

Assessing the Oxygen Reduction Reaction by a 2-electron Mechanism on Ceria Surfaces

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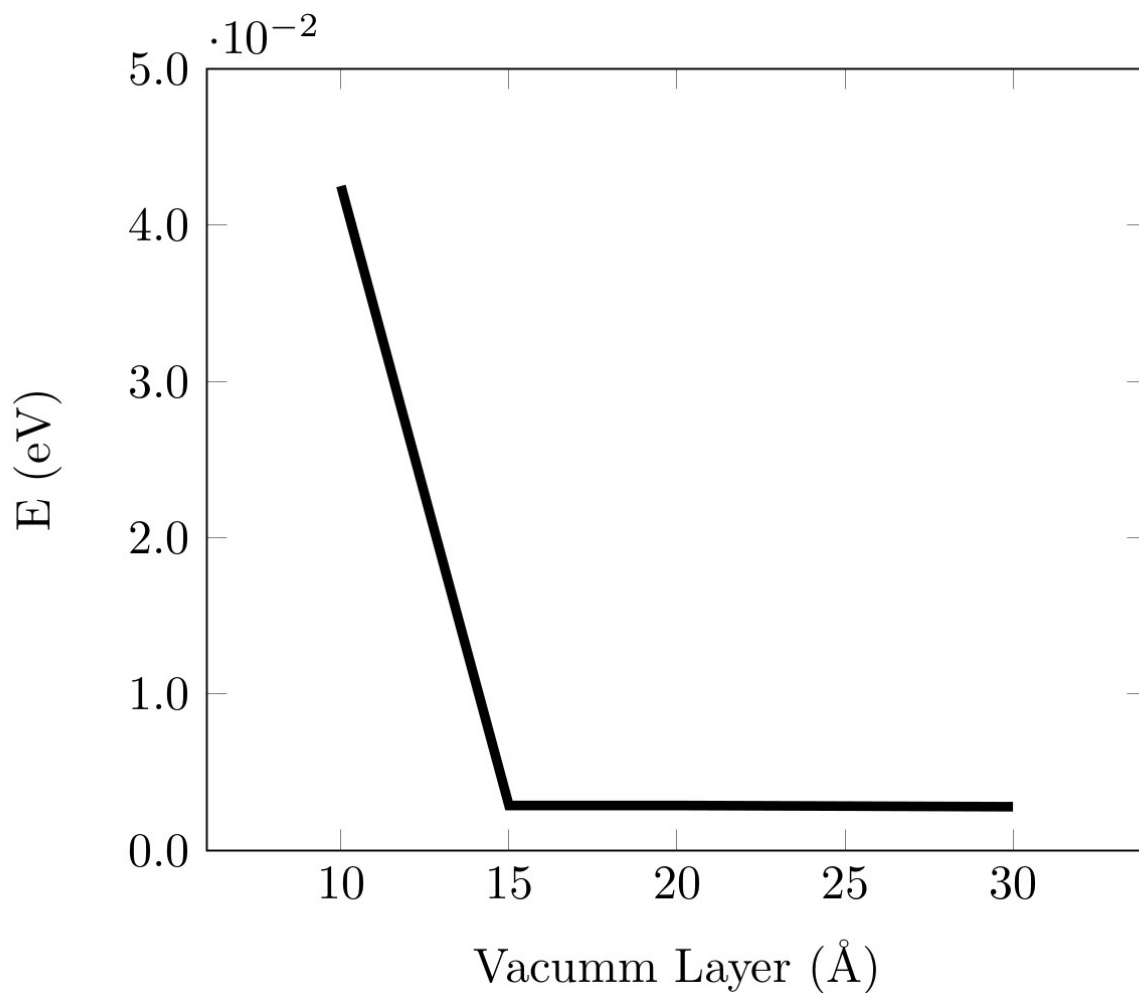


Figure S1: Vacuum layer convergence test regarding the adsorption energy variation of intermediate species (*OOH) over the ceria surface.

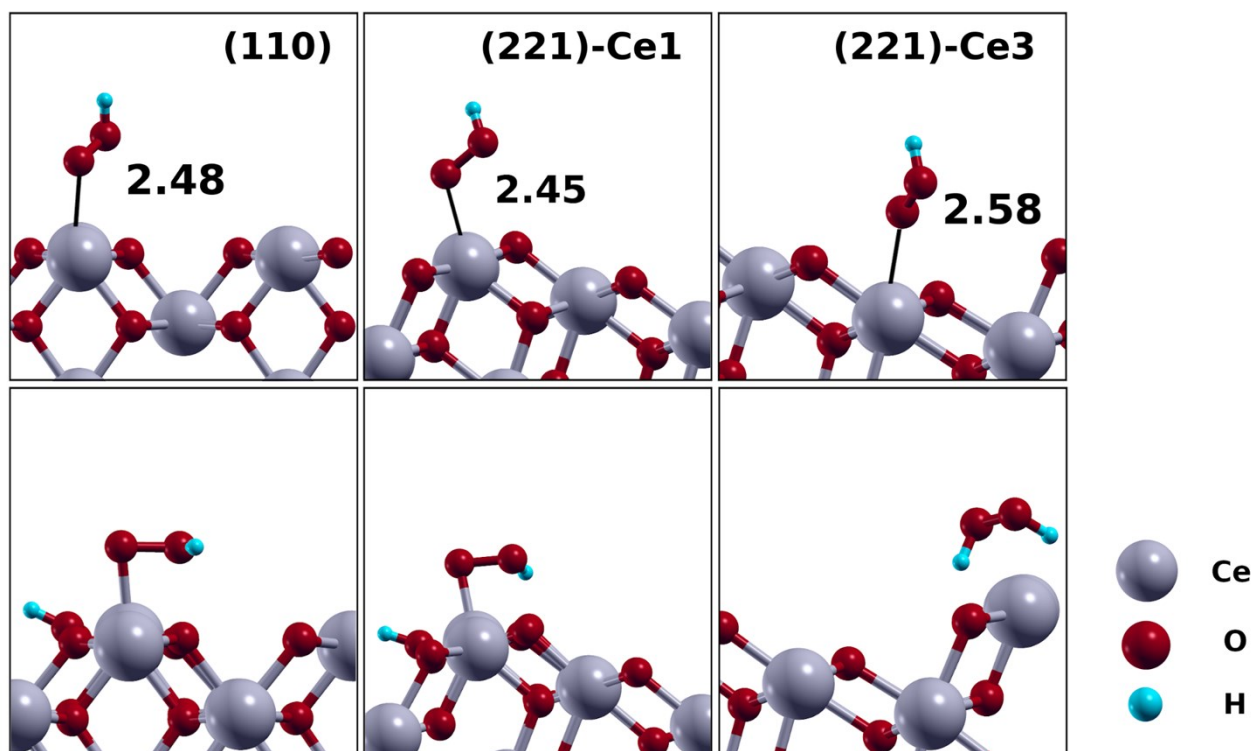


Figure S2: Unstable sites for hydrogen peroxide molecule, along with intermediate reaction step (*OOH). Following the order of the columns, from left to right: (110), where the molecule breaks into $\text{*OOH} + \text{*H}$, (221)-Ce1, where the molecule breaks into $\text{*OOH} + \text{*H}$, (221)-Ce3, where the molecule migrates over the surface to another site.

