849332	0.00000000
Al	2.03083603	0.10292654	0.00000000
O	-3.79337399	-0.08268377	0.00000000
H	-3.86926988	0.88750624	0.00000000

Frequencies -- -166.6, 67.8, 70.9, 89.6, 299.2, 395.6, 506.0, 616.9, 636.1, 755.5, 788.4, 3720.6

(6-6-5) AlO + AlO<sub>2</sub>H(1) (Doublet reaction surface)

O	0.03333831	0.21072622	0.00000000
Al	-0.26180764	1.83837372	0.00000000
O	0.15283825	3.47761918	0.00000000
H	1.00714160	3.91376467	0.00000000
O	0.00796347	-3.78919297	0.00000000
Al	0.06486442	-2.07737250	0.00000000

Frequencies -- -298.6, 100.9, 134.7, 166.5, 167.1, 236.5, 241.4, 463.7, 639.2, 773.8, 1020.8, 3902.0

(6-6-6) AlO<sub>2</sub> + AlOH(1) (Doublet reaction surface)

Al	0.57555117	-2.24608573	0.00000000
O	-0.59471572	-3.46715905	0.00000000
H	-1.55213069	-3.51475445	0.00000000
Al	-0.02710676	2.11244652	0.00000000
O	0.05017179	0.39136098	0.00000000
O	-0.15266189	3.73230610	0.00000000

Frequencies -- -260.9, 72.3, 87.2, 131.7, 231.9, 250.5, 272.8, 436.9, 648.0, 862.6, 1009.6, 3918.2

(6-7-1) Al<sub>2</sub>O<sub>3</sub>H + O (Doublet reaction surface)

Al	-1.01597475	-0.00564703	0.00000000
O	0.21371033	1.25843290	0.00000000
O	0.20050018	-1.28461210	0.00000000
Al	1.42502825	-0.02357717	0.00000000
O	3.13025925	-0.04978126	0.00000000
H	3.68107230	0.73400471	0.00000000
O	-4.66931574	0.03169918	0.00000000

Frequencies -- -127.7, 65.2, 65.6, 163.9, 201.7, 298.0, 357.5, 440.8, 601.5, 631.4, 680.1, 758.6, 768.5, 954.0, 3930.3

(6-7-2) Al<sub>2</sub>O<sub>2</sub>H + O<sub>2</sub> (Doublet reaction surface)

Al	-0.19352309	0.89348088	-0.00229603
O	1.31714283	0.13147673	-0.00103202
O	-0.63451692	2.53334693	0.00201885
Al	2.52122070	-1.11276740	0.00031305
O	-1.61651431	-1.17636597	0.00553418
O	-2.84420935	-1.54247184	-0.00336976
H	-0.03528684	3.28283787	0.00056877

Frequencies -- -275.5, 38.7, 50.8, 94.2, 117.7, 146.7, 209.2, 269.1, 341.1, 487.7, 582.2, 851.5, 1025.5, 1143.2, 3894.4

(6-7-3) Al<sub>2</sub>O<sub>3</sub>(3) + OH (Doublet reaction surface)

Al	1.53600300	-0.01032495	0.00000000
O	0.28880001	-1.25062796	0.00000000
O	0.34975599	1.28646504	0.00000000
Al	-0.91701800	0.04870003	0.00000000
O	3.27972100	-0.05659394	0.00000000
O	-4.36344600	0.07032300	0.00000000
H	-4.48545299	-0.89540500	0.00000000

Frequencies -- -164.5, 68.0, 74.8, 77.8, 157.6, 170.0, 351.0, 393.0, 434.7, 624.1, 667.9, 748.0, 749.7, 920.8, 3718.8

(6-7-4) AlO<sub>2</sub> + AlO<sub>2</sub>H(1) (Doublet reaction surface)

Al	2.24854195	0.10073399	0.00000000
O	2.53737601	1.69842896	0.00000000
O	2.35232190	-1.57910601	0.00000000
H	3.14712696	-2.11292222	0.00000000
O	-4.15112105	0.03505918	0.00000000
Al	-2.45309005	0.01096513	0.00000000
O	-0.79957706	-0.07177791	0.00000000

Frequencies -- -160.7, 56.4, 96.9, 130.8, 160.6, 173.4, 233.1, 251.5, 258.5, 511.0, 705.3, 769.0, 851.3, 1115.0, 3938.0

(6-7-5) AlO<sub>3</sub> + AlOH(1) (Doublet reaction surface)

Al	1.72402224	0.04088779	0.00420372
O	0.08283725	0.12818990	0.02652375
O	3.37603028	0.70543168	-0.02954159
O	3.31321119	-0.76424629	0.02923395
O	-4.47589876	0.06715618	0.02131494
Al	-2.74810378	-0.18671195	-0.05080603
H	-5.05637970	0.80346229	0.22558169

