



START Al₂O₃-cluster-Oi-char

memory stack 1024 mb heap 1024 mb global 2048 mb noverify

geometry units angstroms noautosym noautoz

Oi	-0.54181487	0.29839834	-0.75904939
Al	1.67860004	-2.78406099	-4.59177338
Al	-0.73053772	-1.39834221	-4.08081205
Al	-0.69260258	1.34120656	-4.63579976
O	-1.50898682	0.07937235	-3.24965966
O	-1.70448434	-2.81435777	-3.24189191
O	0.94535977	-1.57982045	-3.27709540
Al	-3.09225557	2.75173623	-4.15044640
O	-4.06480402	1.36379827	-3.27906199
O	-1.47040687	2.61116002	-3.28818540
Al	4.11404235	-1.35328138	-4.10573471
O	3.34441359	0.07730660	-3.25117194
O	3.08126635	-2.87607626	-3.27057047
Al	1.70340618	2.79958683	-4.07409194
O	0.65788363	1.33157610	-3.23975618
O	-2.45510818	-1.64138119	3.26105601
Al	-0.75297591	-1.43878828	2.46933539
Al	-3.12568079	-0.06674761	4.07456758
O	-1.45790552	-2.73063297	1.12406145
Al	-3.10106857	2.69978794	2.48151217
O	-3.85498578	1.46698360	1.07644279
Al	1.72036418	-2.79647592	4.53938018
O	0.21917644	-2.84870677	3.25960188
Al	1.68671176	-2.80111195	1.93139265
O	2.36173349	-1.57789030	3.24143550
Al	4.04533745	-1.40762328	2.49430429
Al	1.64905538	-0.06995469	4.05776967
O	3.33128451	-2.64886393	1.05557348
O	0.67923936	-1.44457355	1.12723895
Al	-0.71989200	1.31752813	4.54171426
O	-2.15406908	1.29692691	3.24613634
Al	-0.72200392	1.30756438	1.88648935
O	-0.02539914	0.03789549	3.26505489

O	0.03324760	2.55402799	3.22791277
Al	1.75286012	2.73827497	2.43616880
O	0.94483688	1.40565565	1.07335878
O	-1.70246001	2.71185286	1.07930816
O	-1.57464415	-0.25267349	1.20985843
O	2.55985794	1.23019627	3.22658798
O	3.36163362	-0.22871437	1.10413897
O	-0.03318401	-2.90411406	-1.08124719
Al	1.60069620	-2.71468944	-1.90879153
Al	-0.81313010	-1.45479369	-0.17523604
Al	-3.19929322	-0.05728755	0.23089572
Al	-3.15975312	0.03280109	-2.34860480
O	-2.46378927	-1.31036477	-1.06265892
O	-2.48936157	1.27636993	-1.12086974
Al	-0.85511150	1.47236852	-2.01432929
Al	-3.14049642	2.69388125	-0.22907709
Al	4.11917997	-1.41795112	-0.24263270
Al	1.75198298	-0.08541588	0.32666531
O	0.65111356	-0.49077004	-1.11484640
Al	1.73001593	0.00692263	-2.51860782
O	2.54579965	-1.39295480	-1.12456561
O	2.35622422	1.18832580	-1.08113260
Al	1.61530485	2.68963410	-0.21040870
O	-0.11000537	2.83874464	-1.05337691
O	-4.82111106	2.54889066	3.22319147
O	5.01159904	-2.79654835	3.33297901
O	-4.78442105	2.88329265	-1.08892988
O	4.84252318	-3.11740797	-1.10408703
O	-2.32551398	-4.19755699	-5.35108546
O	-4.45507305	-3.02427607	-3.15809304
O	-0.77388409	-5.48683000	-7.47388240
O	-2.31804600	-4.54953169	7.35038399
O	-0.17800924	-5.48283653	5.21474625
O	-5.28098027	-1.54164458	-5.15712896
O	-7.17270312	2.08710346	-2.07940995
O	-3.23914747	-1.40112123	-7.79510956
O	-4.67210236	0.12198012	7.63135512
O	-6.23942936	0.08943219	-3.36856692
O	-6.70591667	2.15203348	-5.77133153