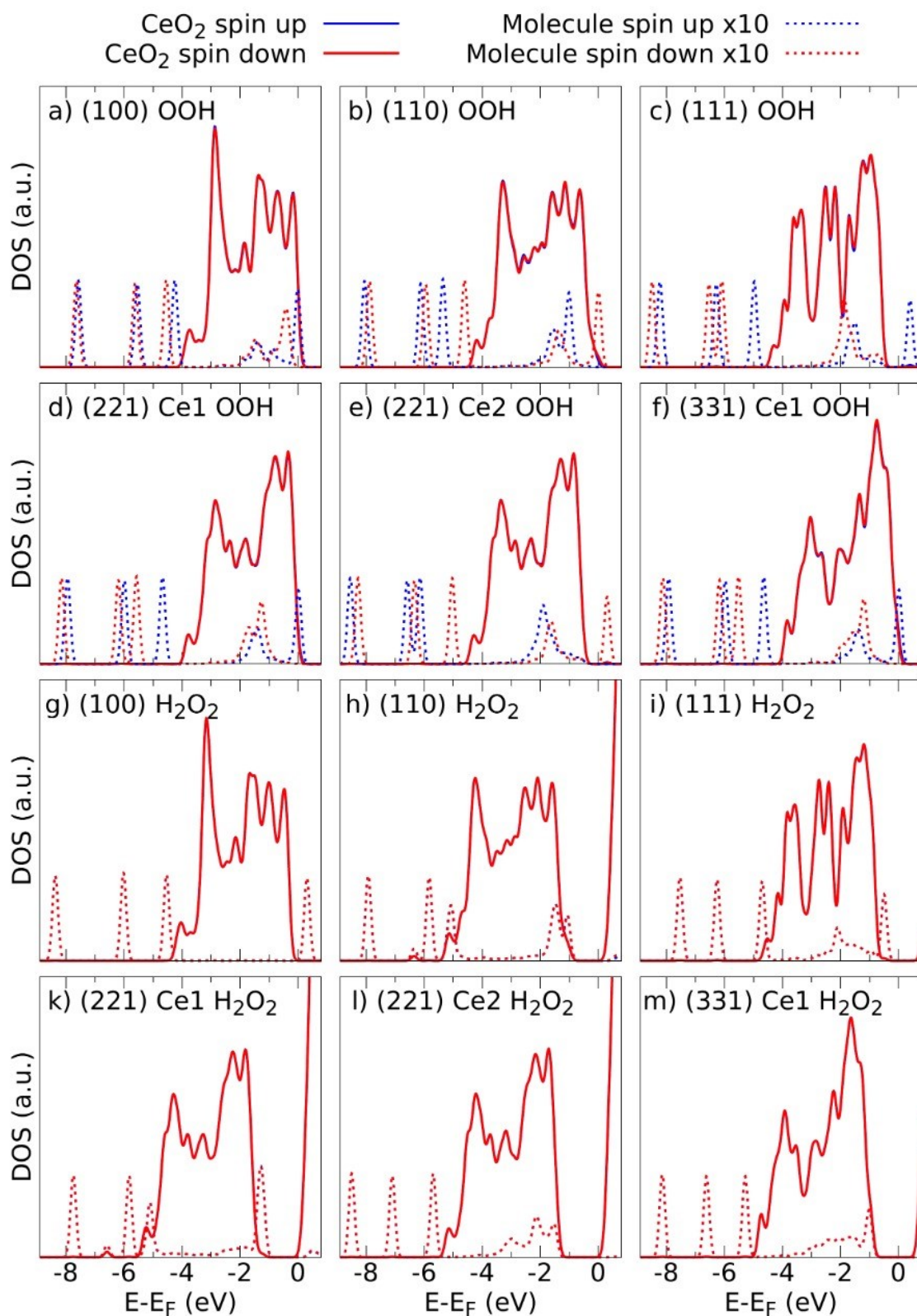


Figure S3: Density of States (DOS) of selected ceria surfaces and sites with adsorbed species *OOH and H₂O₂. For better visualization, molecular species contributions have been magnified by twenty times. The surface DOS were normalized to account for the different number of atoms in each case.

Structures Optimized Atomic Coordinates

100-OOH

Ce	2.7500769090	0.0000000000	1.7734174790
Ce	2.7500769090	5.5001538170	1.7734174790
Ce	8.2502307260	0.0000000000	1.7734174790
Ce	8.2502307260	5.5001538170	1.7734174790
Ce	10.9922608510	2.7405087640	23.4031887210
Ce	10.9917314470	8.2407709680	23.4012728380
Ce	5.4925138900	2.7487589540	23.4141600240
Ce	5.4923075280	8.2299139490	23.4142010500
Ce	2.7419471620	10.9908262210	23.4031542280
Ce	2.7502353940	5.4910852160	23.4141467880
Ce	8.2422189370	10.9902991190	23.4012936390
Ce	8.2314087730	5.4908703880	23.4141783580
Ce	2.7453402990	2.7442467440	20.6490450170
Ce	2.7451694650	8.2407012250	20.6482037250
Ce	8.2418026330	2.7440677710	20.6482106720
Ce	8.2412028180	8.2401080160	20.6470686940
Ce	10.9935764460	10.9924953630	20.6449668250
Ce	10.9928034560	5.4921741730	20.6479977880
Ce	5.4932722280	10.9916962040	20.6480034560
Ce	5.4929839090	5.4918659440	20.6440050610
Ce	10.9957595780	2.7455443210	17.8884802900
Ce	10.9955363470	8.2440693250	17.8880552250
Ce	5.4953099580	2.7444848440	17.8863013790
Ce	5.4955963370	8.2449937640	17.8854807260
Ce	2.7461975170	10.9951043550	17.8884887080
Ce	2.7451475000	5.4946542210	17.8863054330
Ce	8.2447203390	10.9948816300	17.8880605750
Ce	8.2456567280	5.4949393910	17.8854807320
Ce	2.7480801220	2.7478586550	15.1301301040
Ce	2.7480604330	8.2485105290	15.1298996710
Ce	8.2487318420	2.7478378120	15.1298966530
Ce	8.2487271290	8.2485057390	15.1295875260
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Ce	5.4984310260	10.9984470740	15.1296469380
Ce	5.4984403860	5.4982168440	15.1288748010
Ce	10.9907443820	10.9891569680	25.7244943250
Ce	-0.0100864040	5.4909952630	25.7366766630
Ce	5.4924939810	-0.0117006830	25.7366868700
Ce	5.4876379550	5.4859976170	25.8018317830
Ce	0.0000000000	2.7500769090	12.3716886990
Ce	0.0000000000	8.2502307260	12.3716886990
Ce	5.5001538170	2.7500769090	12.3716886990
Ce	5.5001538170	8.2502307260	12.3716886990

Ce	2.7500769090	0.0000000000	12.3716849970
Ce	2.7500769090	5.5001538170	12.3716849970
Ce	8.2502307260	0.0000000000	12.3716849970
Ce	8.2502307260	5.5001538170	12.3716849970
Ce	2.7500769090	2.7500769090	9.6150052340
Ce	2.7500769090	8.2502307260	9.6150052340
Ce	8.2502307260	2.7500769090	9.6150052340
Ce	8.2502307260	8.2502307260	9.6150052340
Ce	0.0000000000	0.0000000000	9.6150447140
Ce	0.0000000000	5.5001538170	9.6150447140
Ce	5.5001538170	0.0000000000	9.6150447140
Ce	5.5001538170	5.5001538170	9.6150447140
Ce	0.0000000000	0.0000000000	4.1042991380
Ce	0.0000000000	5.5001538170	4.1042991380
Ce	5.5001538170	0.0000000000	4.1042991380
Ce	5.5001538170	5.5001538170	4.1042991380
Ce	0.0000000000	2.7500769090	6.8584163580
Ce	0.0000000000	8.2502307260	6.8584163580
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Ce	5.5001538170	8.2502307260	6.8584163580
Ce	2.7500769090	0.0000000000	6.8607432510
Ce	2.7500769090	5.5001538170	6.8607432510
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Ce	8.2502307260	5.5001538170	6.8607432510
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Ce	2.7500769090	8.2502307260	4.1040885740
Ce	8.2502307260	2.7500769090	4.1040885740
Ce	8.2502307260	8.2502307260	4.1040885740
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O	6.9257911560	9.6758867650	2.7402562040

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O	1.3751295370	6.8750996490	8.2371202020
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O	9.6252691800	1.3750424140	13.7503855520
O	9.6252691800	6.8751961210	13.7503855520
O	5.3357639740	5.3335182390	28.2380309030
O	6.3042309530	6.3018709990	28.7020527530
H	6.2115247170	6.2092291980	29.6680922210

100-HOOH

Ce	2.7500769090	0.0000000000	1.7734174790
Ce	2.7500769090	5.5001538170	1.7734174790
Ce	8.2502307260	0.0000000000	1.7734174790
Ce	8.2502307260	5.5001538170	1.7734174790
Ce	10.9959689000	2.7368005780	23.4152542010
Ce	10.9969813090	8.2388659370	23.4170847660
Ce	5.4961151290	2.7420855720	23.4114984130
Ce	5.4980263920	8.2403962070	23.4046043590
Ce	2.7527047240	10.9893651820	23.4156259400
Ce	2.7423012910	5.4883256580	23.4010070680
Ce	8.2513336990	10.9905336280	23.4175852180
Ce	8.2375389400	5.4901011490	23.4122921380
Ce	2.7493153530	2.7398541750	20.6525222370