Frequencies -- -164.3, 19.2, 59.2, 70.0, 85.1, 149.8, 221.9, 256.7, 387.5, 501.3, 594.6,



732.3, 771.2, 1074.0, 3896.7

(6-8-1)  $\text{AlO}_2\text{H}(1) + \text{H}$  (Doublet reaction surface)

O	-0.08262145	1.96871631	0.00000000
H	0.82529870	2.30399921	0.00000000
H	0.06909029	-3.22906968	0.00000000
Al	-0.03412131	-0.01569094	0.00000000
O	0.02626997	-1.82758472	0.00000000

Frequencies -- -1627.4, 177.2, 192.4, 245.6, 571.3, 695.5, 943.3, 949.0, 3772.8

(6-8-2)  $\text{AlOH}_2 + \text{O}$  (Doublet reaction surface)

O	-2.15282536	-0.29100450	0.00000000
Al	-0.52086770	0.25886177	0.00000000
H	-2.45070644	-1.20181086	0.00000000
H	-0.32794118	1.83842501	0.00000000
O	3.34656632	-0.20922265	0.00000000

Frequencies -- -111.7, 95.4, 144.4, 413.3, 538.8, 627.7, 812.6, 1858.3, 3922.9

(6-8-3)  $\text{AlOH}(1) + \text{OH}$  (Doublet reaction surface)

H	-3.27553856	0.47799166	0.00000000
O	-2.57908292	-0.21455808	0.00000000
H	2.96761258	-0.36643890	0.00000000
O	2.02236309	-0.17825444	0.00000000
Al	0.36628343	0.23314980	0.00000000

Frequencies -- -176.5, 92.2, 238.6, 381.5, 381.9, 514.6, 806.7, 3599.9, 3848.0

(6-9-1)  $\text{AlO}_2\text{H}_2 + \text{O}$  (Doublet reaction surface)

O	3.27914102	0.30056967	0.00000000
Al	-0.72036223	0.36360752	0.00000000
O	0.47603046	-0.84676930	0.00000000
H	1.42217126	-0.63582977	0.00000000
O	-2.40666316	0.12581319	0.00000000
H	-2.84552893	-0.72797655	0.00000000

Frequencies -- -61.4, 57.0, 114.2, 199.9, 265.2, 518.9, 558.3, 739.1, 778.2, 945.2, 3686.6, 3889.3

(6-9-2)  $\text{AlOH}_2 + \text{O}_2$  (Doublet reaction surface)

O	-1.52771044	0.27834636	0.00000000
O	-2.57707456	-0.44632846	0.00000000
O	2.44180838	-0.31236421	0.00000000
Al	0.76358340	0.25028849	0.00000000
H	2.73252832	-1.22725434	0.00000000
H	0.64470049	1.81627450	0.00000000

Frequencies -- -283.0, 116.5, 196.7, 280.7, 351.1, 416.1, 606.7, 667.6, 738.5, 1166.8, 1970.9, 3897.7

(6-9-3)  $\text{AlO}_2 + \text{H}_2\text{O}$  (Doublet reaction surface)

H	0.00000000	-0.76126900	2.72383036
H	-0.00000000	0.76126900	2.72383036
O	0.00000000	-0.00000000	2.12787336
Al	0.00000000	0.00000000	-0.67616964
O	0.00000000	-1.65390300	-0.85502764

O                    -0.00000000      1.65390300     -0.85502764  
 Frequencies -- -134.8, 88.1, 212.4, 216.0, 220.0, 352.4, 398.3, 771.0, 841.3, 1657.1,  
 3767.5, 3850.3

(6-10-1) Al<sub>2</sub>OH + H (Singlet reaction surface)

H                    4.45322804      1.51175803      0.00000000  
 O                    -0.19912176     -0.02630613      0.00000000  
 Al                   -1.91992619      0.08324317      0.00000000  
 Al                   1.52844553      -0.06767262      0.00000000  
 H                    2.22899466      -1.50372618      0.00000000  
 Frequencies -- -547.3, 128.7, 135.6, 262.2, 265.1, 496.7, 617.3, 981.0, 1826.6

(6-10-2) Al + AlOH<sub>2</sub> (Singlet reaction surface)

Al                    3.41521547      0.12036240      0.00000000  
 O                    -2.85175714      0.45317251      0.00000000  
 Al                   -1.31685791     -0.35731723      0.00000000  
 H                    -2.92776872      1.40883132      0.00000000  
 H                    -1.53682240     -1.95379861      0.00000000  
 Frequencies -- -87.3, 76.4, 122.8, 444.9, 563.3, 660.5, 785.8, 1776.9, 3910.2

(6-10-3) Al<sub>2</sub>OH + H (Triplet reaction surface)