O	-4.52163631	3.85411455	-8.87215684
O	-6.51237613	4.23543424	8.13010536
O	1.20099145	-4.97554134	-6.15318017
O	3.32912129	-5.70456243	-7.09059760
O	-0.49235802	-3.42840881	-8.82003755
O	0.35440739	-5.02027710	7.94962393
O	2.71127677	-4.37716873	8.05010727
O	3.73643492	-5.37490806	5.36510660
O	0.62270635	-0.61940433	-7.77110211
O	-1.98910582	-0.47101889	-7.74559318
O	-1.27821706	-2.97579717	-7.59303157
O	-2.27954873	-1.54908393	7.33124948
O	0.34262181	-2.33810922	7.59181335
O	0.20659692	-0.72884462	7.74093365
O	-1.51071684	3.21449042	-7.75311533
O	-4.01375205	4.17658952	-7.46400055
O	-3.75605365	1.22003112	-7.48178884
O	-3.73248557	3.44234164	7.77600428
O	-2.39271937	1.58563594	7.60924849
O	-3.26980383	2.27598593	8.66531007
O	-5.53927438	5.50957413	-5.08830211
O	-6.28815578	5.18009436	-3.80571162
O	-6.49669115	4.48585487	-7.63614019
O	-5.26002870	6.05156958	6.40550754
O	-6.24132161	5.33857827	5.42636017
O	5.49462592	-5.29749642	-5.71283723
O	6.75144146	-4.44777976	-5.57616461
O	5.46955035	-4.42943000	-3.39831627
O	4.84943253	-3.33018296	-8.05733882
O	3.89068219	-5.34324490	8.35603050
O	5.67023658	-4.21854315	5.59034517
O	5.45631985	-1.96236629	-7.89678814
O	3.09561687	-0.10549168	-7.48954478
O	3.37616072	-3.03254573	-7.58836633
O	2.91830006	-1.01795012	7.78654573
O	4.86075230	-2.70258534	7.40114030
O	4.26346654	-0.22980031	7.84613294
O	2.15171252	4.13734201	-5.64061577
O	1.18298856	4.08383047	-2.78183789

O	2.87819754	2.42559186	-8.04299459
O	1.06084808	4.48509973	-6.78846240
O	0.48078278	0.95682425	-7.45752118
O	0.30483788	2.69524245	7.60996176
O	2.74563379	1.53903129	7.27353750
O	1.46572860	3.64268359	8.07289908
O	3.47460715	2.32812913	6.10318505
O	-0.41902346	4.91874184	-4.24680558
O	-2.85178398	5.31731639	-3.34147585
O	-1.63071250	4.78596673	-7.82012646
O	-0.43458284	5.08261442	8.16348467
O	-1.46667544	5.21699920	5.44419919
O	7.70730814	-2.10186648	-5.52500994
O	7.81443369	-3.19621718	-3.13522587
O	6.98145361	-3.43493733	6.19714369
O	5.62723731	2.43004950	-4.35637515
O	5.58068883	1.37427887	-3.18940285
O	6.02903417	0.16479919	5.39296753
O	-1.61877631	-5.40510491	1.38487901
O	-4.76770830	-3.36613945	3.95672758
O	-2.32664541	-4.11560854	3.30921865
O	-4.71623059	-3.53734082	2.49409437
O	-7.18520498	1.12239281	3.63536587
O	-7.14979034	0.50713344	2.31023092
O	-7.28840689	3.95420424	3.51168821
O	-6.16051755	5.07107762	1.69212414
O	2.08440475	-5.27783072	1.19186649
O	-5.13145367	5.30361301	2.67089880
O	-0.88203424	5.89981370	0.09530961
O	7.54937637	-3.52301623	3.24049089
O	7.43467955	-1.88951085	3.28033529
O	7.79300602	-2.79891612	0.58669063
O	5.43424682	-4.30271525	1.29524380
O	4.38543841	2.74185810	3.42480918
O	5.47256524	1.57794788	0.66928096
O	0.18544525	5.28805187	2.96534789
O	3.08839354	3.58448124	3.62794600
O	-2.29050413	-4.08781257	-1.08333331
O	-0.28759396	-5.42137321	-1.18635766