Ce	2.7493927600	8.2412662410	20.6520369800
Ce	8.2493393790	2.7409286790	20.6552065150
Ce	8.2506221370	8.2414238710	20.6534825780
Ce	0.0021061280	10.9901132610	20.6586301180
Ce	10.9955532250	5.4900908490	20.6511415010
Ce	5.5024420200	10.9922652540	20.6506665410
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Ce	0.0026211340	8.2439521140	17.8943291660
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Ce	2.7496112710	5.4935245580	17.8904059250
Ce	8.2546084930	10.9940844360	17.8948419230
Ce	8.2513978940	5.4939871140	17.8900647520
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Ce	2.7520121700	8.2473681850	15.1315517380
Ce	8.2515434600	2.7477465860	15.1319032750
Ce	8.2516688510	8.2475871450	15.1314863240
Ce	0.0017807650	10.9973851650	15.1326102130
Ce	0.0008098290	5.4972909500	15.1312761080
Ce	5.5019895800	10.9977325890	15.1311009240
Ce	5.5008620590	5.4976072980	15.1316186790
Ce	0.0068100910	10.9878318940	25.7363973520
Ce	-0.0087640920	5.4844631710	25.7276164240
Ce	5.5054032350	-0.0115534230	25.7302003990
Ce	5.4740679420	5.4964638780	25.7195432190
Ce	0.0000000000	2.7500769090	12.3716886990
Ce	0.0000000000	8.2502307260	12.3716886990
Ce	5.5001538170	2.7500769090	12.3716886990
Ce	5.5001538170	8.2502307260	12.3716886990
Ce	2.7500769090	0.0000000000	12.3716849970
Ce	2.7500769090	5.5001538170	12.3716849970
Ce	8.2502307260	0.0000000000	12.3716849970
Ce	8.2502307260	5.5001538170	12.3716849970
Ce	2.7500769090	2.7500769090	9.6150052340
Ce	2.7500769090	8.2502307260	9.6150052340
Ce	8.2502307260	2.7500769090	9.6150052340
Ce	8.2502307260	8.2502307260	9.6150052340
Ce	0.0000000000	0.0000000000	9.6150447140
Ce	0.0000000000	5.5001538170	9.6150447140
Ce	5.5001538170	0.0000000000	9.6150447140
Ce	5.5001538170	5.5001538170	9.6150447140
Ce	0.0000000000	0.0000000000	4.1042991380
Ce	0.0000000000	5.5001538170	4.1042991380
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Ce	5.5001538170	8.2502307260	6.8584163580
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Ce	2.7500769090	8.2502307260	4.1040885740
Ce	8.2502307260	2.7500769090	4.1040885740
Ce	8.2502307260	8.2502307260	4.1040885740
O	1.3770966510	1.3649829830	19.2778798840
O	1.3730672730	6.8670761280	19.2707135710
O	6.8785799700	1.3661408850	19.2711740330
O	6.8758544100	6.8684404020	19.2639804960
O	4.1277018740	1.3657716310	19.2705797960
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110-OOH

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O	5.5004360850	3.8891945150	7.7806341730
O	5.5004360850	11.6675835450	7.7806341730
O	2.7504627520	5.8333944990	9.7329576270
O	2.7497546040	13.6128658200	9.7219007720
O	8.2502599630	5.8327626810	9.7242214500
O	8.2498131150	13.6121299840	9.7241912010
O	4.1168503640	5.7408329180	17.9859268430
O	4.8130085430	6.7595591330	18.6505274620
H	4.7952213000	6.4399361700	19.5765603770

110-HOOH

Ce	1.3750384540	0.0000000000	2.1094769160
Ce	1.3750384540	7.7783890300	2.1094769160
Ce	6.8751922710	0.0000000000	2.1094769160
Ce	6.8751922710	7.7783890300	2.1094769160
Ce	4.1433498120	1.9273936340	15.3963118220
Ce	4.1524404930	9.8182854770	15.4265586640
Ce	9.6555154080	1.9559802630	15.3994445770
Ce	9.6223418200	9.7455847040	15.4022046630
Ce	1.3970979250	3.9065327390	13.7209616860
Ce	1.3782038280	11.6581761410	13.7060506540
Ce	6.8798744460	3.8895314450	13.7363977730
Ce	6.8913447340	11.6948876720	13.7154225200
Ce	1.3942362850	0.0001891700	13.7100887400
Ce	1.3377843570	7.7725436360	13.6332675260
Ce	6.8955260570	0.0120973820	13.7175391700
Ce	6.8395542680	7.7952933380	13.7381235190
Ce	4.1215864750	5.8343241370	11.7040507380
Ce	4.1321163240	13.6156625250	11.6293516490
Ce	9.6018006170	5.8351480750	11.6353871450
Ce	9.6334893510	13.6223362480	11.6288455620
Ce	4.1317885420	1.9435469450	11.6386343240
Ce	4.1210918790	9.7315245320	11.6509763900

Ce	9.6344570540	1.9553301840	11.6351835910
Ce	9.6037807470	9.7332532970	11.6297300740
Ce	1.3791897530	3.9024413440	9.7519068950
Ce	1.3707356380	11.6627576900	9.7451914300
Ce	6.8670894820	3.8966123460	9.7531341460
Ce	6.8720160830	11.6739022780	9.7446980640
Ce	1.3762907560	0.0005083250	9.7464342060
Ce	1.3739692510	7.7768203070	9.7348260720
Ce	6.8773763750	0.0060423340	9.7456580920
Ce	6.8614662310	7.7745404540	9.7545338750
Ce	4.1251153630	1.9445972570	7.7511731640
Ce	4.1251153630	9.7229862880	7.7511731640
Ce	9.6252691800	1.9445972570	7.7511731640
Ce	9.6252691800	9.7229862880	7.7511731640
Ce	1.3750384540	3.8891945150	5.8698462730
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Ce	6.8751922710	3.8891945150	5.8698462730
Ce	6.8751922710	11.6675835450	5.8698462730
Ce	1.3750384540	0.0000000000	5.8698462730
Ce	1.3750384540	7.7783890300	5.8698462730
Ce	6.8751922710	0.0000000000	5.8698462730
Ce	6.8751922710	7.7783890300	5.8698462730
Ce	4.1251153630	5.8337917730	7.7511731640
Ce	4.1251153630	13.6121808030	7.7511731640
Ce	9.6252691800	5.8337917730	7.7511731640
Ce	9.6252691800	13.6121808030	7.7511731640
Ce	4.1568411440	5.7329574580	15.6043600680
Ce	4.1613578370	13.6405920700	15.3935507000
Ce	9.6156884350	5.8399410280	15.4005365540
Ce	9.6532747930	13.6256899060	15.4011393750
Ce	1.3750384540	3.8891945150	2.1094769160
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Ce	6.8751922710	3.8891945150	2.1094769160
Ce	6.8751922710	11.6675835450	2.1094769160
Ce	4.1251153630	1.9445972570	3.7800833660
Ce	4.1251153630	9.7229862880	3.7800833660
Ce	9.6252691800	1.9445972570	3.7800833660
Ce	9.6252691800	9.7229862880	3.7800833660
Ce	4.1251153630	5.8337917730	3.7800833660
Ce	4.1251153630	13.6121808030	3.7800833660
Ce	9.6252691800	5.8337917730	3.7800833660
Ce	9.6252691800	13.6121808030	3.7800833660
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O	2.6511591350	7.8375348980	15.8436839590
O	8.3679761060	0.0107725550	15.5464445210
O	8.3211774980	7.7907491080	15.5307258360
O	10.9616461310	0.0120397730	15.5445171950
O	10.9668595760	7.8003779480	15.5944381250

