

Supplementary Materials for

Revealing the catalytic mechanism of CO oxidation on AlN₃C-doped graphene: Synergistic roles of Al, N, and C

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Contents

Figure S1. The geometry of $\text{N}_3\text{C-Gr}$ and $\text{AlN}_3\text{C-Gr}$	3
Figure S2. The orbital charge density isosurfaces for HOMO, HOMO-1, and LUMO of O_2 on $\text{AlN}_3\text{C-Gr}$	3
Figure S3. The orbital charge density isosurfaces for HOMO-14, HOMO, and LUMO of CO on $\text{AlN}_3\text{C-Gr}$	4
Figure S4. The orbital charge density isosurfaces (isovalue = $0.015 \text{ bohr}^{-3/2}$) for HOMO, and LUMO of CO_2 on $\text{AlN}_3\text{C-Gr}$	4
Table S1. Energy of the $\text{AlN}_x\text{C}_{4-x}\text{-Gr}$ configurations in the work.....	5
Table S2. Energy of the adsorption configurations in the work.....	5
Table S3. Energy of the involved structures along the PESs in the work.....	5
Coordinates of the referred structures in the work.....	5

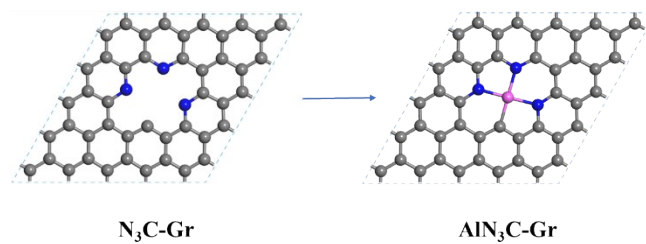


Figure S1. The geometry of $\text{N}_3\text{C-Gr}$ and $\text{AlN}_3\text{C-Gr}$.

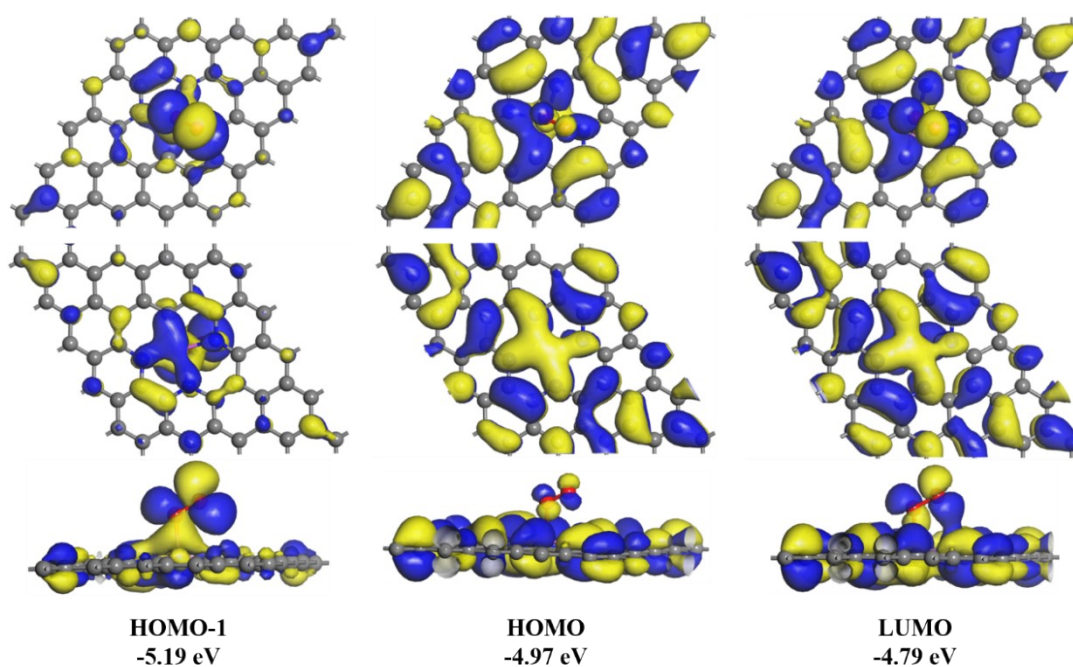


Figure S2. The orbital charge density isosurfaces for HOMO, HOMO-1, and LUMO of O_2 on $\text{AlN}_3\text{C-Gr}$.

The yellow and blue colors of orbital charge density isosurfaces (isovalue = $0.015 \text{ bohr}^{-3/2}$) represent charge accumulation and depletion in the work, respectively.

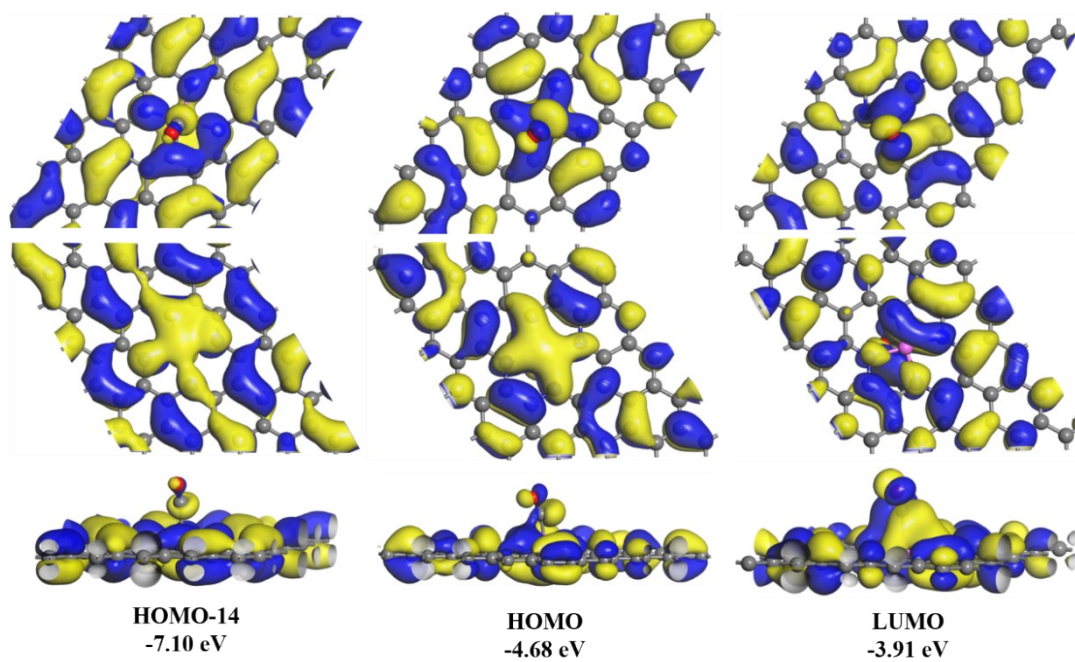


Figure S3. The orbital charge density isosurfaces for HOMO-14, HOMO, and LUMO of CO on AlN₃C-Gr.

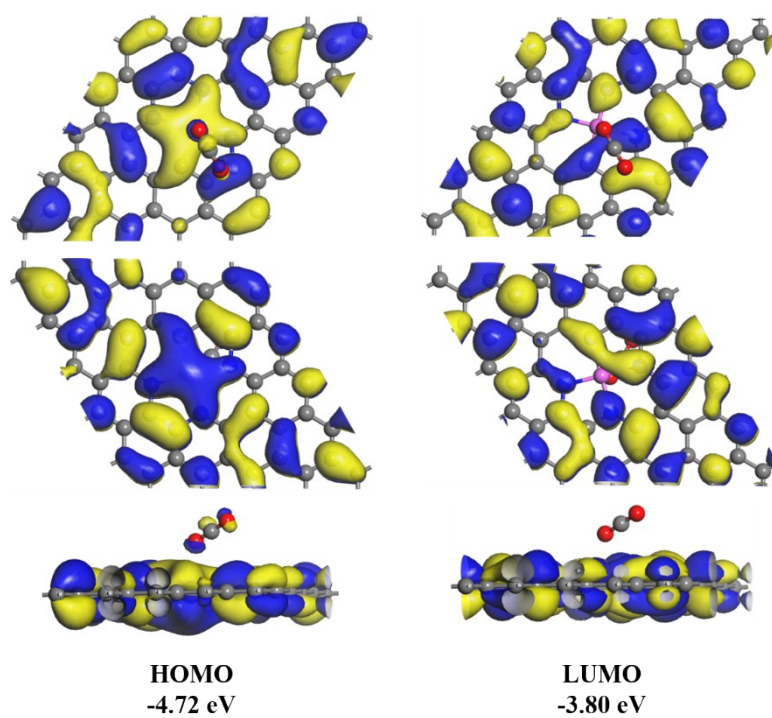


Figure S4. The orbital charge density isosurfaces (isovalue = 0.015 bohr^{-3/2}) for HOMO, and LUMO of CO₂ on AlN₃C-Gr.

Table S1. Energy of the $\text{AlN}_x\text{C}_{4-x}\text{-Gr}$ configurations in the work

$\text{AlN}_x\text{C}_{4-x}\text{-Gr}$	Energy/Hartree
$\text{AlN}_4\text{-Gr}$	-2137.081973
$\text{AlN}_3\text{C-Gr}$	-2120.40804
a- $\text{AlN}_2\text{C}_2\text{-Gr}$	-2103.714841
b- $\text{AlN}_2\text{C}_2\text{-Gr}$	-2103.726734
$\text{AlNC}_3\text{-Gr}$	-2087.017327
$\text{AlN}_4\text{-Gr}$	-2070.309544

Table S2. Energy of the adsorption configurations in the work

Adsorption configuration	Energy/Hartree
$\text{O}_2\text{-AlN}_3\text{C-Gr}$	-2270.692378
$\text{CO-AlN}_3\text{C-Gr}$	-2233.661353
$\text{CO}_2\text{-AlN}_3\text{C-Gr}$	-2308.897289

Table S3. Energy of the involved structures along the PESs in the work

Structure	Energy/Hartree
IS1	-2270.692378
IM1	-2270.691509
TS1-1	-2270.676335
IM2	-2270.68592
TS1-2	-2270.678861
FS1	-2270.74822
IS2	-2383.984472
TS2	-2383.990601
FS2	-2384.09058
IS3	-2459.125894
TS3	-2459.11413
FS3	-2459.24084
IS4	-2383.931716
TS4	-2383.9190
FS4	-2384.03643
IS5	-2308.780483
TS5	-2308.7870
FS5	-2308.89729

Coordinates of the referred structures in the work **$\text{AlN}_4\text{-Gr}$:**

\$cell vectors

23.46283956792041 0.0000000000000000 0.0000000000000000

	-11.66312693572874	20.34693000729107	0.000000000000000
	0.000000000000000	0.000000000000000	35.13265428020583
\$coordinates			
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C	2.32777600746975	1.52128671562211	17.44190102413231
C	4.66636115388815	2.83182774393201	17.44190102413231
C	7.03526327479558	1.50978420781230	17.44190102413231
C	9.33871916277162	2.94495503622319	17.44190102413231
C	11.70933433552917	1.58699994606797	17.44190102413231
C	14.01947024473035	2.98363125768983	17.44190102413231
C	16.38783153735917	1.61413861475382	17.44190102413231
C	18.74170507646510	2.94652523611661	17.44190102413231
C	21.08977086357930	1.58671404562307	17.44190102413231
C	-2.36793468884583	6.95731549632333	17.44190102413231
C	-0.04438490267654	5.56047560240098	17.44190102413231
C	2.28693947377373	6.85594086244804	17.44190102413231
C	4.63137817536567	5.49813896861032	17.44190102413231
N	6.85322086625277	6.89797335467569	17.44190102413231
C	9.23020027944106	5.67440941468449	17.44190102413231
C	11.56808254222727	7.10161446733261	17.44190102413231
C	13.97212237810147	5.70970293001136	17.44190102413231
C	16.36293124170948	7.02195106131354	17.44190102413231
C	18.73043725752220	5.65158472429063	17.44190102413231
C	-4.62601315596941	11.04862575461460	17.44190102413231
C	-2.26834313629139	9.67071685544324	17.44190102413231
C	0.15527858404140	10.93206364320631	17.44190102413231
N	2.39782599118685	9.47826789142598	17.44190102413231
N	9.40330940834990	11.29255649155026	17.44190102413231
C	11.64585681549535	9.83876073976994	17.44190102413231
C	14.06947853582813	11.10010752753301	17.44190102413231
C	16.42714855550616	9.72219862836164	17.44190102413231
C	-6.92930185798545	15.11923965868562	17.44190102413231
C	-4.56179584217273	13.74887332166270	17.44190102413231
C	-2.17098697856472	15.06112145296488	17.44190102413231
C	0.23305285730948	13.66920991564363	17.44190102413231
C	2.57093512009569	15.09641496829175	17.44190102413231
N	4.94791453328398	13.87285102830056	17.44190102413231
C	7.16975722417108	15.27268541436592	17.44190102413231
C	9.51419592576302	13.91488352052821	17.44190102413231
C	11.84552030221329	15.21034878057526	17.44190102413231
C	14.16907008838257	13.81350888665291	17.44190102413231
C	-9.28863546404255	19.18411033735318	17.44190102413231
C	-6.94056967692835	17.82429914685963	17.44190102413231
C	-4.58669613782242	19.15668576822243	17.44190102413231