O	-6.64489696	4.75476237	-1.10769535
O	-5.15911657	5.42651461	-1.07114628
O	3.50155195	-5.49120471	-1.24909599
O	-0.07684880	5.41257702	-1.17253233
O	7.61355272	-4.33269524	-2.04482736
O	7.41713548	-1.90215291	-0.60856143
O	1.99785081	4.18272007	-1.47491356
O	4.87300887	2.44957774	-0.46169259
H	-1.43778130	-6.21007027	-7.45633449
H	-2.81247619	-3.75055984	7.67199132
H	-5.71017226	-1.25717138	-4.23878366
H	-2.72285402	-2.30444514	-7.91734292
H	-5.07443237	-0.62997389	8.12357271
H	-7.21584897	0.03229907	-3.23286798
H	-7.66375380	1.95338798	-5.88792438
H	-3.89970631	0.99584605	-8.42518426
H	-7.06653146	3.52234336	8.51023462
H	1.32976367	-4.96302209	-3.36165427
H	2.26661083	-5.63329070	-6.90998219
H	-0.63719382	-4.47050235	-8.58700178
H	-0.05357222	-5.36394058	8.77604561
H	1.44689041	-4.88215682	8.01131908
H	-7.46227200	4.60917288	-7.72226651
H	-6.67446973	6.06531665	-3.57572296
H	-5.53418485	4.18354398	-8.64965065
H	-5.93174460	6.62800716	6.87082156
H	5.46908410	-5.09547070	-4.22486250
H	7.13130898	-4.31036790	-6.49047197
H	3.60513417	-6.14931096	-7.91974080
H	4.20289147	-4.98346525	9.23541396
H	3.23730669	0.76629158	-7.99127106
H	3.86602144	0.73461510	7.88386387
H	3.09952761	3.05661286	-8.75992153
H	0.80228341	4.47547607	8.39775650
H	0.35055056	5.53801444	-4.15516229
H	-2.58054553	5.11033294	-4.35491941
H	-2.69354547	4.87439755	-7.77546649
H	-0.77817725	5.97048811	8.38733369
H	7.60767914	-1.19489828	-5.89337020

H	5.87340657	-2.80262532	7.27621775
H	6.48492860	2.11699004	-4.76180590
H	6.63858395	0.20482966	6.18832872
H	-1.80569592	-6.29854169	1.01477004
H	-2.14845816	-5.09429873	2.25722621
H	-4.69777867	-1.15030740	1.78940115
H	-7.77428895	3.12923335	3.76759415
H	-7.44260895	4.27261016	2.57932117
H	2.19966561	-5.07240374	2.27787577
H	-3.57187966	4.80666084	1.57242731
H	-2.66456659	4.93502206	-1.19145463
H	6.06785653	-0.61105544	1.05822569
H	4.11904378	2.94451372	0.21529456
H	0.66261931	4.94127806	2.05668343
H	0.21254106	6.25983296	3.11130709
H	7.34673945	-5.12383872	-2.59434043
H	8.30439110	-1.52290913	-0.84551399
H	1.39528807	5.02657479	-1.14806732
H	5.52702735	0.48488273	-0.39153087
Al	-0.72104726	-4.17495303	-6.24930332
Al	-3.10194726	-2.80035303	-4.57450332
Al	-0.72104726	-4.17495303	6.74619668
O	-4.75374726	-0.16285303	-5.41190332
Al	-3.10194726	-0.05105303	-6.24930332
Al	-5.48284726	1.32354697	-4.57450332
O	-3.83104726	-1.53745303	-3.24600332
Al	-3.10194726	-0.05105303	6.74619668
O	-3.83104726	-1.31385303	5.41769668
Al	-5.48284726	4.07284697	-6.24930332
O	-6.21194726	2.58634697	-3.24600332
Al	-5.48284726	4.07284697	6.74619668
O	-6.21194726	2.80994697	5.41769668
O	2.38895274	-4.28675303	-5.41190332
Al	4.04075274	-4.17495303	-6.24930332
O	0.93075274	-4.06315303	-3.24600332
Al	4.04075274	-4.17495303	6.74619668
O	0.73715274	-4.17495303	5.41769668
O	-2.17924726	-1.42565303	-5.41190332
Al	-0.72104726	-1.42565303	-6.74050332

O	0.00805274	-2.68845303	-5.41190332
O	0.00805274	-0.16285303	-5.41190332
Al	1.67975274	-0.06255303	-6.29520332
Al	-0.72104726	-1.42565303	6.25509668
Al	1.65985274	-0.05105303	6.74619668
O	0.93075274	-1.31385303	5.41769668
O	-1.64374726	-0.05105303	5.41769668
O	-1.45014726	-2.91215303	5.41769668
O	-4.56014726	2.69814697	-5.41190332
Al	-3.10194726	2.69814697	-6.74050332
O	-2.37284726	1.43534697	-5.41190332
O	-2.37284726	3.96094697	-5.41190332
Al	-0.72104726	4.07284697	-6.24930332
O	-3.83104726	4.18464697	-3.24600332
Al	-3.10194726	2.69814697	6.25509668
Al	-0.72104726	4.07284697	6.74619668
O	-1.43024726	2.79844697	5.37179668
O	-4.02464726	4.07284697	5.41769668
O	-3.83104726	1.21174697	5.41769668
Al	6.42175274	-2.80035303	-4.57450332
O	2.58265274	-1.42565303	-5.41190332
Al	4.04075274	-1.42565303	-6.74050332
O	4.76985274	-2.68845303	-5.41190332
O	4.76985274	-0.16285303	-5.41190332
Al	4.04075274	1.32354697	-4.57450332
O	5.69265274	-1.53745303	-3.24600332
Al	4.04075274	-1.42565303	6.25509668
O	5.69265274	-1.31385303	5.41769668
O	3.13795274	-0.06255303	5.39469668
O	3.31175274	-2.91215303	5.41769668
O	0.22165274	2.68664697	-5.45780332
Al	1.67975274	2.68664697	-6.78640332
O	2.40885274	1.42384697	-5.45780332
O	3.31175274	2.58634697	-3.24600332
Al	1.65985274	2.69814697	6.25509668
O	0.73715274	4.07284697	5.41769668
O	0.95065274	1.20024697	5.37179668
Al	-0.72104726	-4.17495303	4.08909668
Al	-3.10194726	-2.80035303	4.58029668