O	5.4709187040	15.5508211750	15.5511839190
O	5.3053660500	7.9269030340	15.4711095730
O	2.7341971090	5.9112616150	13.7002179160
O	2.7665367930	13.5955017460	13.6148069060
O	8.2429178830	5.8390975070	13.6195173980
O	8.2738032110	13.6196374090	13.6283307310
O	10.9730999840	5.8643437930	13.6064826950
O	0.0123048620	13.6126123720	13.6168183490
O	5.5073206870	5.7994815490	13.7199456600
O	5.5165400450	13.6302387810	13.5951256890
O	2.6770410260	1.9445972570	1.9601089810
O	2.6770410260	9.7229862880	1.9601089810
O	8.1771948430	1.9445972570	1.9601089810
O	8.1771948430	9.7229862880	1.9601089810
O	2.7592291710	-0.0139562470	11.6680691460
O	2.7217817610	7.7782824760	11.6726578400
O	8.2622688560	0.0060530390	11.6868744440
O	8.2286731990	7.7880366320	11.6822262180
O	2.7645445750	1.9133099350	13.5911735860
O	2.7564550730	9.6645230400	13.6517175700
O	8.2731974650	1.9623153110	13.6300078970
O	8.2484480320	9.7454185270	13.6224880400
O	0.0143947730	1.9567443700	13.6140950190
O	10.9844182890	9.7148878480	13.6069746180
O	5.5127055090	1.9313027540	13.5925911560
O	5.5028988210	9.8177489260	13.6001428800
O	10.9359305000	3.9203824170	15.5348676020
O	10.9589074520	11.6640326130	15.5396998230
O	5.4688258060	3.7546973430	15.5889602270
O	5.4647404170	11.7569278060	15.5734093360
O	0.0730357720	5.8337917730	1.9601089810
O	0.0730357720	13.6121808030	1.9601089810
O	5.5731897000	5.8337917730	1.9601089810
O	5.5731897000	13.6121808030	1.9601089810
O	2.7540053380	3.9200388300	11.7171293300
O	2.7420162280	11.6423182220	11.7054413270
O	8.2534851900	3.8948234270	11.6792311870
O	8.2485491990	11.6818734120	11.6770960670
O	10.9972379510	3.9069755480	11.6725720220
O	10.9940952390	11.6690482920	11.6822192530
O	5.4997650320	3.9030611090	11.6923010550
O	5.4939148550	11.6893569110	11.6529250460
O	2.6770410260	5.8337917730	1.9601089810
O	2.6770410260	13.6121808030	1.9601089810
O	8.1771948430	5.8337917730	1.9601089810
O	8.1771948430	13.6121808030	1.9601089810
O	0.0730357720	1.9445972570	1.9601089810
O	0.0730357720	9.7229862880	1.9601089810

O	5.5731897000	1.9445972570	1.9601089810
O	5.5731897000	9.7229862880	1.9601089810
O	2.7478803670	3.8891945150	3.8858678670
O	2.7478803670	11.6675835450	3.8858678670
O	8.2480339640	3.8891945150	3.8858678670
O	8.2480339640	11.6675835450	3.8858678670
O	10.9924573750	5.8412613760	9.7125836730
O	0.0010156700	13.6108593140	9.7169630630
O	5.4893975470	5.8484634530	9.7443867860
O	5.5030277650	13.6205072730	9.7085729300
O	0.0016904170	1.9445972570	5.8217789370
O	0.0016904170	9.7229862880	5.8217789370
O	5.5018441240	1.9445972570	5.8217789370
O	5.5018441240	9.7229862880	5.8217789370
O	2.7483863810	1.9445972570	5.8217789370
O	2.7483863810	9.7229862880	5.8217789370
O	8.2485404180	1.9445972570	5.8217789370
O	8.2485404180	9.7229862880	5.8217789370
O	0.0021965410	3.8891945150	3.8858678670
O	0.0021965410	11.6675835450	3.8858678670
O	5.5023505780	3.8891945150	3.8858678670
O	5.5023505780	11.6675835450	3.8858678670
O	0.0016904170	5.8337917730	5.8217789370
O	0.0016904170	13.6121808030	5.8217789370
O	5.5018441240	5.8337917730	5.8217789370
O	5.5018441240	13.6121808030	5.8217789370
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O	8.2485404180	5.8337917730	5.8217789370
O	8.2485404180	13.6121808030	5.8217789370
O	0.0002820480	0.0000000000	7.7806341730
O	0.0002820480	7.7783890300	7.7806341730
O	5.5004360850	0.0000000000	7.7806341730
O	5.5004360850	7.7783890300	7.7806341730
O	0.0063065970	-0.0006450410	11.6739784440
O	-0.0201872650	7.7877349390	11.6663990870
O	5.5063731550	0.0049988270	11.6658311070
O	5.4751163690	7.7687248960	11.7454254820
O	2.7497947510	0.0000000000	7.7806341730
O	2.7497947510	7.7783890300	7.7806341730
O	8.2499484580	0.0000000000	7.7806341730
O	8.2499484580	7.7783890300	7.7806341730
O	2.7497947510	3.8891945150	7.7806341730
O	2.7497947510	11.6675835450	7.7806341730
O	8.2499484580	3.8891945150	7.7806341730
O	8.2499484580	11.6675835450	7.7806341730
O	2.8290303930	3.8123026770	15.4792864250
O	2.8495222550	11.6332208660	15.5521440680

O	8.3401284950	3.9171470750	15.5784234950
O	8.3581943190	11.6733533220	15.5705626860
O	2.7478803670	0.0000000000	3.8858678670
O	2.7478803670	7.7783890300	3.8858678670
O	8.2480339640	0.0000000000	3.8858678670
O	8.2480339640	7.7783890300	3.8858678670
O	0.0044262620	1.9494291090	9.7225100830
O	10.9923868710	9.7271632610	9.7165971700
O	5.4998014720	1.9534488140	9.7178434760
O	5.4931622950	9.7055816230	9.7401160100
O	2.7507199310	1.9561354380	9.7339664740
O	2.7487318170	9.7266431430	9.7215402100
O	8.2506532590	1.9497502330	9.7241793910
O	8.2382084230	9.7252220660	9.7233822120
O	0.0021965410	0.0000000000	3.8858678670
O	0.0021965410	7.7783890300	3.8858678670
O	5.5023505780	0.0000000000	3.8858678670
O	5.5023505780	7.7783890300	3.8858678670
O	0.0002820480	3.8891945150	7.7806341730
O	0.0002820480	11.6675835450	7.7806341730
O	5.5004360850	3.8891945150	7.7806341730
O	5.5004360850	11.6675835450	7.7806341730
O	2.7491528790	5.8310152010	9.7349272430
O	2.7505752620	13.5988141280	9.7220190280
O	8.2363057090	5.8385891450	9.7187342570
O	8.2532083780	13.6164719960	9.7197782020
O	3.9638316570	5.4086651410	17.8330219930
O	5.3990099360	5.6746957520	17.8133282730
H	5.7789627760	4.7659677450	17.8213434950
H	1.7672435270	7.8305357330	16.2777246790

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Ce	5.8266454740	3.3640178510	6.0047050620
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Ce	7.7688605160	0.0000000000	6.0047050620
Ce	9.7110757900	3.3640178510	6.0047050620
Ce	11.6532911230	6.7280358020	6.0047050620
Ce	0.0000000000	0.0000000000	6.0047050620
Ce	1.9422152750	3.3640178510	6.0047050620
Ce	3.8844306070	6.7280358020	6.0047050620
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Ce	5.8219449300	5.6107636780	9.1903839270
Ce	7.7591968470	8.9776528510	9.1957776090
Ce	7.7673780030	2.2556951360	9.2163045470
Ce	9.6996338640	5.6047693850	9.2155231930

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Ce	11.6408795900	2.2517287390	9.2027941540
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Ce	1.9422151580	1.1213397540	2.8456536130
Ce	3.8844303160	4.4853574030	2.8456536130
Ce	5.8266457650	7.8493755570	2.8456536130
Ce	5.8266457070	1.1213397540	2.8456536130
Ce	7.7688608650	4.4853574030	2.8456536130
Ce	9.7110763140	7.8493755570	2.8456536130
Ce	9.7110759070	1.1213397540	2.8456536130
Ce	11.6532910650	4.4853574030	2.8456536130
Ce	13.5955065140	7.8493755570	2.8456536130
Ce	1.9323974510	1.1311887170	12.3441079680
Ce	3.8695926760	4.4959007810	12.3504753740
Ce	5.8112439620	7.8625820380	12.3490873400
Ce	5.8121205700	1.1285431600	12.3567139570
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Ce	11.6700152390	4.5054853600	12.3597035620
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O	9.7043231770	3.3693080290	8.4127813310
O	11.6459986610	6.7348138490	8.4024447590
O	11.6460666020	0.0036980270	8.3984357660
O	13.5902483690	3.3714160930	8.3975613920
O	15.5331103880	6.7318198790	8.3960120450
O	3.8844303740	2.2426790040	2.0626843520
O	5.8266454740	5.6066965520	2.0626843520
O	7.7688609230	8.9707147060	2.0626843520
O	7.7688608070	2.2426790040	2.0626843520
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O	15.5377216720	8.9707147060	2.0626843520
O	3.8543030520	2.2295863060	11.5352557720
O	5.7965844120	5.6260034560	11.5638080140
O	7.7658404290	9.0164094910	11.5305304600
O	7.7804962160	2.2804527590	11.5924108620
O	9.6897877630	5.5853588690	11.5906184620
O	11.6416524600	8.9806505300	11.5521742770
O	11.6377587460	2.2549923070	11.5539026360
O	13.5948311700	5.6145899880	11.5456402780