C	-2.21833484519360	17.78719312528641	17.44190102413231
C	0.09180106400757	19.18382443690827	17.44190102413231
C	2.46241623676512	17.82586934675306	17.44190102413231
C	4.76587212474117	19.26104017516395	17.44190102413231
C	7.13477424564860	17.93899663904423	17.44190102413231
C	9.47335939206700	19.24953766735414	17.44190102413231
C	11.82106610098184	17.89074965773261	17.44190102413231
Al	5.90056769882351	10.38541219054326	17.44190102413231
\$end			

AlN₃C-Gr:

\$cell vectors

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-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

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C	7.05083645487932	1.49453707540499	17.44190102413231
C	9.35013293282206	2.91502710532069	17.44190102413231
C	11.71814693914253	1.57577014463526	17.44190102413231
C	14.02216145472756	2.98605084601274	17.44190102413231
C	16.38568146177621	1.62520397599858	17.44190102413231
C	18.73902945670842	2.95515766379258	17.44190102413231
C	21.09150052990150	1.58546334550505	17.44190102413231
C	-2.36064382309942	6.96567275152961	17.44190102413231
C	-0.04531047541475	5.54587329934957	17.44190102413231
C	2.29436531887779	6.83981764545028	17.44190102413231
C	4.67214406165051	5.46036854011855	17.44190102413231
N	6.89121849273710	6.83474472858006	17.44190102413231
C	9.23814328967320	5.64507638279422	17.44190102413231
C	11.56910675300003	7.09635306728897	17.44190102413231
C	13.96860920715976	5.71103017159635	17.44190102413231
C	16.36059352010176	7.01944482526835	17.44190102413231
C	18.72212421434835	5.65164182614494	17.44190102413231
C	-4.64675701223527	11.04376110257090	17.44190102413231
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C	2.38603749411501	9.48337881257830	17.44190102413231
N	9.40449997360317	11.29706240176585	17.44190102413231
C	11.63264186432724	9.83753528639295	17.44190102413231
C	14.06211980434740	11.10314259209592	17.44190102413231

C	16.41559714536369	9.72443930497394	17.44190102413231
C	-6.92719940161112	15.11747265137518	17.44190102413231
C	-4.56863830047611	13.75062621838816	17.44190102413231
C	-2.16984954296146	15.07465001930125	17.44190102413231
C	0.21386520940482	13.70676424828384	17.44190102413231
C	2.56624060198474	15.11206924408242	17.44190102413231
N	4.95618621980159	13.91833444578109	17.44190102413231
C	7.16244794871276	15.29882664780847	17.44190102413231
C	9.51516670830905	13.92051357779295	17.44190102413231
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C	-9.28958595848890	19.18500162856975	17.44190102413231
C	-6.93834221895029	17.81996899440175	17.44190102413231
C	-4.58333671688796	19.14311252309129	17.44190102413231
C	-2.22033731615866	17.79356878533213	17.44190102413231
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C	2.46538756653502	17.84101916204439	17.44190102413231
C	4.76234863778454	19.27086542820562	17.44190102413231
C	7.13714239373666	17.95261534531675	17.44190102413231
C	9.47877467439873	19.25560280193381	17.44190102413231
C	11.81948485941867	17.89469808740297	17.44190102413231
Al	5.89572934042911	10.39771918500010	17.44190102413231

\$end

a-AlN₂C₂-Gr:

\$cell vectors

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0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

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C	7.11059004281671	1.56588565245902	17.42914063146576
C	9.42261200451529	2.96525254862695	17.43238636269708
C	11.78056583649086	1.62462357685491	17.42574397725746
C	14.08287819827633	3.04208036201396	17.42311753006428
C	16.44050993399279	1.68678107027809	17.41650761200921
C	18.79399999853509	3.01531272404522	17.41607425245532
C	21.14926704436230	1.64743895278871	17.41155776544261
C	-2.32313983276318	7.03039996823688	17.43218678494157
C	-0.01464106511368	5.61605727598729	17.43519041202067
C	2.30455846569121	6.91206805650293	17.45778430071426

C	4.70537354251462	5.52248501136701	17.45556861195051
C	6.94700868059377	6.91816050518402	17.46235670094356
C	9.32924747370848	5.70268687012778	17.44280080966782
C	11.66941566448878	7.15441818115422	17.43307221044826
C	14.03902011911810	5.78172415696931	17.42608121589200
C	16.42813121120143	7.08606183802048	17.42460401698009
C	18.77197305035570	5.71287139979007	17.42308631367842
C	-4.59332045748029	11.10936810773182	17.42982053224882
C	-2.25787881377903	9.73322306758717	17.43775577570658
C	0.16482963404289	11.01252045073896	17.45052297327691
C	2.40088291799130	9.55176805962333	17.47143284954175
N	9.51496435076641	11.38808067885149	17.42964186053343
C	11.71693689648209	9.90386781032559	17.42854324557394
C	14.13856565873112	11.17289345295442	17.42301226476021
C	16.48010320175338	9.78978914864487	17.42584868698204
C	-6.85792649028415	15.18176622506964	17.41921468058806
C	-4.50896827433824	13.81296464552891	17.42704786938644
C	-2.10826548693090	15.13521511799767	17.42950598355586
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C	2.62698275479100	15.16977450496060	17.42919794118995
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C	9.60304754113950	13.98253370891383	17.41692260531488
C	11.91406534583896	15.28378122665746	17.41065810651875
C	14.23439542797484	13.87465356813132	17.41721020840303
C	-9.23129880936286	19.24646726680241	17.41204551509383
C	-6.87269779154292	17.88439617173325	17.41713725552597
C	-4.52032505969737	19.20451461928300	17.42238625140733
C	-2.16163352966522	17.85574253417944	17.42471349259396
C	0.15860566609268	19.24294094525659	17.42405449974075
C	2.52577361368110	17.90104740844596	17.42147730070011
C	4.82039759449142	19.32801665539902	17.41495598812359
C	7.19857347454767	18.01451486844716	17.40937165089272
C	9.53947078213822	19.31706178455106	17.40631214083265
C	11.88091822679829	17.96172186937268	17.40673303953247
Al	5.97265319914642	10.47235761839047	17.47332472239562
Send			

b-AlN₂C₂-Gr:

\$cell vectors

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-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

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C	4.68398245505095	2.79488179161021	17.44804807833950
C	7.05250861683555	1.48282375730758	17.44879993611395
C	9.34875318141724	2.90163915539501	17.44976355470824
C	11.71545915710851	1.57363915339644	17.44990289177434
C	14.02106544759013	2.97774336619259	17.44930106502613
C	16.38111900717551	1.63774473713599	17.44844900641364
C	18.73788886526252	2.95916150779182	17.44766897471239
C	21.09168178865196	1.58629968726537	17.44640028629139
C	-2.35563725451346	6.96836472497617	17.44821280954528
C	-0.04368521646095	5.54532124420805	17.44705470789711
C	2.29309378641897	6.83669036792164	17.45177256979488
C	4.68001731453247	5.43473380807955	17.44968991775033
N	6.88187466443330	6.78599274630743	17.45085536287421
C	9.24386521975296	5.62560854519701	17.45027943860201
C	11.59178944748314	7.05949726057251	17.45118264832126
C	13.96615569447346	5.69876084882981	17.44981744591787
C	16.36832413645580	7.02037860697685	17.44903492544732
C	18.72258572515232	5.65649872275263	17.44810349455812
C	-4.63400050106617	11.04305814901884	17.44893960766158
C	-2.28505594217097	9.67265497934402	17.44947006323349
C	0.14186317261567	10.95652549215938	17.45311600444303
C	2.38480617124867	9.47827371745163	17.45859004213943
C	9.41632922828807	11.29255066363489	17.45859004213943
C	11.65927222881080	9.81429889081686	17.45311600444303
C	14.08619134170772	11.09816940363222	17.44947006323349
C	16.43513590060292	9.72776623395741	17.44893960766158
C	-6.92145032561557	15.11432565833389	17.44810349455812
C	-4.56718873691905	13.75044577599939	17.44903492544732
C	-2.16502029493671	15.07206353414643	17.44981744591787
C	0.20934595394334	13.71132712051401	17.45118264832126
C	2.55727017978379	15.14521583588951	17.45027943860201
N	4.91926073510345	13.98483163666881	17.45085536287421
C	7.12111808689400	15.33609057489669	17.44968991775033
C	9.50804161500751	13.93413401505460	17.45177256979488
C	11.84482061599770	15.22550313876820	17.44705470789711
C	14.15677265405020	13.80245965800007	17.44821280954528
C	-9.29054638911521	19.18452469382115	17.44640028629139
C	-6.93675346572578	17.81166287518442	17.44766897471239
C	-4.57998360763876	19.13307964584026	17.44844900641364
C	-2.21993004805338	17.79308101678365	17.44930106502613
C	0.08567624431796	19.19718522957981	17.44990289177434

C	2.45238222000924	17.86918522758123	17.44976355470824
C	4.74862678459093	19.28800062566867	17.44879993611395
C	7.11715294448579	17.97594259136603	17.44804807833950
C	9.47625252308012	19.26221832113712	17.44666854236347
C	11.82406034179127	17.90181836946180	17.44591061100925
Al	5.90056770071324	10.38541219054326	17.45703143760552
\$end			

AINC₃-Gr:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.02102989088131	2.93074848717578	17.40597769710305
C	2.38287908334846	1.57245967138689	17.40735246718981
C	4.73193385674045	2.86568697413755	17.42497592264040
C	7.11010674724997	1.57197983023951	17.42543651125802
C	9.41970724223788	2.97362593831488	17.43227514475572
C	11.77291023092561	1.63598215556413	17.42525620115007
C	14.08367367848865	3.04403562195124	17.42084653657576
C	16.43539806419797	1.68943755466803	17.41214249583856
C	18.78572227623223	3.01248490952589	17.40535756268815
C	21.14557996948420	1.64845614133918	17.39812164828773
C	-2.33557505458623	7.02420743399103	17.42085758013523
C	-0.03444258488087	5.60404141462700	17.42352412542706
C	2.28111940643684	6.90066256345293	17.44992178336641
C	4.69800844265684	5.52184750092039	17.45439203067057
C	6.94136842258741	6.91150808718840	17.47608543462998
C	9.32818555723035	5.71047489447178	17.44863141222785
C	11.67660151815442	7.15537408966592	17.43573103998832
C	14.03775227351495	5.78304915355966	17.42360588064840
C	16.42761372481991	7.08540058883428	17.41853551112900
C	18.76288751548785	5.71116096332091	17.41229732487943
C	-4.59394432410429	11.10688175538492	17.42606998713936
C	-2.26935485408473	9.72799147419370	17.43140798345204
C	0.14136075113082	11.00879919449472	17.44763503901064
C	2.36424547857721	9.52191579146515	17.46277710642486
N	9.58658843855110	11.39446509588806	17.43481959106316
C	11.75259109060635	9.91049394412054	17.43139062631757
C	14.16843724178003	11.17451753838829	17.42347058570649
C	16.49107524832209	9.78681364446997	17.42259771176072
C	-6.84653423098620	15.18422826420023	17.41587881131029

C	-4.51659669241372	13.80935371905475	17.42490629001214
C	-2.12430582998946	15.13070927203277	17.43251809361553
C	0.21863885223834	13.76585326489649	17.44761250024715
C	2.59293880952592	15.18085324924578	17.45198573846068
C	5.00724031746229	13.99273282915153	17.47355558645686
C	7.24206168706009	15.36277827367089	17.43874743972629
C	9.65319735193706	13.96897903601105	17.42905096396112
C	11.94828704441253	15.27935152531705	17.41370370252535
C	14.25568170366871	13.87307654065741	17.41642264614317
C	-9.23017054082103	19.24693631572390	17.40299893315058
C	-6.86874111132830	17.88686096419479	17.41207949425928
C	-4.51649631016196	19.21030057706333	17.41976497828428
C	-2.16441205445803	17.86320543870254	17.42684918169194
C	0.15229121238643	19.25951915728265	17.42653799671148
C	2.50891919928461	17.91476961879780	17.43048581033112
C	4.82043855241545	19.32042499438640	17.41742127380365
C	7.20692503789885	18.02969088668094	17.41181114181117
C	9.53948511571088	19.32564257735038	17.39826785072884
C	11.88761027801993	17.96211282725178	17.40193394208804
Al	5.97233679474241	10.45638593664094	17.48846387963161
\$end			