Al	-3.10194726	-2.80035303	1.92319668
O	-4.02464726	-1.42565303	1.08579668
Al	-5.48284726	1.32354697	4.58029668
Al	-5.48284726	1.32354697	1.92319668
O	-4.75374726	0.06074697	3.25179668
Al	-5.48284726	4.07284697	4.08909668
O	-6.40564726	2.69814697	1.08579668
Al	4.04075274	-4.17495303	4.08909668
O	2.38895274	-4.06315303	3.25179668
O	0.93075274	-4.28675303	1.08579668
Al	-0.72104726	4.07284697	4.08909668
O	-2.37284726	4.18464697	3.25179668
O	-3.83104726	3.96094697	1.08579668
Al	6.42175274	-2.80035303	4.58029668
Al	6.42175274	-2.80035303	1.92319668
O	5.49895274	-1.42565303	1.08579668
Al	4.04075274	1.32354697	4.58029668
Al	4.04075274	1.32354697	1.92319668
O	4.76985274	0.06074697	3.25179668
O	3.11805274	2.69814697	1.08579668
O	0.93075274	3.96094697	1.08579668
Al	-3.10194726	-2.80035303	-1.91750332
Al	-5.48284726	1.32354697	-1.91750332
Al	-0.72104726	-4.17495303	0.24839668
Al	-0.72104726	-4.17495303	-2.40860332
O	-4.56014726	-0.05105303	-1.08010332
Al	-5.48284726	4.07284697	0.24839668
Al	-5.48284726	4.07284697	-2.40860332
Al	4.04075274	-4.17495303	0.24839668
O	2.58265274	-4.17495303	-1.08010332
Al	4.04075274	-4.17495303	-2.40860332
Al	6.42175274	-2.80035303	-1.91750332
Al	4.04075274	1.32354697	-1.91750332
Al	-0.72104726	4.07284697	0.24839668
O	-2.17924726	4.07284697	-1.08010332
Al	-0.72104726	4.07284697	-2.40860332
O	4.96355274	-0.05105303	-1.08010332

END

BASIS "ao basis" PRINT

#BASIS SET: (3s) -> [2s]

H S

5.4471780 0.1562850

0.8245470 0.9046910

H S

0.1831920 1.0000000

#BASIS SET: (6s,3p) -> [3s,2p]

O S

322.0370000 0.0592394

48.4308000 0.3515000

10.4206000 0.7076580

O SP

7.4029400 -0.4044530 0.2445860

1.5762000 1.2215600 0.8539550

O SP

0.3736840 1.0000000 1.0000000

#BASIS SET: (6s,3p) -> [3s,2p]

Oi S

322.0370000 0.0592394

48.4308000 0.3515000

10.4206000 0.7076580

Oi SP

7.4029400 -0.4044530 0.2445860

1.5762000 1.2215600 0.8539550

Oi SP

0.3736840 1.0000000 1.0000000

#BASIS SET: (9s,6p) -> [4s,3p]

Al S

775.7370000 0.0668347

116.9520000 0.3890610

25.3326000 0.6694680

Al SP

29.4796000 -0.1079020 0.1175740

6.6331400 0.1462450 0.4611740

1.7267500 0.9237300 0.6055350

Al SP

0.9461600 -0.3203270 0.0519383

0.2025060 1.1841200 0.9726600

Al SP

0.0639088 1.0000000 1.0000000
END

set fock:replicated logical .false.

set geometry:actlist 1:158

DFT

set atomscf:z -1

set atomscf:list_z Oi

print "convergence"

direct

XC b3pw91

iterations 9999

convergence energy 1e-6

convergence damp 30

END

DRIVER

MAXITER 999

xyz Al2O3_Oi_cluster_char

EPREC 1e-6

END

task dft optimize

title "Optimized geometry"

dft

XC b3pw91

iterations 9999

end

task dft energy