O	15.5297954890	8.9746316700	11.5473771010
O	3.8844300250	2.2426790040	6.8014205150
O	5.8266451240	5.6066965520	6.8014205150
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O	5.8266458240	3.3640178510	3.6488352620
O	7.7688611560	6.7280358020	3.6488352620
O	7.7688612150	0.0000000000	3.6488352620
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O	11.6405797850	0.0026469330	13.1355745610
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O	15.5105508270	6.7461204050	13.1420108960
O	1.9422148080	1.1213397540	5.1931696170
O	3.8844299660	4.4853574030	5.1931696170
O	5.8266454160	7.8493755570	5.1931696170
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O	7.7688605160	4.4853574030	5.1931696170
O	9.7110759650	7.8493755570	5.1931696170
O	9.7110759070	1.1213397540	5.1931696170
O	11.6532910650	4.4853574030	5.1931696170
O	13.5955065140	7.8493755570	5.1931696170
O	1.9133862550	1.1440543780	10.0019185030
O	3.8797184860	4.4878818010	10.0037533850
O	5.8217122240	7.8558610800	10.0036091990
O	5.8463495320	1.1414887670	10.0327180100
O	7.7408935360	4.5029359200	9.9945272430
O	9.7043420110	7.8277853130	10.0312138850
O	9.6984340310	1.1173696000	10.0117622870
O	11.6521071670	4.5013129950	10.0111088510
O	13.5895391240	7.8544566990	10.0064072680
O	8.0867115350	4.0625994810	14.9034409280
O	8.5186685110	5.0814134550	15.7113469760

H	8.7366136270	4.6166352740	16.5502455000
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Ce	7.7688605160	0.0000000000	6.0047050620
Ce	9.7110757900	3.3640178510	6.0047050620
Ce	11.6532911230	6.7280358020	6.0047050620
Ce	0.0000000000	0.0000000000	6.0047050620
Ce	1.9422152750	3.3640178510	6.0047050620
Ce	3.8844306070	6.7280358020	6.0047050620
Ce	3.8769559300	2.2510021690	9.1965298690
Ce	5.8219449300	5.6107636780	9.1903839270
Ce	7.7591968470	8.9776528510	9.1957776090
Ce	7.7673780030	2.2556951360	9.2163045470
Ce	9.6996338640	5.6047693850	9.2155231930
Ce	11.6539738980	8.9720298180	9.2016197760
Ce	11.6408795900	2.2517287390	9.2027941540
Ce	13.5896168750	5.6117667900	9.1873401040
Ce	15.5307719320	8.9760347960	9.1880555870
Ce	1.9422151580	1.1213397540	2.8456536130
Ce	3.8844303160	4.4853574030	2.8456536130
Ce	5.8266457650	7.8493755570	2.8456536130
Ce	5.8266457070	1.1213397540	2.8456536130
Ce	7.7688608650	4.4853574030	2.8456536130
Ce	9.7110763140	7.8493755570	2.8456536130
Ce	9.7110759070	1.1213397540	2.8456536130
Ce	11.6532910650	4.4853574030	2.8456536130
Ce	13.5955065140	7.8493755570	2.8456536130
Ce	1.9330057010	1.1338360050	12.3458874600
Ce	3.8627019050	4.4972672700	12.3480578610
Ce	5.8052223920	7.8772221570	12.3531533050
Ce	5.8147226330	1.1194060940	12.3599505370
Ce	7.7223164740	4.4647278560	12.3842989360
Ce	9.7045210800	7.8736251470	12.3632408020
Ce	9.7101602980	1.1157427620	12.3729989890
Ce	11.6591055810	4.5010912430	12.3653096980
Ce	13.5935153080	7.8528586420	12.3609479200
O	3.8856889340	0.0013471740	8.4190866600
O	5.8197560460	3.3615908130	8.3992776200
O	7.7680092370	6.7377135490	8.3996902320
O	7.7605590670	0.0043634220	8.4024168810
O	9.7043231770	3.3693080290	8.4127813310
O	11.6459986610	6.7348138490	8.4024447590
O	11.6460666020	0.0036980270	8.3984357660

O	13.5902483690	3.3714160930	8.3975613920
O	15.5331103880	6.7318198790	8.3960120450
O	3.8844303740	2.2426790040	2.0626843520
O	5.8266454740	5.6066965520	2.0626843520
O	7.7688609230	8.9707147060	2.0626843520
O	7.7688608070	2.2426790040	2.0626843520
O	9.7110759070	5.6066965520	2.0626843520
O	11.6532913560	8.9707147060	2.0626843520
O	11.6532911230	2.2426790040	2.0626843520
O	13.5955062230	5.6066965520	2.0626843520
O	15.5377216720	8.9707147060	2.0626843520
O	3.8543030520	2.2295863060	11.5352557720
O	5.7965844120	5.6260034560	11.5638080140
O	7.7658404290	9.0164094910	11.5305304600
O	7.7930466330	2.2764737250	11.5857794670
O	9.6631518500	5.5752473300	11.6058313260
O	11.6416524600	8.9806505300	11.5521742770
O	11.6341500780	2.2632651880	11.5620287830
O	13.5948311700	5.6145899880	11.5456402780
O	15.5297954890	8.9746316700	11.5473771010
O	3.8844300250	2.2426790040	6.8014205150
O	5.8266451240	5.6066965520	6.8014205150
O	7.7688605740	8.9707147060	6.8014205150
O	7.7688608070	2.2426790040	6.8014205150
O	9.7110759070	5.6066965520	6.8014205150
O	11.6532913560	8.9707147060	6.8014205150
O	11.6532911230	2.2426790040	6.8014205150
O	13.5955062230	5.6066965520	6.8014205150
O	15.5377216720	8.9707147060	6.8014205150
O	3.8844305490	0.0000000000	3.6488352620
O	5.8266458240	3.3640178510	3.6488352620
O	7.7688611560	6.7280358020	3.6488352620
O	7.7688612150	0.0000000000	3.6488352620
O	9.7110764890	3.3640178510	3.6488352620
O	11.6532918220	6.7280358020	3.6488352620
O	0.0000000000	0.0000000000	3.6488352620
O	1.9422152750	3.3640178510	3.6488352620
O	3.8844306070	6.7280358020	3.6488352620
O	3.8793288770	0.0059842590	13.1397266080
O	5.7866902940	3.3480043920	13.1037620610
O	7.7467141360	6.8436466470	13.2049029350
O	13.5937048310	10.0886968690	13.1373493230
O	9.7505567450	3.3252737240	13.2423665620
O	11.6613725800	6.7353001820	13.1338206410
O	11.6405797850	0.0026469330	13.1355745610
O	13.5937170520	3.3778191880	13.1346759440
O	15.5105508270	6.7461204050	13.1420108960
O	1.9422148080	1.1213397540	5.1931696170

O	3.8844299660	4.4853574030	5.1931696170
O	5.8266454160	7.8493755570	5.1931696170
O	5.8266453580	1.1213397540	5.1931696170
O	7.7688605160	4.4853574030	5.1931696170
O	9.7110759650	7.8493755570	5.1931696170
O	9.7110759070	1.1213397540	5.1931696170
O	11.6532910650	4.4853574030	5.1931696170
O	13.5955065140	7.8493755570	5.1931696170
O	1.9133862550	1.1440543780	10.0019185030
O	3.8797184860	4.4878818010	10.0037533850
O	5.8217122240	7.8558610800	10.0036091990
O	5.8463495320	1.1414887670	10.0327180100
O	7.7408935360	4.5029359200	9.9945272430
O	9.7043420110	7.8277853130	10.0312138850
O	9.6984340310	1.1173696000	10.0117622870
O	11.6521071670	4.5013129950	10.0111088510
O	13.5895391240	7.8544566990	10.0064072680
O	7.9099775350	4.9399490050	14.9902909020
O	9.2551774030	4.6379124680	15.4811570360
H	9.5462815080	4.0037892660	14.7435084700
H	7.9775845500	5.8934726750	14.6746248650