AIC₄-Gr:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.02841794902178	2.93401432698281	17.41328151314259
C	2.38393493569546	1.57057994569255	17.41357810754763
C	4.73404810122636	2.85504585829757	17.42917435362846
C	7.11119066391965	1.56614621545603	17.43175098197180
C	9.42495773289260	2.96362930790065	17.44001832778850
C	11.77651609104403	1.63329726859054	17.43158898519974
C	14.09164011565556	3.03117311226434	17.42754677220125
C	16.43976062545889	1.69069414884183	17.41990279223113
C	18.79193962825127	3.01533172902086	17.41304263286313
C	21.14911762560732	1.65059387134137	17.40723244879388
C	-2.32352196184182	7.03081602545837	17.42057896269482
C	-0.02544588792787	5.61064516272627	17.42544163808499
C	2.29796883951526	6.90162525041224	17.44255730711826
C	4.69815321457528	5.51144005538494	17.45348373002914
C	6.95474930682710	6.86242085238339	17.48215543714416

C	9.35316358865392	5.69338175475337	17.45625661776892
C	11.71548282214877	7.11542957473104	17.43660991003508
C	14.05690998626806	5.75952538922147	17.42723021472942
C	16.44317543993525	7.08347250882785	17.41971573769064
C	18.77390240781699	5.71478039545236	17.41603925094803
C	-4.58472004176488	11.11045186944396	17.42197340672026
C	-2.26114007477965	9.73393011995520	17.42547777531768
C	0.14456652788269	11.02831571710609	17.43449288576204
C	2.35263696469069	9.53174672880301	17.43988024928000
C	9.56884176539826	11.36716510317266	17.41868257906468
C	11.77503663768886	9.87052961729696	17.42325331444526
C	14.18109404343986	11.16432803685657	17.41806593308421
C	16.50501623037770	9.78773803612935	17.41992017015257
C	-6.85342294789540	15.18346240166546	17.41462728160251
C	-4.52269389564574	13.81486105561521	17.42128018336802
C	-2.13629321128732	15.13909804220163	17.42943868662910
C	0.20425955198749	13.78307593211268	17.43991570432156
C	2.56716634668803	15.20429913230118	17.45044261456318
C	4.96633995448694	14.03612171576910	17.46900676245070
C	7.22243081901062	15.38647307712065	17.43672537041159
C	9.62259495132438	13.99603231364248	17.42378961871954
C	11.94572108168344	15.28763365635095	17.41433006547757
C	14.24406526994000	13.86759809800940	17.41341052285542
C	-9.22870793626399	19.24779294369417	17.40833918012707
C	-6.87153453094243	17.88300172770781	17.41455554948853
C	-4.51927205327792	19.20763087781859	17.42386697843791
C	-2.17130206205017	17.86721567186581	17.42899445359108
C	0.14399748221357	19.26481896978924	17.43079273019971
C	2.49558693391866	17.93417951928175	17.43433721768277
C	4.80929464470430	19.33193728908781	17.42401899934577
C	7.18687606038533	18.04345250160195	17.41741078204421
C	9.53647438704101	19.32792389252300	17.40643691566923
C	11.89169367570959	17.96461994579907	17.40722348015369
Al	5.96158671540434	10.44879093459253	17.46461406950671

\$end

O₂ on AlN₃C-Gr:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	-0.01750039648533	2.90240057518365	17.32351511914353
---	-------------------	------------------	-------------------

C	2.33602556529443	1.54309470123538	17.33481457021202
C	4.69591935987429	2.84010506561293	17.37837659920634
C	7.05730836056631	1.52171113677143	17.41000942968045
C	9.35553306710917	2.93780915782400	17.44138223572949
C	11.72317124280818	1.60301769934043	17.43655004162171
C	14.02596710425082	3.01468708107866	17.43000374497609
C	16.38934510216063	1.65871040378521	17.39937420978598
C	18.74402205832859	2.98399374873458	17.36279959620665
C	21.09866721040588	1.61334279439080	17.32981001796383
C	-2.35365735254750	6.99419525909788	17.36896715961148
C	-0.03683634820655	5.58023123394867	17.34744817926313
C	2.30247652985286	6.88469769794554	17.40782025944342
C	4.69582527796943	5.49457877750317	17.43617342676390
N	6.90313594282999	6.84184696564412	17.52929260497928
C	9.23658821703741	5.66716742292486	17.49273777116329
C	11.57339995564299	7.12349926086424	17.48485889634611
C	13.96636825842690	5.74426841134104	17.44205877468977
C	16.36619880494672	7.04849148239246	17.41094273706769
C	18.72620720007771	5.68147267425750	17.37476438204924
C	-4.63838703539272	11.06998812957952	17.41435477175693
C	-2.28568689904739	9.69916209588971	17.40935319393765
C	0.14298512569279	10.97713400812989	17.47964758727286
C	2.39665940277865	9.51566632166088	17.51034298886705
N	9.43408547290374	11.32496243732800	17.48393989040618
C	11.63744811816450	9.87383617881226	17.46308019014941
C	14.07446039057584	11.13272527192511	17.41844081317343
C	16.42439213106038	9.75308714106855	17.41240474258156
C	-6.91722755495502	15.14255722744740	17.39525339173960
C	-4.56113963099637	13.77500002689080	17.42721772363974
C	-2.15624836200902	15.09759040817712	17.46510536239441
C	0.21822016829754	13.73048472744246	17.51851986404551
C	2.58205177228694	15.14814388904141	17.53547710788909
N	4.94942202450567	13.97445576845691	17.60307149077252
C	7.14625701904848	15.31863544113151	17.46186681401209
C	9.52425910477247	13.92267237824143	17.42561567997138
C	11.84424997162028	15.23265644757051	17.37262399131266
C	14.16927563200346	13.83340427667563	17.39042149620854
C	-9.28581595486954	19.21152904833293	17.34179349697725
C	-6.93116363884051	17.84536604613738	17.37976359771085
C	-4.57444496020614	19.16608522061472	17.40807645150391
C	-2.21226860701387	17.82099252298338	17.44454673897306
C	0.10056145070864	19.21889465274758	17.44482792833074
C	2.47018992942619	17.87715764951078	17.46062479718561
C	4.76743058754563	19.29988351645017	17.41773672767543

C	7.13994282045526	17.97916030173837	17.38775446525710
C	9.48250476511261	19.28107700929739	17.33638399342801
C	11.82328444481079	17.91844232797789	17.33872965566491
Al	5.90281823980618	10.40997987738742	18.20091358892661
O	6.22846008432077	10.54992990261250	21.81577317652697
O	5.55785949200970	8.43307583721064	22.92431947638211

\$end

CO on AlN₃C-Gr:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.07860071475323	2.92711951192740	17.37556469807070
C	2.43031053445357	1.57040199774227	17.38437035316110
C	4.78870993550352	2.87055458360264	17.41965724877735
C	7.15351427412603	1.55160644533183	17.42887599799867
C	9.45356422555905	2.97135567615037	17.44591377441078
C	11.82161437667111	1.63264643368501	17.43290774569387
C	14.12597440411166	3.04190109692456	17.42743633471678
C	16.48953719833923	1.68095612555808	17.40771707283809
C	18.84319657667314	3.01100670905913	17.38941441202365
C	21.19484391446889	1.64101015931353	17.37239109768557
C	-2.25650943508091	7.02249810301166	17.39835419042577
C	0.05930961757131	5.60396012427828	17.39599390737784
C	2.39914774500716	6.89982271436093	17.45087824745759
C	4.77861855989056	5.51803342699806	17.46785569247345
N	6.99791542119070	6.88472302783452	17.52656388013903
C	9.34226823661999	5.69950219972700	17.48087107533468
C	11.67507755985927	7.15120153091823	17.46493937263105
C	14.07236534381764	5.76775749731511	17.43510401752168
C	16.46560805184243	7.07538039920445	17.41399439342598
C	18.82636894725475	5.70746791312881	17.39623188625794
C	-4.54304523500845	11.10130883587929	17.41385188917890
C	-2.18987028607695	9.73045518006272	17.41784460269127
C	0.23618006680797	11.01448772177549	17.46331729219659
C	2.48591311408001	9.54477711231022	17.49355640241037
N	9.52692125267160	11.35178318793920	17.45275795803412
C	11.74011275846121	9.89634129006222	17.43995685877711
C	14.17049036307442	11.15953258280411	17.41217861417399
C	16.52182735114866	9.78044894672550	17.41173258211670
C	-6.82471831230265	15.17460695040196	17.40183056273065

C	-4.46676731680600	13.80733929746167	17.42147908649130
C	-2.06839330693263	15.13282408910569	17.44532313862069
C	0.31225107700726	13.76660329341605	17.47828799924579
C	2.66663870098769	15.17268825288574	17.47672253122658
N	5.04704431992142	13.98161037172162	17.51912176827249
C	7.25835325219942	15.35058684541523	17.45150846356137
C	9.61956268733559	13.96894530628944	17.42927072021220
C	11.94241394380168	15.26642146359036	17.39098679077130
C	14.26599204751695	13.86467995269157	17.39666666688587
C	-9.18799064239673	19.24178095388230	17.38000229279715
C	-6.83656313266165	17.87727718035737	17.39875311916966
C	-4.48149826863255	19.20064250809192	17.41767202156318
C	-2.11887362516028	17.85162922590468	17.43369090867131
C	0.19595739930530	19.24657179322356	17.43237043797503
C	2.56594132605833	17.90036667051423	17.43710908686017
C	4.86481973044180	19.32709009622377	17.41653568389079
C	7.23918491729576	18.00533540852171	17.40529929487281
C	9.58084110299332	19.31034471902470	17.37510490502778
C	11.92141540725623	17.95052484523961	17.37492780367480
Al	6.01875003684493	10.45219813347261	17.80097481287832
C	5.50875920675607	10.54611845540949	21.91744911967399
O	4.41830839326084	10.66857909180393	23.77657735672089

\$end

CO₂ on AlN₃C-Gr:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	-0.03197208922588	2.86330079050335	17.41762695537455
C	2.32101465243219	1.50641184603334	17.41940421255949
C	4.67907923747649	2.80577486652417	17.40265656579934
C	7.04408227135242	1.48702323331419	17.41872783233620
C	9.34398857714377	2.90768699709092	17.42072355508927
C	11.71191793129274	1.56808907878994	17.43802913970837
C	14.01561950445202	2.97864219363696	17.44204769711523
C	16.37885574077711	1.61696203754963	17.44863651448839
C	18.73226582833034	2.94759799206380	17.43943943853600
C	21.08453492948491	1.57780191958334	17.43741853140286
C	-2.36778722784711	6.95799938064907	17.41633281045292
C	-0.05352784175490	5.53837982850640	17.40211972862230
C	2.28658183365594	6.83558577008925	17.39275309699335

C	4.66607752867350	5.45295343999723	17.38669050031585
N	6.88485403687758	6.82538572577548	17.40030781952940
C	9.23224555270285	5.63724264219581	17.41462613264902
C	11.56284074431272	7.08976799913244	17.43628360346617
C	13.96166174244479	5.70401923098084	17.43978552486826
C	16.35407622319324	7.01212380138272	17.43745557759382
C	18.71467056759354	5.64348292793111	17.43040255655696
C	-4.65315024106476	11.03682404835715	17.43621549395717
C	-2.30000804297674	9.66556251594348	17.42245758478910
C	0.12942635964323	10.94784191715612	17.42724193481085
C	2.38029894011452	9.47900005258503	17.41979791054146
N	9.40541981858150	11.29202221873157	17.45609263111525
C	11.62728189805864	9.83275829307500	17.44485696586237
C	14.05705414402551	11.09651061904724	17.44525888037354
C	16.40982688553828	9.71707385740656	17.43890777353937
C	-6.93334386878325	15.11075469578782	17.44664504928828
C	-4.57507669564972	13.74331913501215	17.44365975255259
C	-2.17565062610969	15.06759541845335	17.44877868992313
C	0.20696673017046	13.70024977651589	17.45330760566456
C	2.55990618899116	15.10368369400688	17.46933810136028
N	4.94866680112900	13.90867235358277	17.49742056541336
C	7.15485686406660	15.28994736142934	17.48579176342717
C	9.51055283615021	13.91266094560246	17.47126349417616
C	11.83479290147844	15.20460312120455	17.45886547350160
C	14.15676043319135	13.80227140159377	17.45039415253670
C	-9.29615793462283	19.17843848501573	17.43970182700846
C	-6.94492866093772	17.81344073519199	17.44204887063515
C	-4.59001160183748	19.13631373446893	17.43605075897195
C	-2.22672678443317	17.78646235496580	17.44571480136763
C	0.08826083974665	19.18073854816123	17.44696469079314
C	2.45895639578438	17.83242230657299	17.45943996914086
C	4.75578494432021	19.26297301728021	17.46098458781173
C	7.13053731338047	17.94351816595652	17.46748053837393
C	9.47219582344115	19.24804406561946	17.45419503428094
C	11.81320596846836	17.88827852146047	17.45378159621986
Al	5.89749072013515	10.39554307277059	17.57143777968603
O	5.99283691413266	9.76552223250049	22.23471658617390
C	4.91417198232831	8.00931621864923	23.09612247005705
O	3.85991639343665	6.27665171555419	23.96441864310155