H                    4.15194712      0.86754637      0.00000000  
 O                    -0.05233457     -0.03468169      0.00000000  
 Al                   -1.77031256     -0.06835011      0.00000000  
 Al                   1.67857754      -0.08078719      0.00000000  
 H                    -2.54071525      1.34869209      0.00000000  
 Frequencies -- -520.5, 107.7, 128.1, 143.3, 223.1, 493.9, 596.1, 989.8, 1763.8

(6-10-4) Al + AlOH<sub>2</sub> (Triplet reaction surface)

Al                    2.51462120      0.16366304      0.00000000  
 O                    -2.36476688      0.37833896      0.00000000  
 Al                   -0.80059437     -0.34845368      0.00000000  
 H                    -2.56365259      1.31541541      0.00000000  
 H                    -0.80056124     -1.93984877      0.00000000  
 Frequencies -- -103.6, 112.2, 183.2, 365.7, 540.1, 634.1, 807.9, 1861.9, 3927.0

(6-11-1) Al<sub>2</sub>O<sub>2</sub>H + H (Singlet reaction surface)

Al                    -0.40027540      1.02502276      0.00000000  
 O                    0.90583498      2.13289892      0.00000000  
 H                    0.78251655      3.08373236      0.00000000  
 O                    -0.14858337     -0.65741840      0.00000000  
 Al                    0.15310714      -2.35330010      0.00000000  
 H                    -3.62734203      2.38002890      0.00000000  
 Frequencies -- -518.5, 73.6, 113.2, 197.7, 224.0, 245.6, 319.8, 498.9, 601.9, 827.4,  
 1029.2, 3913.9

(6-11-2) Al<sub>2</sub>OH + OH (Singlet reaction surface)

H                    4.82311516      0.74238099      0.00000000  
 O                    -1.12552505     -0.04099606      0.00000000  
 Al                    0.59335419      -0.20463908      0.00000000  
 H                    1.26255480      -1.65145403      0.00000000  
 Al                    -2.83544033      0.17880201      0.00000000

O                    4.00820627    0.19661544    0.00000000  
 Frequencies -- -145.0, 61.0, 65.0, 143.7, 145.1, 288.8, 439.5, 492.6, 586.9, 979.7,  
 1842.9, 3615.1

(6-11-3) Al + AlO<sub>2</sub>H<sub>2</sub> (Singlet reaction surface)

Al                    -1.61150340    0.64425334    0.00000000  
 O                    0.15766596    0.20451617    0.00000000  
 H                    0.26066497    -0.75961222    0.00000000  
 O                    -2.53942011    -0.82278159    0.00000000  
 H                    -3.49841107    -0.82075559    0.00000000  
 Al                    3.32625566    -0.14221556    0.00000000  
 Frequencies -- -123.3, 84.4, 103.3, 207.3, 308.2, 354.2, 517.3, 585.5, 775.4, 793.1,  
 3728.2, 3904.3

(6-11-4) AlO + AlOH<sub>2</sub> (Singlet reaction surface)

O                    3.51197170    0.28008187    0.00000000  
 Al                    -3.38411488    0.04772454    0.00000000  
 H                    3.82178334    1.18734533    0.00000000  
 Al                    1.85931434    -0.24021442    0.00000000  
 H                    1.64604691    -1.81080298    0.00000000  
 O                    -1.71764961    0.11064640    0.00000000  
 Frequencies -- -115.1, 104.2, 115.1, 139.6, 165.2, 405.6, 549.6, 623.0, 791.6, 873.4,  
 1884.9, 3916.3

(6-12-1) AlO<sub>2</sub>H<sub>2</sub> + H (Singlet reaction surface)

Al                    0.00909038    0.37726857    0.00000000  
 O                    1.42369503    -0.58865896    0.00000000  
 O                    -1.54759746    -0.32035553    0.00000000  
 H                    2.31426037    -0.23429819    0.00000000  
 H                    -1.71643345    -1.26521355    0.00000000  
 H                    0.27521758    3.86713624    0.00000000  
 Frequencies -- -515.8, 177.4, 209.9, 213.9, 287.0, 313.8, 575.5, 596.8, 758.0, 916.4,  
 3891.6, 3919.1

(6-12-2) AlOH<sub>2</sub> + OH (Singlet reaction surface)

Al                    -0.45432556    0.18990741    0.00000000  
 O                    -2.13315471    -0.19657131    0.00000000  
 H                    -0.07833594    1.72672052    0.00000000  
 H                    -2.51682454    -1.07483156    0.00000000  
 H                    3.56038382    -0.67227051    0.00000000  
 O                    2.75078083    -0.10948055    0.00000000  
 Frequencies -- -198.9, 114.5, 125.1, 330.5, 413.4, 510.0, 596.3, 625.2, 810.4, 1902.6,  
 3546.3, 3921.2