221-Ce1-OOH

Ce	1.9445951940	2.4093844220	2.8000527150
Ce	9.7229868580	2.4093844220	2.8000527150
Ce	5.8337906370	2.4093844220	2.8000527150
Ce	13.6121826120	2.4093844220	2.8000527150
Ce	0.0000208070	10.9489391440	3.6444218520
Ce	7.7784124720	10.9489391440	3.6444218520
Ce	3.8892167170	10.9489391440	3.6444218520
Ce	11.6676082260	10.9489391440	3.6444218520
Ce	1.9445888540	7.8041438960	4.5298469320
Ce	9.7229803630	7.8041438960	4.5298469320
Ce	-1.9446067450	7.8041438960	4.5298469320
Ce	5.8337846090	7.8041438960	4.5298469320
Ce	0.0000089450	4.6047904270	5.2434760540
Ce	7.7784006100	4.6047904270	5.2434760540
Ce	3.8892043880	4.6047904270	5.2434760540
Ce	11.6675954310	4.6047904270	5.2434760540
Ce	5.8337863200	1.3053169250	6.3566574820
Ce	13.6121782950	1.3053169250	6.3566574820
Ce	1.9445902540	1.3053169250	6.3566574820
Ce	9.7229816080	1.3053169250	6.3566574820
Ce	3.8891978160	9.7009476410	7.3076483830
Ce	11.6675893240	9.7009476410	7.3076483830
Ce	0.0000019060	9.7009476410	7.3076483830

Ce	7.7783935700	9.7009476410	7.3076483830
Ce	-1.9445979550	6.4819932090	8.1585764310
Ce	5.8337937090	6.4819932090	8.1585764310
Ce	1.9445979550	6.4819932090	8.1585764310
Ce	9.7229894640	6.4819932090	8.1585764310
Ce	0.0018013900	3.2693260220	9.0094287790
Ce	7.7779780870	3.2684551970	9.0140765940
Ce	3.8927360580	3.2667743920	9.0111554740
Ce	11.6701637030	3.2711596360	9.0117891100
Ce	1.9454394000	0.0058357640	9.9637263680
Ce	9.7291250400	0.0089677320	9.9643731460
Ce	5.8355759280	-0.0014889130	9.9926231420
Ce	13.6170258390	0.0092322280	9.9618954240
Ce	0.0083696050	8.3957099680	11.0799510470
Ce	7.7831189710	8.3910526230	11.0775297000
Ce	3.8860344400	8.3967645640	11.0786170010
Ce	11.6744666970	8.3882135630	11.0788228410
Ce	1.9453791830	5.1883871080	11.7996524780
Ce	9.7335657930	5.1897086900	11.8046336160
Ce	5.8327881000	5.1916881280	11.8039401760
Ce	13.6233426750	5.1898980470	11.8014661910
Ce	0.0073820530	2.0502945980	12.6764503540
Ce	7.7838051300	2.0523743760	12.6774970010
Ce	3.8953888770	2.0488575220	12.6787141810
Ce	11.6791470580	2.0517532530	12.6773415630
Ce	1.9404918530	10.5760349090	13.6175783940
Ce	9.7412223270	10.5904765110	13.5313571680
Ce	-1.9259454990	10.6035265900	13.5331565090
Ce	5.8282457860	10.6059158610	13.5314997800
O	0.0000278850	1.0936971120	2.2401547390
O	7.7784193940	1.0936971120	2.2401547390
O	3.8892236400	1.0936971120	2.2401547390
O	11.6676151490	1.0936971120	2.2401547390
O	0.0000530100	3.6598501530	3.0304604640
O	7.7784442070	3.6598501530	3.0304604640
O	3.8892489200	3.6598501530	3.0304604640
O	11.6676399620	3.6598501530	3.0304604640
O	1.9445652470	9.6970730690	3.1665399670
O	9.7229567560	9.6970730690	3.1665399670
O	-1.9446308190	9.6970730690	3.1665399670
O	5.8337610010	9.6970730690	3.1665399670
O	1.9445956990	0.6173987810	4.1099962430
O	9.7229875190	0.6173987810	4.1099962430
O	5.8337917650	0.6173987810	4.1099962430
O	13.6121832740	0.6173987810	4.1099962430
O	3.8892287350	6.6033288830	4.0372105540
O	11.6676205550	6.6033288830	4.0372105540
O	0.0000329800	6.6033288830	4.0372105540

O	7.7784249560	6.6033288830	4.0372105540
O	1.9446021160	3.2313913800	4.8946937290
O	9.7229937810	3.2313913800	4.8946937290
O	5.8337975600	3.2313913800	4.8946937290
O	13.6121886020	3.2313913800	4.8946937290
O	0.0000032280	9.1016627900	5.0340550170
O	7.7783944260	9.1016627900	5.0340550170
O	3.8891991380	9.1016627900	5.0340550170
O	11.6675911140	9.1016627900	5.0340550170
O	0.0000087900	11.6608973020	5.8961619820
O	7.7784002980	11.6608973020	5.8961619820
O	13.6122023700	5.8211656850	5.8086849850
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O	1.9446152620	5.8211656850	5.8086849850
O	9.7230066150	5.8211656850	5.8086849850
O	11.6675960530	11.6608973020	5.8961619820
O	3.8892045440	11.6608973020	5.8961619820
O	-0.0000275740	2.6100309870	6.7405680980
O	7.7783636230	2.6100309870	6.7405680980
O	-1.9446299240	8.4026813220	6.8008587780
O	5.8337614290	8.4026813220	6.8008587780
O	3.8891683360	2.6100309870	6.7405680980
O	11.6675603110	2.6100309870	6.7405680980
O	1.9445656750	8.4026813220	6.8008587780
O	9.7229571830	8.4026813220	6.8008587780
O	0.0000562380	5.2025083220	7.6500997840
O	7.7784479020	5.2025083220	7.6500997840
O	3.8892516810	5.2025083220	7.6500997840
O	11.6676427230	5.2025083220	7.6500997840
O	1.9445942210	11.0066060770	7.7246176470
O	9.7229852630	11.0066060770	7.7246176470
O	-1.9446015330	11.0066060770	7.7246176470
O	5.8337895090	11.0066060770	7.7246176470
O	0.0000555280	7.7666557540	8.6653878430
O	7.7825415250	7.7683326850	8.6711320430
O	3.8925054580	7.7666193920	8.6652547990
O	11.6682900330	7.7654621270	8.6720553980
O	1.9446019220	1.9573791750	8.5925352150
O	9.7229938970	1.9573791750	8.5925352150
O	5.8337972100	1.9573791750	8.5925352150
O	13.6121887180	1.9573791750	8.5925352150
O	1.9451974800	4.5677306260	9.5141630930
O	9.7268558920	4.5708550970	9.5187162880
O	5.8373787200	4.5729628390	9.5184265160
O	13.6141279170	4.5737597090	9.5154335980
O	0.0010566930	10.3614145910	9.5918161880
O	7.7808311620	10.3665991820	9.5835803540
O	3.8929948570	10.3631749450	9.5938336930

O	11.6698859660	10.3626479090	9.5812617450
O	-0.0010173450	1.3244339370	10.4147989450
O	7.7774874520	1.3239966820	10.4239461260
O	3.8968275930	1.3197536180	10.4222327730
O	11.6802763360	1.3301146610	10.4170467080
O	-1.9408381700	7.1609653550	10.5203879980
O	5.8386161580	7.1621722180	10.5211972560
O	1.9478017700	7.1547263720	10.5114313070
O	9.7256993840	7.1580474680	10.5208001890
O	-1.9507791600	9.7553115850	11.4354552960
O	5.8504979480	9.7595445220	11.4361943310
O	0.0013885300	3.8871527440	11.2894073270
O	7.7852865360	3.8941498170	11.2943442860
O	3.8907694140	3.8900117070	11.2874321270
O	11.6790095830	3.8921185860	11.2942283870
O	1.9469454480	9.7372956290	11.4434914340
O	9.7283942170	9.7528551910	11.4345654390
O	0.0056342220	6.3925129910	12.2986710410
O	7.7852342520	6.4048648300	12.3107945140
O	1.9373444180	0.7128127040	12.1960718660
O	9.7447094720	0.7185259890	12.1948348010
O	3.8898903960	6.3973276760	12.3019201940
O	11.6740892580	6.3984726800	12.3041265670
O	5.8395550330	0.7132513970	12.2420946750
O	13.6232291280	0.7050676540	12.2102150020
O	1.9446305940	3.3173584800	13.1590909590
O	9.7385252030	3.3250281390	13.1634066460
O	3.9159889820	9.3553378460	13.2860522960
O	11.6617501200	9.3450971520	13.3164443820
O	-0.0139766210	9.3576796870	13.2940453700
O	7.7927660840	9.3428488540	13.3215798230
O	5.8369393900	3.3364961340	13.1599213980
O	13.6223260470	3.3125869640	13.1630994620
O	3.8432487650	0.2722877520	14.0724980850
O	11.6832810910	0.2494706560	14.0771965900
O	0.0086710170	0.2501549760	14.0844467110
O	7.8450489860	0.2663173560	14.0589136780
O	1.9178948710	10.0401708500	16.0091063950
O	2.4547497530	11.0189631250	16.8457262540
H	2.1068695230	10.7519894930	17.7230818390