\$end

IS1:

\$cell vectors

	23.46283956792041	0.000000000000000	0.000000000000000
	-11.66312693572874	20.34693000729107	0.000000000000000
	0.000000000000000	0.000000000000000	35.13265428020583
\$coordinates			
C	-0.01750039648533	2.90240057518365	17.32351511914353
C	2.33602556529443	1.54309470123538	17.33481457021202
C	4.69591935987429	2.84010506561293	17.37837659920634
C	7.05730836056631	1.52171113677143	17.41000942968045
C	9.35553306710917	2.93780915782400	17.44138223572949
C	11.72317124280818	1.60301769934043	17.43655004162171
C	14.02596710425082	3.01468708107866	17.43000374497609
C	16.38934510216063	1.65871040378521	17.39937420978598
C	18.74402205832859	2.98399374873458	17.36279959620665
C	21.09866721040588	1.61334279439080	17.32981001796383
C	-2.35365735254750	6.99419525909788	17.36896715961148
C	-0.03683634820655	5.58023123394867	17.34744817926313
C	2.30247652985286	6.88469769794554	17.40782025944342
C	4.69582527796943	5.49457877750317	17.43617342676390
N	6.90313594282999	6.84184696564412	17.52929260497928
C	9.23658821703741	5.66716742292486	17.49273777116329
C	11.57339995564299	7.12349926086424	17.48485889634611
C	13.96636825842690	5.74426841134104	17.44205877468977
C	16.36619880494672	7.04849148239246	17.41094273706769
C	18.72620720007771	5.68147267425750	17.37476438204924
C	-4.63838703539272	11.06998812957952	17.41435477175693
C	-2.28568689904739	9.69916209588971	17.40935319393765
C	0.14298512569279	10.97713400812989	17.47964758727286
C	2.39665940277865	9.51566632166088	17.51034298886705
N	9.43408547290374	11.32496243732800	17.48393989040618
C	11.63744811816450	9.87383617881226	17.46308019014941
C	14.07446039057584	11.13272527192511	17.41844081317343
C	16.42439213106038	9.75308714106855	17.41240474258156
C	-6.91722755495502	15.14255722744740	17.39525339173960
C	-4.56113963099637	13.77500002689080	17.42721772363974
C	-2.15624836200902	15.09759040817712	17.46510536239441
C	0.21822016829754	13.73048472744246	17.51851986404551
C	2.58205177228694	15.14814388904141	17.53547710788909
N	4.94942202450567	13.97445576845691	17.60307149077252
C	7.14625701904848	15.31863544113151	17.46186681401209
C	9.52425910477247	13.92267237824143	17.42561567997138
C	11.84424997162028	15.23265644757051	17.37262399131266
C	14.16927563200346	13.83340427667563	17.39042149620854
C	-9.28581595486954	19.21152904833293	17.34179349697725
C	-6.93116363884051	17.84536604613738	17.37976359771085

C	-4.57444496020614	19.16608522061472	17.40807645150391
C	-2.21226860701387	17.82099252298338	17.44454673897306
C	0.10056145070864	19.21889465274758	17.44482792833074
C	2.47018992942619	17.87715764951078	17.46062479718561
C	4.76743058754563	19.29988351645017	17.41773672767543
C	7.13994282045526	17.97916030173837	17.38775446525710
C	9.48250476511261	19.28107700929739	17.33638399342801
C	11.82328444481079	17.91844232797789	17.33872965566491
Al	5.90281823980618	10.40997987738742	18.20091358892661
O	6.22846008432077	10.54992990261250	21.81577317652697
O	5.55785949200970	8.43307583721064	22.92431947638211
\$end			

IM1:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	-0.00174525845246	2.87294043464504	17.31416619991754
C	2.35110891513849	1.51308421764711	17.32331252160566
C	4.71123951885798	2.81030019934487	17.37664574424640
C	7.07327235868941	1.49146460938261	17.40536764626675
C	9.37148651867077	2.90783147232235	17.44205172790106
C	11.73916558615339	1.57331921709430	17.43075213699282
C	14.04178878898917	2.98507566418429	17.42364528521756
C	16.40513922335372	1.62901804425173	17.38598431344240
C	18.75976814457332	2.95449056779374	17.35117506311177
C	21.11430967729799	1.58366513314711	17.31279833866950
C	-2.33771208727948	6.96466572592623	17.37512486431511
C	-0.02114716539490	5.55086538129506	17.35395502787589
C	2.31748330799434	6.85483248705313	17.43700766336932
C	4.71021409299132	5.46364265881572	17.45119750345832
N	6.91822996584720	6.81173657034590	17.55963861888967
C	9.25332150187901	5.63670719396747	17.50463515047500
C	11.58932902784785	7.09352351800105	17.48710955260207
C	13.98223342576339	5.71469127218885	17.43937158791949
C	16.38219230736382	7.01887579660677	17.40723362987271
C	18.74199655538152	5.65192309676084	17.37141883170453
C	-4.62180156870807	11.04014685395821	17.41236114282040
C	-2.26861560834244	9.66936663100912	17.41862580224326
C	0.16027115353623	10.94683619924322	17.50160666404873
C	2.41292202109320	9.48489808813211	17.56704621301882

N	9.45142681492058	11.29537912444056	17.46455148933636
C	11.65338474171496	9.84480808257815	17.45551774430268
C	14.09085452060061	11.10308501592034	17.40544888181341
C	16.44079912823033	9.72342980382934	17.40676019489689
C	-6.90133914587691	15.11279716847549	17.37948217024768
C	-4.54522743782526	13.74508850070079	17.42039014503986
C	-2.14002616682600	15.06748100120566	17.45939632024682
C	0.23396226533042	13.70086805144028	17.52069253697347
C	2.59697368282814	15.11968880690128	17.52116041804421
N	4.96320974599309	13.94610665648869	17.57552406865666
C	7.16114933080939	15.28893573812230	17.43137448238729
C	9.53943074451081	13.89241305929647	17.39447615116384
C	11.85960567446265	15.20282000208917	17.34254662275793
C	14.18489001189618	13.80357082641020	17.36971884920030
C	-9.27026441214993	19.18166599172831	17.32165677759001
C	-6.91558464784894	17.81545054774305	17.36290210062085
C	-4.55860476937984	19.13618184103403	17.39658549370018
C	-2.19638302874550	17.79116631414846	17.43449575625602
C	0.11601250157237	19.18951764882011	17.43492866794482
C	2.48551986396312	17.84816805833620	17.44552182820492
C	4.78289041618721	19.27040244341527	17.39814825374184
C	7.15544689892379	17.94899535760582	17.36048714023722
C	9.49818358844564	19.25136724916575	17.31049777852603
C	11.83873465852585	17.88858905826487	17.31103228567076
Al	5.92364222801864	10.39339508155554	18.23091059687788
O	6.48882858316770	10.51362760612668	21.80966913626584
O	4.56402796210513	9.72176151392194	23.16292087006102

\$end

TS1-1:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.02204635944614	2.87941667158430	17.33709875965808
C	2.37215460979938	1.52112069562312	17.33348398948097
C	4.72958455489104	2.81389630847648	17.38589721029611
C	7.09049157904515	1.50062869638603	17.39881100148087
C	9.39109369333408	2.91502126606696	17.43915644826933
C	11.75989647889803	1.58232428553403	17.42510654051015
C	14.06357356498618	2.99356544588371	17.42249014854968
C	16.42979412483800	1.64222498676052	17.38153260057207
C	18.78368012857745	2.96134002753242	17.35928053498860

C	21.13480006459870	1.59239819440841	17.31209239368099
C	-2.31852225485142	6.97293283174771	17.43262152777498
C	0.01108581941980	5.55781230365864	17.43216151741355
C	2.34515389301039	6.82980731830109	17.57006365021643
C	4.72015291479366	5.47594420141269	17.49790892355639
N	6.94483053312922	6.81938989312198	17.59150370615317
C	9.27012691000789	5.64470053138577	17.50927882928400
C	11.61277710487528	7.10111104429292	17.49999346910651
C	14.00617508413686	5.72471583086548	17.44649546990658
C	16.40453327511284	7.02965713579440	17.42300626299004
C	18.77535357197208	5.66749455152463	17.39832651538667
C	-4.60483532220923	11.05375764605772	17.42063962290343
C	-2.25039511093020	9.68826949151757	17.45753734752479
C	0.14585516803212	10.97935457049731	17.55918476903541
C	2.43784383505428	9.50432077261329	17.80142233215006
N	9.48703517184796	11.30612460418524	17.53733305515960
C	11.68190779163463	9.84986028427058	17.48774745044255
C	14.11426035657997	11.11132026095935	17.42090985751875
C	16.46126303668858	9.73286812599829	17.41886673665502
C	-6.88807478215009	15.12122370104151	17.37650709315088
C	-4.52956486424717	13.75577374164579	17.42083040587356
C	-2.13050192258960	15.07888736730913	17.46144695277191
C	0.24051284031599	13.69854512827785	17.54467435202710
C	2.62607010966920	15.12926835586246	17.54543705682951
N	4.97827958807481	13.97193735501657	17.61618032248036
C	7.17422247503936	15.29641840918067	17.43990817754240
C	9.56114267345543	13.89889213271465	17.42843681052940
C	11.87612876506737	15.21002091309258	17.34631464972376
C	14.20352776839573	13.81155493251638	17.37709994181027
C	-9.25306308183141	19.18523973973068	17.31566951295477
C	-6.89933536722137	17.82274292716008	17.35513074177154
C	-4.54161506193116	19.14368704140726	17.38664551160599
C	-2.17932333906923	17.80087587815677	17.42816163805972
C	0.13481203752548	19.19820637521679	17.42762010491326
C	2.50487811445262	17.85756454763792	17.44131100817239
C	4.80438004719911	19.27853729297444	17.38569258130267
C	7.17399741999623	17.96064268835667	17.34223756938854
C	9.51674964117710	19.26058903895640	17.29339273920221
C	11.85692677036197	17.89651063711302	17.29943750064454
Al	6.00054324750600	10.39581546356342	18.32321583414642
O	5.74848978738372	10.24985865850140	21.74101801664358
O	3.10121295193160	9.94290400005260	21.48053626650999

\$end

IM2:**\$cell vectors**

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.04061752010731	2.87892578120826	17.34337830445362
C	2.38420938440004	1.51859534877763	17.33691782783024
C	4.73548005442565	2.81171750905642	17.44147578662131
C	7.09838355911301	1.50109547952589	17.39912444657377
C	9.40333836462332	2.91349272518597	17.44558533623081
C	11.77179243146651	1.57908507385783	17.40348528440446
C	14.07976491794911	2.98841390128889	17.38950555351466
C	16.44637020525299	1.63598932329533	17.33056809293723
C	18.79958821348396	2.95715055006673	17.32988584133487
C	21.15035255218137	1.59107448283183	17.26236253483046
C	-2.30394632859726	6.97386472939927	17.52403980318950
C	0.04149598764241	5.55818910559933	17.57544300129562
C	2.36492289814987	6.79448980723189	17.92318881922645
C	4.71799200163137	5.47081100794827	17.68891378532509
N	6.96054922212459	6.82156723178375	17.68617478226445
C	9.28287059182633	5.64619975316594	17.52963073367482
C	11.63066025215914	7.09685146554690	17.47230729196020
C	14.02502181222049	5.71828339021889	17.41363937813778
C	16.42110900592849	7.02708462327456	17.39917313347765
C	18.79642004039226	5.66638321870833	17.41044437282483
C	-4.59830651308917	11.05743813901972	17.40526769865200
C	-2.24696219098784	9.69357371086548	17.52694938993771
C	0.12098478296753	11.00000686764268	17.76666310853914
C	2.37184130643594	9.50826363137103	18.48202430564683
N	9.51005455505530	11.29986673076890	17.48396964603375
C	11.70574402596704	9.84109494648706	17.43800326746799
C	14.12885647644749	11.10759378151210	17.36022998630613
C	16.47413475312116	9.73074620355514	17.38143798009527
C	-6.88316664561852	15.12162299261282	17.32297903029803
C	-4.52495628143176	13.75873433021239	17.39920636809101
C	-2.13239908100744	15.08271907237620	17.46156547450475
C	0.23758829827522	13.69695646576018	17.62655942401365
C	2.63630116438869	15.11359237278780	17.53252635345725
N	4.98092566952243	13.94402424821882	17.54180037149854
C	7.18018853505775	15.27566693731853	17.32949551084485
C	9.57001135469154	13.89461697506646	17.33274843248408
C	11.88474177013822	15.20658797236323	17.24921735424061