221-Ce1-HOOH

Ce	1.9445951940	2.4093844220	2.8000527150
Ce	9.7229868580	2.4093844220	2.8000527150
Ce	5.8337906370	2.4093844220	2.8000527150
Ce	13.6121826120	2.4093844220	2.8000527150

Ce	0.0000208070	10.9489391440	3.6444218520
Ce	7.7784124720	10.9489391440	3.6444218520
Ce	3.8892167170	10.9489391440	3.6444218520
Ce	11.6676082260	10.9489391440	3.6444218520
Ce	1.9445888540	7.8041438960	4.5298469320
Ce	9.7229803630	7.8041438960	4.5298469320
Ce	-1.9446067450	7.8041438960	4.5298469320
Ce	5.8337846090	7.8041438960	4.5298469320
Ce	0.0000089450	4.6047904270	5.2434760540
Ce	7.7784006100	4.6047904270	5.2434760540
Ce	3.8892043880	4.6047904270	5.2434760540
Ce	11.6675954310	4.6047904270	5.2434760540
Ce	5.8337863200	1.3053169250	6.3566574820
Ce	13.6121782950	1.3053169250	6.3566574820
Ce	1.9445902540	1.3053169250	6.3566574820
Ce	9.7229816080	1.3053169250	6.3566574820
Ce	3.8891978160	9.7009476410	7.3076483830
Ce	11.6675893240	9.7009476410	7.3076483830
Ce	0.0000019060	9.7009476410	7.3076483830
Ce	7.7783935700	9.7009476410	7.3076483830
Ce	-1.9445979550	6.4819932090	8.1585764310
Ce	5.8337937090	6.4819932090	8.1585764310
Ce	1.9445979550	6.4819932090	8.1585764310
Ce	9.7229894640	6.4819932090	8.1585764310
Ce	0.0016549980	3.2715528620	9.0070453600
Ce	7.7737401010	3.2667761380	9.0070461050
Ce	3.8938387680	3.2639128640	9.0125819980
Ce	11.6698339350	3.2689333280	9.0061770070
Ce	1.9369701520	0.0067482180	9.9679635940
Ce	9.7312062400	-0.0003986290	9.9688131000
Ce	5.8323399920	-0.0167115540	10.0192010520
Ce	13.6135319490	0.0087999510	9.9612109480
Ce	0.0002794560	8.4081270230	11.0908997590
Ce	7.7706630870	8.3794059430	11.0738970460
Ce	3.8805264620	8.3665899140	10.9983217670
Ce	11.6578893280	8.3906152380	11.0773959550
Ce	1.9415766460	5.1987133960	11.7982918380
Ce	9.7210909560	5.1818234170	11.7979225720
Ce	5.8378472990	5.1732045420	11.8085021670
Ce	13.6135658940	5.2073569520	11.7939453800
Ce	0.0027757930	2.0701502840	12.6675830590
Ce	7.7963872910	2.0144724020	12.6674553400
Ce	3.8762165300	2.0575072350	12.6895799930
Ce	11.6912002900	2.0681131750	12.6703305980
Ce	1.8877958390	10.5641549460	13.7152448770
Ce	9.7633484320	10.6193727240	13.5389550940
Ce	-1.9666431500	10.6215857420	13.5407148860
Ce	5.9528361880	10.6245547180	13.5611586760

O	0.0000278850	1.0936971120	2.2401547390
O	7.7784193940	1.0936971120	2.2401547390
O	3.8892236400	1.0936971120	2.2401547390
O	11.6676151490	1.0936971120	2.2401547390
O	0.0000530100	3.6598501530	3.0304604640
O	7.7784442070	3.6598501530	3.0304604640
O	3.8892489200	3.6598501530	3.0304604640
O	11.6676399620	3.6598501530	3.0304604640
O	1.9445652470	9.6970730690	3.1665399670
O	9.7229567560	9.6970730690	3.1665399670
O	-1.9446308190	9.6970730690	3.1665399670
O	5.8337610010	9.6970730690	3.1665399670
O	1.9445956990	0.6173987810	4.1099962430
O	9.7229875190	0.6173987810	4.1099962430
O	5.8337917650	0.6173987810	4.1099962430
O	13.6121832740	0.6173987810	4.1099962430
O	3.8892287350	6.6033288830	4.0372105540
O	11.6676205550	6.6033288830	4.0372105540
O	0.0000329800	6.6033288830	4.0372105540
O	7.7784249560	6.6033288830	4.0372105540
O	1.9446021160	3.2313913800	4.8946937290
O	9.7229937810	3.2313913800	4.8946937290
O	5.8337975600	3.2313913800	4.8946937290
O	13.6121886020	3.2313913800	4.8946937290
O	0.0000032280	9.1016627900	5.0340550170
O	7.7783944260	9.1016627900	5.0340550170
O	3.8891991380	9.1016627900	5.0340550170
O	11.6675911140	9.1016627900	5.0340550170
O	0.0000087900	11.6608973020	5.8961619820
O	7.7784002980	11.6608973020	5.8961619820
O	13.6122023700	5.8211656850	5.8086849850
O	5.8338108610	5.8211656850	5.8086849850
O	1.9446152620	5.8211656850	5.8086849850
O	9.7230066150	5.8211656850	5.8086849850
O	11.6675960530	11.6608973020	5.8961619820
O	3.8892045440	11.6608973020	5.8961619820
O	-0.0000275740	2.6100309870	6.7405680980
O	7.7783636230	2.6100309870	6.7405680980
O	-1.9446299240	8.4026813220	6.8008587780
O	5.8337614290	8.4026813220	6.8008587780
O	3.8891683360	2.6100309870	6.7405680980
O	11.6675603110	2.6100309870	6.7405680980
O	1.9445656750	8.4026813220	6.8008587780
O	9.7229571830	8.4026813220	6.8008587780
O	0.0000562380	5.2025083220	7.6500997840
O	7.7784479020	5.2025083220	7.6500997840
O	3.8892516810	5.2025083220	7.6500997840
O	11.6676427230	5.2025083220	7.6500997840

O	1.9445942210	11.0066060770	7.7246176470
O	9.7229852630	11.0066060770	7.7246176470
O	-1.9446015330	11.0066060770	7.7246176470
O	5.8337895090	11.0066060770	7.7246176470
O	-0.0024560090	7.7724095000	8.6612246080
O	7.7757449140	7.7660627440	8.6697492940
O	3.8924780650	7.7636911930	8.6662038560
O	11.6641390930	7.7631079480	8.6739628580
O	1.9446019220	1.9573791750	8.5925352150
O	9.7229938970	1.9573791750	8.5925352150
O	5.8337972100	1.9573791750	8.5925352150
O	13.6121887180	1.9573791750	8.5925352150
O	1.9485006730	4.5665685180	9.5148717560
O	9.7183977500	4.5733263870	9.5172044730
O	5.8396221270	4.5693878070	9.5194116930
O	13.6126669160	4.5787767420	9.5156132380
O	0.0222794350	10.3550589880	9.6228543890
O	7.7573952840	10.3467634530	9.6010390170
O	3.8913512150	10.3527800950	9.5701700780
O	11.6498654540	10.3693623560	9.5698072780
O	-0.0015421160	1.3304447590	10.4095719970
O	7.7679045300	1.2910139110	10.4504343740
O	3.9020751920	1.3230585020	10.4281811190
O	11.6881796640	1.3244820470	10.3948246810
O	-1.9411776820	7.1698690790	10.5238494090
O	5.8288752560	7.1538041540	10.5065882110
O	1.9493297950	7.1458934920	10.4923596380
O	9.7066754570	7.1640740150	10.5214336370
O	-2.0039972030	9.7654698970	11.4121376530
O	5.7769139190	9.7489891280	11.4813754670
O	-0.0003902780	3.8995320750	11.2858431140
O	7.7824683190	3.8657649260	11.2895686670
O	3.8924525870	3.9079201370	11.2968892630
O	11.6687659360	3.8908906160	11.2857091730
O	2.0366494260	9.7014764840	11.4974337620
O	9.7116144730	9.7548033880	11.4413414040
O	0.0137169370	6.4094843680	12.2963303450
O	7.7666469080	6.3935024050	12.2943400330
O	1.9316792770	0.7253799270	12.1860832810
O	9.8082942950	0.7270725350	12.1829540680
O	3.8880244210	6.4345823190	12.3441831920
O	11.6607702550	6.3956868030	12.2902862090
O	5.7955326780	0.6870438980	12.2969805670
O	13.6260388060	0.7238363420	12.1998017170
O	1.9398088920	3.3318351650	13.1558541520
O	9.7222322890	3.3075512880	13.1572342290
O	3.9433696960	9.0692520110	13.5724947690
O	11.6299878300	9.3647866240	13.3332476270