C	14.21247804611619	13.80944654240201	17.30379146176187
C	-9.24401869763965	19.18108818906833	17.26111463717628
C	-6.89269817852859	17.82163978630653	17.30522035360484
C	-4.53519048254525	19.14533101998806	17.35153375769673
C	-2.17365743181018	17.80036734151818	17.39846452586503
C	0.14612908572366	19.19227469687551	17.39852787326419
C	2.51552065703582	17.84639479981174	17.39278407338398
C	4.81649262096303	19.26826348320138	17.31104908155656
C	7.18226169311825	17.94822780754564	17.24319922848802
C	9.52542185892636	19.25591518689036	17.20401090257986
C	11.86729781977225	17.89324715757393	17.20836160958880
Al	6.10098778463874	10.38008421544823	18.36217320717622
O	5.55230984070185	10.36573048508158	21.70179034474778
O	2.76002636582172	10.04592709871851	21.20105015300859

\$end

TS1-2:

\$cell vectors

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-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.02876522021231	2.87911211954254	17.27768759765344
C	2.37282181540233	1.52379356771801	17.29463200269772
C	4.72295692821245	2.83081067065483	17.41278926405347
C	7.08506131496470	1.51554860192781	17.38243815544145
C	9.38998443354734	2.92760164153312	17.43937261404077
C	11.75938753785804	1.57694153105809	17.39258320683525
C	14.07139966542187	2.97581574349989	17.38680452450051
C	16.43500539422700	1.61346614437388	17.32180674247584
C	18.78653254355148	2.94187037012895	17.29807538416392
C	21.13665782978574	1.57687685329173	17.22444408598103
C	-2.31451373755946	6.97093385110680	17.46037418548637
C	0.02812977712607	5.56348729105173	17.49390928608750
C	2.35311414510370	6.79982552453485	17.91680421888644
C	4.70648251884244	5.48713689429348	17.69460818209521
N	6.94010127051375	6.85089584927379	17.74356276190569
C	9.27395967521132	5.66594084894028	17.54850162379668
C	11.63123676413618	7.09498146438320	17.47431904525999
C	14.02056989903920	5.70693003660240	17.41183105385535
C	16.41737109174846	7.01652043440568	17.37031448142626
C	18.78495158355750	5.65189977376101	17.36090676337190
C	-4.60163500298641	11.05898283138991	17.35113527870766

C	-2.25828545449524	9.69007043452976	17.48769375198498
C	0.09421912732150	11.00885568974695	17.83410268127896
C	2.23006132145402	9.45477718595662	18.72221589441130
N	9.54090189251967	11.28643189673806	17.42775989551362
C	11.72681190223319	9.83891047977836	17.40286892566236
C	14.14204245622438	11.10670764924784	17.31077364074575
C	16.47794528191727	9.72360342997598	17.33259524939466
C	-6.88678946035973	15.12995885422963	17.28995713773848
C	-4.53341944633871	13.76324387626104	17.36106613153493
C	-2.14573206068987	15.08913075438131	17.45047766520334
C	0.21723056407931	13.69965508348380	17.66415935385553
C	2.62010421216726	15.08612549835829	17.55882658467650
N	4.95272940238265	13.88248589521459	17.54651059890276
C	7.16153988617682	15.23002160999334	17.31655575860260
C	9.56924847225488	13.87766270754152	17.28529857355679
C	11.88047883901806	15.20228101818326	17.20792426649224
C	14.21295901543007	13.80984926949541	17.25932730208192
C	-9.25405728942249	19.18878022855326	17.23748039755910
C	-6.90212674026211	17.82958333133117	17.28874893000211
C	-4.54746470348190	19.16025413050535	17.33300481540691
C	-2.18824382336761	17.80583900193912	17.37917456818796
C	0.13684419608797	19.18547444560513	17.38454596163044
C	2.50477251088758	17.82446866474168	17.39252084776286
C	4.80465285940088	19.24143547226240	17.30767305181918
C	7.16735652366079	17.91043043344904	17.23821964897057
C	9.50922641659609	19.23716975568593	17.18443241395912
C	11.85843350569321	17.88821983601566	17.18199546283258
Al	6.24655831834246	10.39882284363860	18.60816873446509
O	6.04914314462009	10.72560029261184	21.87091135217874
O	2.86474481338341	9.93944274555672	21.17389731893572
\$end			

FS1:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	-0.02484948847310	2.91178002104546	17.29239681573982
C	2.31788705931930	1.54772608170677	17.29372413291385
C	4.67296620967790	2.85789717345099	17.48644354508548
C	7.02782604598134	1.52240672228132	17.41627051563121
C	9.35206399670603	2.90461863366396	17.47167864243938

C	11.71218160855842	1.58135957845749	17.37175983467352
C	14.02308476546360	2.98298982984095	17.36601162417254
C	16.38117089149599	1.63565736266585	17.27600922605717
C	18.73265962268835	2.95936535065920	17.27176395631737
C	21.08306106216016	1.59494099287467	17.21464481289413
C	-2.36941350536330	6.98273952389939	17.44855536397940
C	-0.02304856813762	5.60127779410413	17.50350797041542
C	2.30842186524484	6.88323864229416	17.97828537366031
C	4.69770888894069	5.51655548920324	17.91552962507130
N	6.97037455642449	6.75411381491034	18.18886238401860
C	9.27174900178071	5.60162314533292	17.72696970419120
C	11.59927448447861	7.07769924433790	17.57530222425822
C	13.97475298269213	5.71104683331159	17.41964808927482
C	16.36688518560066	7.02671360389581	17.34224683093628
C	18.72766874638813	5.66537973823116	17.33787104159248
C	-4.67136615589116	11.06407685461121	17.33092242981375
C	-2.33155645182595	9.69280302574965	17.49817600610854
C	0.01354783398393	11.01527810350672	17.84221966158789
C	2.13369443724352	9.49617706779749	18.67716458926541
N	9.48486457761873	11.26091858149232	17.57812023487841
C	11.68016757875092	9.83948689915881	17.45685183614487
C	14.07971286922245	11.10694003642834	17.26881120822446
C	16.41682259685095	9.73077806055816	17.29218090697114
C	-6.96643409006002	15.13224899442325	17.24442091375111
C	-4.61215438266942	13.76839327790644	17.33150822790497
C	-2.21321648418953	15.09524300172301	17.38562659773557
C	0.14796693130762	13.73162466882257	17.56532454968675
C	2.54337138208447	15.15515393959592	17.34863911490271
N	4.80728355658811	13.94303786976308	17.15142001727335
C	7.01390944328247	15.20978866764154	17.15342596911394
C	9.45755354323357	13.81982603321889	17.21868189906564
C	11.78077879350733	15.17945398830845	17.12746235102987
C	14.12599935416569	13.80806475954161	17.20756076066456
C	-9.32790371591716	19.19703275513768	17.18547017973738
C	-6.97477440576132	17.83631398965754	17.23551536395830
C	-4.61541711765642	19.16463624665221	17.30413563947074
C	-2.25473068312261	17.82183076013900	17.32412688774087
C	0.06624259564581	19.21145014848776	17.33916529422850
C	2.42535695000870	17.87819903411457	17.31120695305649
C	4.74107932049291	19.26620155200380	17.23496318787430
C	7.09004506321798	17.92046927656545	17.17247347870862
C	9.43761648097035	19.24485821225013	17.15329671373671
C	11.77921693864448	17.88114139060351	17.11530603955480
Al	7.11693936008024	9.88507648334277	20.10959864638222

O	8.84665435218323	10.17066168224340	22.75316311108233
O	3.78071165985291	10.45635081608091	20.21890425293424
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\$coordinates

C	-0.04332618361501	2.96772979627338	17.22665926262900
C	2.31424354262839	1.62382038844973	17.28826369935581
C	4.66098046866231	2.94034632679613	17.53937709631996
C	7.01918758063041	1.60104464952140	17.51573998053962
C	9.33209916680713	2.99757211880297	17.58799357767052
C	11.69717948481239	1.64203827048102	17.49255204699000
C	14.00452419293790	3.04170927271534	17.42120799583004
C	16.36157655185253	1.67634000651488	17.30333580154998
C	18.71013987739927	3.00823862500316	17.22604315899992
C	21.06829668674764	1.65282113845708	17.14263065162216
C	-2.41077023341837	7.03044540103238	17.39656796460064
C	-0.06463698606425	5.64854848809751	17.44458381539963
C	2.24562872842445	6.91944682852922	17.98701302463571
C	4.66045038725617	5.60307742375666	17.92859975707782
N	6.90611392632557	6.92093885234258	18.13082082747922
C	9.22615540381846	5.72506983892966	17.75632992168150
C	11.57094948919520	7.16326767600099	17.53989896686609
C	13.94765049281295	5.77415959651904	17.41370556201586
C	16.33732995215371	7.08592319637360	17.30682296608076
C	18.69327474069675	5.71314889284344	17.28475370126426
C	-4.69468856235182	11.12604626170345	17.33121849320575
C	-2.37780049541015	9.73912464637073	17.49821795991824
C	-0.05205664650289	11.04213626502602	17.96419166960846
C	1.98104083207810	9.47190701848720	18.84047005714329
N	9.49949202536596	11.35818841463987	17.34762561131818
C	11.67561134134917	9.91472753724261	17.34653100635754
C	14.07646081307778	11.18135499080717	17.20291868812276
C	16.39798719578572	9.79315315216518	17.25766213211236
C	-6.95296363847118	15.20724000535512	17.24225554650435
C	-4.60725824211930	13.83187195067320	17.38706384027829
C	-2.20732390050233	15.15348751484821	17.54502966022285
C	0.14943161645312	13.76710573379816	17.80032406112074
C	2.57059951607425	15.14241363471807	17.65661030805675

N	4.91190955118886	13.92605592530932	17.56438533312591
C	7.08024189918498	15.28729197308056	17.23882466368675
C	9.50590773059798	13.93845077691316	17.11845980537452
C	11.81635390448299	15.27764236063357	17.02979569051389
C	14.14569964319408	13.88580430531269	17.13096909879249
C	-9.31560437674086	19.28061259020491	17.16948051724377
C	-6.96524082627785	17.91285948552039	17.26820665649119
C	-4.61189535413002	19.23911279476436	17.40732836751253
C	-2.25283448468564	17.87774050718815	17.48301691982084
C	0.07373683749724	19.25242153681951	17.50105757955668
C	2.44000529434742	17.88445766342136	17.48804747470051
C	4.73658099752772	19.30655682536811	17.31354812530411
C	7.09843196066825	17.97687990497266	17.17128307597180
C	9.44206480934118	19.30929408232181	17.08261699768572
C	11.79705525406575	17.96980985750341	17.04593191071712
Al	6.70719712331195	10.46572544125137	19.50239336345964
O	8.47758093402763	11.13302223860620	22.20088063172504
O	3.51617072886994	10.31754784705479	20.57655411414780
C	12.26551218860614	14.86646375248630	23.08685583517574
O	11.07906347126466	16.66760255353007	23.22261883957910

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TS2:

\$cell vectors

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\$coordinates

C	-0.02160063730394	3.03427264672374	17.28826080051594
C	2.32101148336148	1.67110471681711	17.28718180847254
C	4.67233975223938	2.98148188508499	17.52605619198747
C	7.02483081306569	1.64242924158819	17.47083258559705
C	9.35186470996834	3.02266728490039	17.55211810228620
C	11.71092374259893	1.70003070358978	17.45270015131196
C	14.02377779228432	3.10147946378646	17.41933954991094
C	16.37904391403546	1.75476746928725	17.31373140417180
C	18.73375856268072	3.07777550272390	17.27980858657188
C	21.08353317999687	1.71437695631015	17.20590888491829
C	-2.36502811810051	7.10589358962621	17.45804715216961
C	-0.02109066069404	5.72198686603002	17.52496681778874
C	2.31051580084408	7.00459019086693	18.02716069835712
C	4.70194717803218	5.63790759713494	17.97717128373359
N	6.97801265367719	6.87368933462015	18.26900840341328

C	9.27816342010925	5.72071324353411	17.79859585933627
C	11.60467154040187	7.19972231842755	17.61459311505181
C	13.97770199101703	5.82926823197202	17.44982674148068
C	16.36962986539858	7.14685053289147	17.34026010327957
C	18.72929477068100	5.78562507514543	17.33819898088476
C	-4.66402696606828	11.18350977180818	17.31534084800766
C	-2.32463883722485	9.81510481554547	17.51131301174317
C	0.01935078040213	11.13610344461190	17.86709388090679
C	2.14416296250677	9.62051399058472	18.70575834517778
N	9.48638782537685	11.38006142194966	17.55301344885504
C	11.68392655581834	9.96080797778754	17.45041851299618
C	14.08277350366956	11.22718266725480	17.22274066228553
C	16.41983625270660	9.85131229691269	17.26624272271099
C	-6.96675463296425	15.25146295472330	17.17902818652522
C	-4.61189036336332	13.88714835034238	17.30138781138910
C	-2.21485336306928	15.21329844085568	17.38829639146660
C	0.14688984788761	13.84998672924711	17.57491512331014
C	2.54106869599911	15.27658945436960	17.35705589459220
N	4.79928155855498	14.06731660221374	17.11859479040135
C	7.00867440302854	15.32966217070510	17.12476798141059
C	9.45463942492211	13.93590491709058	17.16231682250667
C	11.78005967712773	15.29820389990233	17.03993923390625
C	14.12731723026800	13.92621714918340	17.12388400154439
C	-9.33000769352103	19.31911262305629	17.14061991877448
C	-6.97805206013607	17.95886142873181	17.19569433884623
C	-4.61875352172668	19.28522228417929	17.32148683262987
C	-2.25876080187390	17.94122217706054	17.35799537193524
C	0.06443241187287	19.33037522257563	17.41144318756820
C	2.42206369972424	18.00042706034082	17.36011839797845
C	4.73905628174871	19.38711655683416	17.27088415652536
C	7.08607282110872	18.04019925492982	17.17269826730037
C	9.43468330099146	19.36418956611652	17.13010415224782
C	11.77698929358354	18.00025285215854	17.05194232071795
Al	7.15026306268894	10.03517684363591	20.13394734798356
O	8.83260931424827	10.36635313850141	22.81177806910955
O	3.81332913968335	10.59827265524413	20.21889389345563
C	11.51827299551578	13.95187772133743	22.75497534709784
O	10.43284109240783	15.61313884910026	23.63824758078565

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FS2:

\$cell vectors

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C	4.66875827525716	3.00090964159109	17.54992059457750
C	7.03537185089982	1.67255905193263	17.49376383386765
C	9.34467062465571	3.08015665590715	17.53258454190409
C	11.71127069442575	1.71965149750927	17.45082059191352
C	14.01854975535541	3.11918372581588	17.37741591535672
C	16.37618358866787	1.74654797700521	17.26705715498661
C	18.72530908317037	3.08747000561499	17.23473860715243
C	21.08337530471749	1.73489535880066	17.17287511543005
C	-2.39313842726804	7.10593028810756	17.45674031017815
C	-0.05951062773922	5.71853939330677	17.49587659302883
C	2.25457013388075	6.98116181801380	18.02376216954050
C	4.64774065625730	5.64858101406358	17.85635354688634
N	6.88586182215086	7.01522046534813	17.81675151457599
C	9.23777602140081	5.81185377078222	17.60681663315498
C	11.58158709014459	7.24370014386115	17.47375402659724
C	13.96887262553295	5.84675372418740	17.38654032189098
C	16.35341092810341	7.16042294843283	17.33566968829112
C	18.70711013997430	5.78574757664148	17.32177051453630
C	-4.66904756965018	11.20113528706025	17.39839062245573
C	-2.34500916455566	9.81278986513755	17.55272220615439
C	0.00184679343716	11.11365828870271	18.00015730571593
C	2.05734291798796	9.55909666697990	18.83070393741151
N	9.49383188177158	11.45304569680460	17.38772697919062
C	11.68572296726728	9.98381866069581	17.37525796528500
C	14.08666000512507	11.25833475329244	17.29058342510165
C	16.41657020125025	9.86945439903664	17.32571611339692
C	-6.93393977124005	15.28529168852863	17.33070797802391
C	-4.58463400442414	13.90970118095645	17.45024025891026
C	-2.19166079402148	15.23301740793710	17.56302241162196
C	0.18024006335384	13.84658633338108	17.76768286522742
C	2.55677883209403	15.20512666604803	17.51536928808348
N	4.93884491179982	13.97504026830628	17.32749622028886
C	7.14344108523730	15.38993539364262	17.14423068840137
C	9.53338949417963	14.06949226657816	17.16366426526394
C	11.84869100753800	15.37454729144583	17.13551342525047
C	14.16929883217110	13.97015427369572	17.24147200369196
C	-9.29346521473445	19.35825584120185	17.24350409611403
C	-6.94641314285411	17.99115551784076	17.33161140695139
C	-4.59554480874859	19.31663603870373	17.41921896648691

C	-2.23543522634252	17.95087073315063	17.47771652716833
C	0.08961648013584	19.32503847348220	17.45772719130104
C	2.45530123460109	17.94807665402208	17.39235134877807
C	4.75025069617000	19.38487314578816	17.24115492276600
C	7.12312182208584	18.06255103947118	17.13240770382775
C	9.46593774782412	19.39436271732962	17.11317786589762
C	11.82032662280324	18.05785223546139	17.12625862761360
Al	6.20661627705907	10.59242199891046	18.23999193655374
O	8.56839620539457	11.77204812841876	23.05993995386167
O	3.77531290128641	10.42726394558486	20.51992118024898
C	10.48489014977060	12.87986010715789	23.28535577972399
O	12.39156331975587	13.98052669504716	23.52382927106958

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IS3:

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\$coordinates

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C	4.66726080903256	2.79761449999313	17.61571969984766
C	7.02832009975891	1.45810290060208	17.58694726655073
C	9.34095202914585	2.85577289640909	17.64952376327843
C	11.70639205273955	1.49397830606654	17.55411432581669
C	14.01120767047212	2.89400451823085	17.46838723463788
C	16.36811332049902	1.52358051621523	17.35025821712880
C	18.71584327115547	2.85994661922807	17.27200725288678
C	21.07606322490560	1.50838928568615	17.19142036605632
C	-2.40739559262970	6.88138733052183	17.45623728587066
C	-0.06659789439292	5.49967848880011	17.51218114058664
C	2.23968460056746	6.77014945444057	18.07254475970718
C	4.65726764059659	5.45772651591292	17.98909034387314
N	6.90359567918113	6.79550355459109	18.12668849722128
C	9.23634323861174	5.58872933422249	17.77972188518138
C	11.57527149315403	7.01916906509384	17.55466259961624
C	13.95372316362041	5.62631049341477	17.44736708907420
C	16.34229187029080	6.93811777617843	17.34926839559206
C	18.69497850832241	5.56345207411566	17.33387335621067
C	-4.68715324163389	10.97923212002387	17.38750127597142
C	-2.37165340718788	9.58818067643060	17.56074581887493
C	-0.04533824305043	10.88650659254732	18.04823501669962

C	1.97920704751558	9.32088542048757	18.91653830645271
N	9.50011848658393	11.21333135459355	17.28605547312054
C	11.67712634234248	9.77248926532949	17.35921069260075
C	14.08378593388965	11.03928502168219	17.23875843445524
C	16.40391055933205	9.64784263154818	17.30479193568477
C	-6.93756349682925	15.06396391664114	17.29281292020446
C	-4.59489697472815	13.68552125487714	17.44900931776860
C	-2.19495630063894	15.00671322371315	17.62031139040124
C	0.16315174621651	13.61708978946075	17.87563784672339
C	2.57710810512477	14.97642100085690	17.71299897028748
N	4.94896520211221	13.75437599815853	17.59735186237918
C	7.11548849828134	15.14889680884194	17.25241828384496
C	9.52783191358096	13.81056643378793	17.11880578021294
C	11.83643698777362	15.14110625604439	17.07329301528569
C	14.16198246457064	13.74284894847554	17.16716310641244
C	-9.30082045589103	19.13981947311780	17.23396147429106
C	-6.95179669101502	17.77080003083156	17.32942273371233
C	-4.60050777379395	19.09648230830427	17.47842722481805
C	-2.24075815019962	17.72998046120697	17.55660766637081
C	0.08653483949313	19.09922820508581	17.56895701147983
C	2.45371761387272	17.72272558907407	17.54375949970520
C	4.74614757162933	19.15556260383086	17.35970039622878
C	7.11393415507983	17.83181858442949	17.20624595158775
C	9.45622965780219	19.16571907483964	17.12728267209046
C	11.81244155346381	17.83093965580122	17.10213593725680
Al	6.56398848837199	10.39856777218570	19.15719174428212
O	8.11222247554883	10.94684736374517	22.35922539467000
O	3.57202982370003	10.17484432834915	20.63402970716138
O	10.57317516856302	10.65499671551616	22.57486384937119
C	14.45554214520230	15.03640451933082	23.16579173254148
O	13.09588957076078	16.71122816424959	23.23503709733072

Send

TS3:

\$cell vectors

23.46283956792041	0.0000000000000000	0.0000000000000000
-11.66312693572874	20.34693000729107	0.0000000000000000
0.0000000000000000	0.0000000000000000	35.13265428020583

\$coordinates

C	0.00851400609862	2.88925244851077	17.32157298902336
C	2.36413805709564	1.54549929647122	17.36677166257138
C	4.71149191256896	2.86370449269544	17.62937087728420
C	7.07158024689449	1.52139712854014	17.57509313173166

C	9.38533477564488	2.91505489941254	17.64121420098010
C	11.75097281608031	1.55851644244692	17.52643667322493
C	14.05340667969672	2.96096829005774	17.45100951161368
C	16.41223490495785	1.59398476121980	17.34091202477762
C	18.76214048974310	2.92937996830305	17.28446298012802
C	21.12172939024078	1.57518348671866	17.21193112649438
C	-2.36084612395028	6.94840526000973	17.51592961644598
C	-0.01888891432964	5.56786538397167	17.57536008200299
C	2.29018302237138	6.83824298769292	18.13822696462952
C	4.71163681298877	5.52253008322482	18.05406803999882
N	6.96389729714339	6.84243298483329	18.22719071257480
C	9.28569414123379	5.64390435953369	17.81239742117783
C	11.61912470248804	7.07859002910788	17.55419126223642
C	13.99614314796944	5.69107853387552	17.43840007593917
C	16.38600088596257	7.00412350032365	17.35151483964849
C	18.74216426857511	5.63347060523114	17.36091378559418
C	-4.64821897806488	11.04561039422599	17.41407476725753
C	-2.33023363408982	9.65620575246435	17.61914231322374
C	-0.00502363848205	10.95794999227884	18.09242375635576
C	2.03600993015401	9.40017890694850	18.96399407455360
N	9.53611333974702	11.26713859991493	17.27396862230863
C	11.71183917884621	9.83687359123138	17.33401173518563
C	14.12348315170491	11.10313122917273	17.19420847176059
C	16.44588729708010	9.71359010950061	17.30112047372392
C	-6.90287122810467	15.12520166902093	17.27413392043224
C	-4.56010397037302	13.75100267072952	17.45258448306557
C	-2.15774346985541	15.07173263554304	17.61654249038194
C	0.19655323184224	13.68706520269523	17.88591089304710
C	2.61968859525196	15.05310521206595	17.70318957771717
N	4.97166624394627	13.83547473809694	17.58495751533221
C	7.13673730637533	15.20534259371398	17.24542735920857
C	9.55869118655553	13.85802743076101	17.09854099219648
C	11.86650462990800	15.19696003129544	17.03645102246720
C	14.19699281766576	13.80326973634670	17.12279098395369
C	-9.26461348474986	19.20138747970437	17.22461860596813
C	-6.91371622082710	17.83226809169311	17.30697454668242
C	-4.56068023857538	19.15812058813626	17.45380843788974
C	-2.19917796014053	17.79624883460685	17.52885572108617
C	0.12515827523992	19.16935946025437	17.53507848906029
C	2.49145795036569	17.79728203102733	17.51945237963751
C	4.78650795670281	19.22345741915309	17.34344472643718
C	7.15032500980104	17.89554754575232	17.20354033809802
C	9.49522936069718	19.22968540277132	17.13354105006368
C	11.84703875195678	17.89078383531931	17.09427871492156

Al	6.73230926103970	10.44155438524413	19.39525842105671
O	8.23385861309657	11.17019041705112	22.39076673216405
O	3.62798798742223	10.27871726897881	20.64666734321885
O	10.81804889395286	10.56710375631316	22.49078774954683
C	12.90045181968369	13.22980154118156	22.81218365346885
O	12.00985399275248	15.20868215551659	23.19418594660312

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FS3:

\$cell vectors

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0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	-0.09194816028914	2.94321622173681	17.34458587346256
C	2.25054833559359	1.57881213315470	17.34481629154844
C	4.60605308251116	2.88914677313613	17.53875211286782
C	6.96074477098400	1.55369124599498	17.46825656196607
C	9.28508467810232	2.93601310920247	17.52113094209612
C	11.64510805309230	1.61321365995605	17.42149727132580
C	13.95609411417231	3.01562098939881	17.41261965168512
C	16.31378818439473	1.66838167438332	17.32488780675209
C	18.66547960761125	2.99162487478760	17.32137913713800
C	21.01581236687678	1.62657156323634	17.26480354697845
C	-2.43688944399266	7.01473411031479	17.49888557937121
C	-0.09051560615694	5.63276567691528	17.55586719230654
C	2.24173752533033	6.91513912223825	18.02715734031379
C	4.63187221591516	5.54852329630972	17.96388078131501
N	6.90519843149678	6.78750780777198	18.23191023743156
C	9.20529297101772	5.63420477516905	17.76811330326472
C	11.53228985952394	7.11002047558319	17.60359013744588
C	13.90767405473463	5.74394785898819	17.45684093809430
C	16.29957174641051	7.05972947389820	17.37658265196026
C	18.66000309248389	5.69773531902822	17.38461415995657
C	-4.73952993026358	11.09498177014088	17.36572763613047
C	-2.40020218572874	9.72441344785137	17.54684192836371
C	-0.05517909578127	11.04743537833395	17.89310699469751
C	2.06855405459573	9.52789900452758	18.72240437002583
N	9.41692215820568	11.29410229696913	17.59077287725105
C	11.61272866741524	9.87060907461134	17.46305144741505
C	14.01204820175525	11.13790451234602	17.26746760539069
C	16.34974767133339	9.76178223395254	17.31165487295017
C	-7.03431869519200	15.16351076583436	17.27196934687045

C	-4.68032536067783	13.79907259982103	17.36887117475241
C	-2.28118919024319	15.12641029438677	17.43377983540330
C	0.08001712495515	13.76262721138331	17.61514644008929
C	2.47671314495692	15.18736590498693	17.39600713924017
N	4.74004663618821	13.97702481332932	17.18820378951965
C	6.94668413713934	15.24357009215333	17.18679903892793
C	9.39062192698643	13.85327221464693	17.23179144697967
C	11.71315121947424	15.21202126378493	17.13581317549815
C	14.05788306861078	13.83958058384324	17.21100538557055
C	-9.39574009334871	19.22816440756673	17.22833353351958
C	-7.04281357726224	17.86736461818926	17.27761204073378
C	-4.68298696622557	19.19562561215269	17.35396849973343
C	-2.32235031085734	17.85321953248407	17.37435491619247
C	-0.00092099582154	19.24328733772448	17.39095554226010
C	2.35820957239151	17.91053751289019	17.36090580717049
C	4.67387637736874	19.29861729412177	17.28283248852258
C	7.02259970224704	17.95355969437375	17.21455459547919
C	9.37056293014499	19.27686279153728	17.19610117231450
C	11.71156142879008	17.91278551030149	17.14760717356274
Al	7.05767184560700	9.92590855917486	20.13815641246053
O	8.79294905002738	10.21040893811673	22.77375534706227
O	3.71954053543683	10.49015110761833	20.25929783293683
O	14.35468553250102	10.64303684107177	23.28661690357131
C	13.20744184246719	12.54692112300615	23.27410785770747
O	12.28465096630348	14.57083351783674	23.23750317669576
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IS4:

\$cell vectors

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-11.66312693572874	20.34693000729107	0.000000000000000
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\$coordinates

C	-0.00186429419080	2.86380371843481	17.25419365319350
C	2.35075016953092	1.50422428017378	17.25799249970271
C	4.71101081097425	2.80144597640334	17.30087822217305
C	7.07307872979174	1.48291356087249	17.33301577581844
C	9.37078213648576	2.89916183404926	17.37281819468708
C	11.73810797636110	1.56475958733785	17.37126756101796
C	14.04102614465800	2.97618141684343	17.36779510233588
C	16.40442829893686	1.62038441848940	17.33261200370649
C	18.75930232708351	2.94546933463674	17.29768366094574
C	21.11399664983457	1.57476735201840	17.25852646638577

C	-2.33803347678101	6.95531844887225	17.31800630859669
C	-0.02164420682948	5.54143832756299	17.29189158045277
C	2.31713111784669	6.84578990566009	17.36746856711011
C	4.70993867107778	5.45523806219057	17.37430054499240
N	6.91815393838574	6.80364166203810	17.48875507508911
C	9.25274089108601	5.62814643037534	17.43598865879203
C	11.58861451862054	7.08422642073459	17.42681898386845
C	13.98144376401781	5.70570870660782	17.38283672324765
C	16.38159557909670	7.00972969223715	17.35269437457037
C	18.74150580106576	5.64287114421595	17.31683240694839
C	-4.62236042686364	11.03103961180635	17.35869986939354
C	-2.26910833364255	9.66020055412409	17.36264879606187
C	0.15927658689719	10.93763172879251	17.44398348342479
C	2.41224605471994	9.47540446501783	17.50052968267393
N	9.45161799662292	11.28600818423604	17.41080780684292
C	11.65291278450497	9.83548758483308	17.39891251000940
C	14.09052036032992	11.09406047385289	17.35158670971248
C	16.44027588574303	9.71434100918391	17.35271267278844
C	-6.90191028347285	15.10390616768412	17.32638958344198
C	-4.54582928158100	13.73596724056054	17.36701615344770
C	-2.14055197934083	15.05835026408888	17.40534279258875
C	0.23314352825868	13.69137813785839	17.46607157369294
C	2.59634819481913	15.11128570693921	17.46666613822365
N	4.96185337427989	13.93919797651271	17.51917724496234
C	7.16034076991284	15.28030345784498	17.37769581781091
C	9.53897206073712	13.88314644142268	17.34245385421272
C	11.85889105941068	15.19381993197505	17.29072223682388
C	14.18428375374021	13.79447520796374	17.31738249488502
C	-9.27082229331710	19.17301512410481	17.26390323609907
C	-6.91616734300985	17.80655589600080	17.30622863209664
C	-4.55909534039216	19.12753659156631	17.33593182543000
C	-2.19697164441837	17.78230490457848	17.37813632430900
C	0.11514699188932	19.18102267226357	17.37853206508492
C	2.48462774693623	17.83986610029579	17.39140704885396
C	4.78219723818840	19.26157845987120	17.34486779036479
C	7.15491585942650	17.94047883628174	17.30790158017893
C	9.49774463719215	19.24261189480535	17.25775631228298
C	11.83818187772949	17.87975593789497	17.25801118531463
Al	5.92099057754813	10.38693373376841	18.16707764014693
O	6.48285079172952	10.47781619812718	21.74006759778628
O	4.41142521324919	10.28519361552219	23.09945506632917
C	5.52454299303699	4.20092328548930	23.37857136798681
O	7.65509281073523	4.53824416280022	23.38062523194357

Send

TS4:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	0.00379317544111	2.87038229538210	17.20473063312045
C	2.35439494855888	1.50945953963594	17.21992369290443
C	4.71541304892490	2.80442375580850	17.24122804004923
C	7.07589602609546	1.48895879852580	17.30303396315494
C	9.37165362904173	2.90201229693620	17.35705707567103
C	11.74049007629714	1.56897869381944	17.39061653673163
C	14.04263648044460	2.98112642571115	17.37868771237720
C	16.40560358386469	1.62947221157998	17.34148474596405
C	18.76231298016434	2.95387142359533	17.27637526978704
C	21.11805325876668	1.58049525174299	17.24746736202420
C	-2.33468835729386	6.96114785901510	17.27809174204144
C	-0.01513826339553	5.54986451430913	17.21017591485442
C	2.32157667020985	6.85792960455280	17.26645061904090
C	4.72139754511137	5.46283056224159	17.27686854877689
N	6.92109866081179	6.79890033730077	17.38921899544507
C	9.24887133669438	5.62925505710383	17.39955270008767
C	11.58628926920524	7.08712995280030	17.44492682525776
C	13.97881224668944	5.71377727213343	17.39127726435343
C	16.38391050493817	7.01631815812126	17.35754517492158
C	18.74415086395100	5.65234505181756	17.29510336653371
C	-4.61974036505504	11.03741842391524	17.37718366423651
C	-2.26681258663152	9.66599789750432	17.35591803569029
C	0.16356165426918	10.93795947722244	17.45216106158138
C	2.42118834267834	9.48152243822968	17.46008664853865
N	9.45722348555831	11.29332289076724	17.53545313671319
C	11.64998309485024	9.84379346972438	17.46852245777021
C	14.09297501441080	11.09934545578885	17.40194885013744
C	16.44209458651162	9.72188232789257	17.37663632963084
C	-6.89489100349595	15.10816846007685	17.33409286679736
C	-4.54201333682981	13.74201905635049	17.37665168932479
C	-2.13427376302275	15.06103030769442	17.43147971178656
C	0.23626686003917	13.69118216192087	17.52653501268275
C	2.60584998343999	15.11344888021395	17.58508474114358
N	4.96546517569725	13.94540268437425	17.70856792157233
C	7.15541318809944	15.28187774899546	17.52298452153979
C	9.54388797916087	13.87961675616436	17.46789139884858

C	11.86268556521898	15.19579186874538	17.36852093669185
C	14.18753204177099	13.79859461816416	17.36251270743498
C	-9.26830970968185	19.17816048173630	17.26802729124631
C	-6.91130880611989	17.81180039622371	17.30159269549557
C	-4.55315409436751	19.13136095882684	17.32577709863843
C	-2.19232100574804	17.78753800786313	17.39656619014781
C	0.11821162499691	19.18559330370922	17.41385982035944
C	2.48830666386664	17.84592530302516	17.46380103940787
C	4.78221314023374	19.26760690163871	17.40271709750657
C	7.15451156386041	17.94303379891506	17.38706844932030
C	9.50019837664559	19.24771325961265	17.29872010769516
C	11.84248322698178	17.88254956915843	17.30656447422357
Al	5.91463890001667	10.33010913061791	18.37261784252180
O	6.42272953489780	10.05217035888273	21.80535879380692
O	4.52175466963628	8.49296292862958	22.76799123451595
C	5.47642199409695	5.21706075139999	23.24919844790867
O	7.59570587312979	4.69454817648772	22.97877470312257

\$end

FS4:

\$cell vectors

23.46283956792041	0.000000000000000	0.000000000000000
-11.66312693572874	20.34693000729107	0.000000000000000
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\$coordinates

C	0.07919533597572	2.87836277699357	17.20348860873507
C	2.43239631588458	1.51546094698151	17.21146356289763
C	4.79455448991153	2.80895859584133	17.25306765232302
C	7.15218423952583	1.49226419030062	17.30454612766934
C	9.44694294836024	2.90636204018482	17.34924376301203
C	11.81443516539280	1.57686806795498	17.35022278098450
C	14.11619370136338	2.98910287275735	17.34472405779573
C	16.48051439104036	1.63922779797833	17.30211347189028
C	18.83657668653330	2.95843045968147	17.26137737146862
C	21.19273788462245	1.58622100851815	17.21378166536872
C	-2.25810881045598	6.96824564010495	17.28315403109192
C	0.06324749312126	5.55935146669018	17.24211601290673
C	2.40372122993925	6.86670316831414	17.31701908543338
C	4.80505333583046	5.47112012367861	17.31332418897885
N	6.99940393767237	6.80539466647795	17.44200560535552
C	9.32026079419367	5.63552493406052	17.41093912202162
C	11.66240145842652	7.09577258688707	17.40978253026462
C	14.05038906864430	5.72395192797671	17.36289572090545

C	16.45932482019122	7.02475069623690	17.33009682547728
C	18.82031873584228	5.65906182443637	17.28601654854181
C	-4.54038453086007	11.04123461622055	17.33893620273037
C	-2.18809308558380	9.67190078775781	17.33858326236146
C	0.24027975393683	10.94737545526970	17.43611499832184
C	2.50688663632073	9.49315543918733	17.48981058917513
N	9.54071941867531	11.29636747766009	17.38848995422386
C	11.72913058673992	9.85583480648256	17.38016997008594
C	14.17312428980360	11.10769802447434	17.33205520913184
C	16.52097779831300	9.72763747557815	17.33292780717759
C	-6.81934526157036	15.11230782200570	17.30459772097200
C	-4.46524389330335	13.74497196507012	17.35139840228357
C	-2.05648414328881	15.06493860903051	17.39492264242457
C	0.31194953340950	13.69638399968678	17.46300785521280
C	2.68607831552522	15.13024079758803	17.45639397440204
N	5.02974106911408	13.96789359622211	17.50062552391381
C	7.21649473571775	15.28264980605246	17.33518018686378
C	9.61798480948492	13.86815583555738	17.30251710605222
C	11.93528255960186	15.19675028681337	17.25351865436001
C	14.26275212908318	13.80299375885368	17.29249192376597
C	-9.19400488287240	19.17972104024703	17.22613327814910
C	-6.83578035896779	17.81369368448245	17.27873383885336
C	-4.47733448010381	19.13311762744564	17.31221267474884
C	-2.11586360891715	17.79266831949521	17.36194487874949
C	0.19396395745166	19.19514224288663	17.35961349717292
C	2.56310889115862	17.86015381257987	17.36859122694480
C	4.85964691886917	19.27448512678846	17.31220274423806
C	7.22792471583888	17.95054588922974	17.26364957816131
C	9.57325061739034	19.25137546758467	17.21236098627549
C	11.91402230543674	17.88529296961176	17.21664959688396
Al	5.99409874095810	10.38147986133949	18.53522696710960
O	6.28205479970378	10.41886056216388	21.77462745529101
O	2.66726914385860	6.83612941028034	24.20084182695496
C	4.65526425689381	6.02366140480818	23.63613838753768
O	6.55674176473814	4.98247624838949	23.12831395459632

\$end

IS5:

\$cell vectors

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-11.66312693572874	20.34693000729107	0.000000000000000
0.000000000000000	0.000000000000000	35.13265428020583

\$coordinates

C	-0.03060487804363	2.86237072966559	17.27260002595713
C	2.32190353424796	1.49913022104768	17.28286957628751
C	4.68395312083232	2.79309360613909	17.34464350821965
C	7.04251465282488	1.47559892426116	17.38177442882429
C	9.33891881800591	2.88984258352344	17.42616438840794
C	11.70638494925904	1.56006608778928	17.41177849679237
C	14.00775524099724	2.97276378100597	17.40320095621170
C	16.37174701628327	1.62230552918588	17.35425407514544
C	18.72731867840292	2.94223753068695	17.31616751625994
C	21.08331121654568	1.56980358761889	17.26753281417009
C	-2.36749466800735	6.95246953934018	17.35782918186090
C	-0.04614660174629	5.54376239212000	17.32601572380486
C	2.29386509892387	6.85109113924072	17.42772673459958
C	4.69412812249548	5.45454376358416	17.43273471292124
N	6.88947644681905	6.78769276093701	17.57139193870969
C	9.21301396299661	5.61919368089311	17.50450860307532
C	11.55407682193407	7.0799982337864	17.48256185298296
C	13.94188565650152	5.70752363170360	17.42565809676398
C	16.35027062091314	7.00872304457900	17.39122901019682
C	18.71083366200017	5.64272198624318	17.34818578850259
C	-4.64997955652704	11.02568321145095	17.40497386702655
C	-2.29718033995125	9.65629610971902	17.41667240935539
C	0.13122530710463	10.93165279784947	17.52851139030948
C	2.39772176523215	9.47682712643377	17.61014126234175
N	9.43030735480040	11.27891671483144	17.45080476545722
C	11.61931460862524	9.84055431473996	17.44212489053771
C	14.06340807600024	11.09181026357230	17.38880622256759
C	16.41160977599680	9.71189036132242	17.39389621500307
C	-6.92946786664608	15.09637482483968	17.35973319809485
C	-4.57505879049469	13.72935511341563	17.41388204920785
C	-2.16612336209094	15.04909237863952	17.45921747656636
C	0.20260100172855	13.68134313844492	17.53624328033893
C	2.57675258716942	15.11384064689582	17.51554829994958
N	4.92001885920972	13.95033504719474	17.56038550857414
C	7.10654239496589	15.26490469381339	17.38445988460544
C	9.50743794199688	13.85079072267562	17.35276252565334
C	11.82461952120029	15.17972751293696	17.30008134545313
C	14.15274851061292	13.78693232456185	17.34417613737496
C	-9.30422716344231	19.16350157571827	17.28077543848757
C	-6.94595113316244	17.79757973092215	17.33532626647270
C	-4.58718789558275	19.11656802209367	17.37482132705629
C	-2.22530344460556	17.77644256217845	17.42170794177367
C	0.08485246545693	19.17846785135971	17.41686751790862
C	2.45391221031017	17.84337069377062	17.42178440765159

C	4.75041203153792	19.25774127459836	17.36090436153000
C	7.11827332342105	17.93276993099114	17.30908957918412
C	9.46348038198625	19.23457389937927	17.25784685851026
C	11.80392359972732	17.86854248637269	17.26227843634872
Al	5.88739262465609	10.37121811368828	18.65080322162656
O	6.27560270212604	10.51049601813276	21.88074364067078
C	3.81540805195990	3.87867702370829	28.56864770148564
O	5.65464504693292	2.75722770788677	28.45884157262352

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TS5:

\$cell vectors

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-11.66312693572874	20.34693000729107	0.000000000000000
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\$coordinates

C	-0.02962078804623	2.86228528191940	17.28065524434712
C	2.32304979487223	1.49985875204284	17.29088816800574
C	4.68373888825070	2.79565408110352	17.35151154018668
C	7.04358436253355	1.47685730800560	17.37871780059656
C	9.34125209875723	2.89199685996758	17.41922981540459
C	11.70851591404170	1.55986215232532	17.40487857569697
C	14.01189605045630	2.97241080662198	17.39688039113116
C	16.37488877856265	1.61897195214590	17.34921030730071
C	18.73034679633260	2.94231572755400	17.31857372532188
C	21.08477294804926	1.57048509655889	17.27297235302635
C	-2.36675484400886	6.95286580357024	17.37348967296080
C	-0.04621832630136	5.54181057148427	17.34170963660100
C	2.29495849068034	6.84572527702661	17.46304670987166
C	4.69065597561822	5.45368740584473	17.44382147531437
N	6.89282194614115	6.79293053562465	17.55207299452359
C	9.21809523812547	5.62034929188224	17.49100294588876
C	11.55981404745709	7.08011432944346	17.48026587731506
C	13.95010835186934	5.70384551790680	17.42385089686859
C	16.35289304865885	7.00732972116115	17.39627245678812
C	18.71375382365578	5.64120578149432	17.35567775323404
C	-4.65075707489254	11.02712436383702	17.41492587533779
C	-2.29919402266142	9.65729996625168	17.43400459753888
C	0.12752190310309	10.93532463586582	17.55290488030971
C	2.38375246185110	9.47349012521006	17.65580942322772
N	9.42997794152174	11.27937045130213	17.48318340847191
C	11.62644470970102	9.83430288717943	17.45974548305322
C	14.06420837690390	11.09005603081046	17.40077205153900

C	16.41243584142645	9.71099043972662	17.40182591400438
C	-6.93137590799668	15.09831510113852	17.36738867704845
C	-4.57551965690205	13.73164476228045	17.42068300156663
C	-2.17020487383392	15.05317466517022	17.45917187558524
C	0.20222614620577	13.68600288181571	17.53831149487588
C	2.57323906284892	15.11148816841679	17.50032363638589
N	4.92227344231658	13.94165106212091	17.53562728442424
C	7.11629046592344	15.26742968916983	17.38299117056384
C	9.50687057440456	13.86408683569107	17.37320226073500
C	11.82669098606617	15.18424900016499	17.31302464849078
C	14.15397042075343	13.78882685815010	17.35685540031952
C	-9.30196611558239	19.16617648115847	17.28726497909875
C	-6.94584435796720	17.79999299055227	17.33905495689951
C	-4.58800322925773	19.12037392672995	17.37217648337928
C	-2.22657691970283	17.77725036718456	17.41629332840499
C	0.08629440585879	19.17796078114859	17.40909276511119
C	2.45465430953891	17.83982519528409	17.41067525767306
C	4.75263935534542	19.25740517357895	17.35327699603197
C	7.12143002020600	17.93348777747479	17.31016023564558
C	9.46515193545066	19.23658444892351	17.26444140175358
C	11.80670558271894	17.87138382377218	17.27041024533855
Al	5.90336920268601	10.37793129393772	18.51470626860185
O	6.20973617520719	10.45199352148670	21.83290013856356
C	5.04734014331821	7.26796958467963	25.08887964379437
O	6.88761810715527	6.14711824434447	24.98187183649595
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FS5:

\$cell vectors

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\$coordinates

C	-0.03197208922588	2.86330079050335	17.41762695537455
C	2.32101465243219	1.50641184603334	17.41940421255949
C	4.67907923747649	2.80577486652417	17.40265656579934
C	7.04408227135242	1.48702323331419	17.41872783233620
C	9.34398857714377	2.90768699709092	17.42072355508927
C	11.71191793129274	1.56808907878994	17.43802913970837
C	14.01561950445202	2.97864219363696	17.44204769711523
C	16.37885574077711	1.61696203754963	17.44863651448839
C	18.73226582833034	2.94759799206380	17.43943943853600
C	21.08453492948491	1.57780191958334	17.43741853140286

C	-2.36778722784711	6.95799938064907	17.41633281045292
C	-0.05352784175490	5.53837982850640	17.40211972862230
C	2.28658183365594	6.83558577008925	17.39275309699335
C	4.66607752867350	5.45295343999723	17.38669050031585
N	6.88485403687758	6.82538572577548	17.40030781952940
C	9.23224555270285	5.63724264219581	17.41462613264902
C	11.56284074431272	7.08976799913244	17.43628360346617
C	13.96166174244479	5.70401923098084	17.43978552486826
C	16.35407622319324	7.01212380138272	17.43745557759382
C	18.71467056759354	5.64348292793111	17.43040255655696
C	-4.65315024106476	11.03682404835715	17.43621549395717
C	-2.30000804297674	9.66556251594348	17.42245758478910
C	0.12942635964323	10.94784191715612	17.42724193481085
C	2.38029894011452	9.47900005258503	17.41979791054146
N	9.40541981858150	11.29202221873157	17.45609263111525
C	11.62728189805864	9.83275829307500	17.44485696586237
C	14.05705414402551	11.09651061904724	17.44525888037354
C	16.40982688553828	9.71707385740656	17.43890777353937
C	-6.93334386878325	15.11075469578782	17.44664504928828
C	-4.57507669564972	13.74331913501215	17.44365975255259
C	-2.17565062610969	15.06759541845335	17.44877868992313
C	0.20696673017046	13.70024977651589	17.45330760566456
C	2.55990618899116	15.10368369400688	17.46933810136028
N	4.94866680112900	13.90867235358277	17.49742056541336
C	7.15485686406660	15.28994736142934	17.48579176342717
C	9.51055283615021	13.91266094560246	17.47126349417616
C	11.83479290147844	15.20460312120455	17.45886547350160
C	14.15676043319135	13.80227140159377	17.45039415253670
C	-9.29615793462283	19.17843848501573	17.43970182700846
C	-6.94492866093772	17.81344073519199	17.44204887063515
C	-4.59001160183748	19.13631373446893	17.43605075897195
C	-2.22672678443317	17.78646235496580	17.44571480136763
C	0.08826083974665	19.18073854816123	17.44696469079314
C	2.45895639578438	17.83242230657299	17.45943996914086
C	4.75578494432021	19.26297301728021	17.46098458781173
C	7.13053731338047	17.94351816595652	17.46748053837393
C	9.47219582344115	19.24804406561946	17.45419503428094
C	11.81320596846836	17.88827852146047	17.45378159621986
Al	5.89749072013515	10.39554307277059	17.57143777968603
O	5.99283691413266	9.76552223250049	22.23471658617390
C	4.91417198232831	8.00931621864923	23.09612247005705
O	3.85991639343665	6.27665171555419	23.96441864310155

\$end