O	-0.0814101260	9.4195604440	13.2132096030
O	7.7648985990	9.3694906870	13.3273777360
O	5.8448511620	3.3118285420	13.1588641990
O	13.6176529090	3.3318695960	13.1556127840
O	3.7066257630	0.3566591950	14.1800881020
O	11.7290499560	0.2772909960	14.1080695130
O	-0.0050850460	0.2805318140	14.0833016590
O	7.9399694860	0.1362290120	13.9667676840
O	1.3781078350	10.0365155760	15.8301797970
O	1.5775242800	11.4574512660	16.0347008920
H	4.5946405450	0.1661350000	15.6873004360
H	3.9342888040	8.1232109510	13.8175798930

221-Ce2-OOH

Ce	1.9445951940	2.4093844220	2.8000527150
Ce	9.7229868580	2.4093844220	2.8000527150
Ce	5.8337906370	2.4093844220	2.8000527150
Ce	13.6121826120	2.4093844220	2.8000527150
Ce	0.0000208070	10.9489391440	3.6444218520
Ce	7.7784124720	10.9489391440	3.6444218520
Ce	3.8892167170	10.9489391440	3.6444218520
Ce	11.6676082260	10.9489391440	3.6444218520
Ce	1.9445888540	7.8041438960	4.5298469320
Ce	9.7229803630	7.8041438960	4.5298469320
Ce	-1.9446067450	7.8041438960	4.5298469320
Ce	5.8337846090	7.8041438960	4.5298469320
Ce	0.0000089450	4.6047904270	5.2434760540
Ce	7.7784006100	4.6047904270	5.2434760540
Ce	3.8892043880	4.6047904270	5.2434760540
Ce	11.6675954310	4.6047904270	5.2434760540
Ce	5.8337863200	1.3053169250	6.3566574820
Ce	13.6121782950	1.3053169250	6.3566574820
Ce	1.9445902540	1.3053169250	6.3566574820
Ce	9.7229816080	1.3053169250	6.3566574820
Ce	3.8891978160	9.7009476410	7.3076483830
Ce	11.6675893240	9.7009476410	7.3076483830
Ce	0.0000019060	9.7009476410	7.3076483830
Ce	7.7783935700	9.7009476410	7.3076483830
Ce	-1.9445979550	6.4819932090	8.1585764310
Ce	5.8337937090	6.4819932090	8.1585764310
Ce	1.9445979550	6.4819932090	8.1585764310
Ce	9.7229894640	6.4819932090	8.1585764310
Ce	0.0005244880	3.2657342490	9.0102582060
Ce	7.7782361080	3.2664781070	9.0111063370
Ce	3.8886842150	3.2589828220	9.0213375590
Ce	11.6676659130	3.2650715320	9.0105647510

Ce	1.9527108680	0.0020156920	9.9721564090
Ce	5.8329205080	11.6628284320	9.9649703740
Ce	5.8268804190	0.0021766570	9.9707243410
Ce	9.7240589340	11.6627183070	9.9649859870
Ce	-0.0008858450	8.3720474370	11.0814778090
Ce	7.7783787110	8.3724443920	11.0811750400
Ce	3.8919012650	8.3633709350	11.0762619400
Ce	11.6648139280	8.3680321810	11.0766443310
Ce	1.9396545120	5.1750082150	11.7958812110
Ce	9.7217843870	5.1766804900	11.7987963010
Ce	5.8367564810	5.1745468360	11.7961554360
Ce	13.6110324650	5.1757775620	11.7977870330
Ce	-0.0054858200	2.0367241440	12.6776659870
Ce	7.7841605780	2.0373900140	12.6762138670
Ce	3.8958515200	2.0502325630	12.7488402070
Ce	11.6674253580	2.0384601300	12.6784794940
Ce	1.9781610400	10.5502919380	13.5286694820
Ce	9.7182320900	10.5837407670	13.5318921360
Ce	-1.9714746440	10.5544306410	13.5304532120
Ce	5.8404919880	10.5836617120	13.5325702600
O	0.0000278850	1.0936971120	2.2401547390
O	7.7784193940	1.0936971120	2.2401547390
O	3.8892236400	1.0936971120	2.2401547390
O	11.6676151490	1.0936971120	2.2401547390
O	0.0000530100	3.6598501530	3.0304604640
O	7.7784442070	3.6598501530	3.0304604640
O	3.8892489200	3.6598501530	3.0304604640
O	11.6676399620	3.6598501530	3.0304604640
O	1.9445652470	9.6970730690	3.1665399670
O	9.7229567560	9.6970730690	3.1665399670
O	-1.9446308190	9.6970730690	3.1665399670
O	5.8337610010	9.6970730690	3.1665399670
O	1.9445956990	0.6173987810	4.1099962430
O	9.7229875190	0.6173987810	4.1099962430
O	5.8337917650	0.6173987810	4.1099962430
O	13.6121832740	0.6173987810	4.1099962430
O	3.8892287350	6.6033288830	4.0372105540
O	11.6676205550	6.6033288830	4.0372105540
O	0.0000329800	6.6033288830	4.0372105540
O	7.7784249560	6.6033288830	4.0372105540
O	1.9446021160	3.2313913800	4.8946937290
O	9.7229937810	3.2313913800	4.8946937290
O	5.8337975600	3.2313913800	4.8946937290
O	13.6121886020	3.2313913800	4.8946937290
O	0.0000032280	9.1016627900	5.0340550170
O	7.7783944260	9.1016627900	5.0340550170
O	3.8891991380	9.1016627900	5.0340550170
O	11.6675911140	9.1016627900	5.0340550170

O	0.0000087900	11.6608973020	5.8961619820
O	7.7784002980	11.6608973020	5.8961619820
O	13.6122023700	5.8211656850	5.8086849850
O	5.8338108610	5.8211656850	5.8086849850
O	1.9446152620	5.8211656850	5.8086849850
O	9.7230066150	5.8211656850	5.8086849850
O	11.6675960530	11.6608973020	5.8961619820
O	3.8892045440	11.6608973020	5.8961619820
O	-0.0000275740	2.6100309870	6.7405680980
O	7.7783636230	2.6100309870	6.7405680980
O	-1.9446299240	8.4026813220	6.8008587780
O	5.8337614290	8.4026813220	6.8008587780
O	3.8891683360	2.6100309870	6.7405680980
O	11.6675603110	2.6100309870	6.7405680980
O	1.9445656750	8.4026813220	6.8008587780
O	9.7229571830	8.4026813220	6.8008587780
O	0.0000562380	5.2025083220	7.6500997840
O	7.7784479020	5.2025083220	7.6500997840
O	3.8892516810	5.2025083220	7.6500997840
O	11.6676427230	5.2025083220	7.6500997840
O	1.9445942210	11.0066060770	7.7246176470
O	9.7229852630	11.0066060770	7.7246176470
O	-1.9446015330	11.0066060770	7.7246176470
O	5.8337895090	11.0066060770	7.7246176470
O	-0.0010709240	7.7613143300	8.6685008020
O	7.7794165030	7.7629488210	8.6674515240
O	3.8903772980	7.7620678690	8.6696374020
O	11.6672701250	7.7604795320	8.6703292960
O	1.9446019220	1.9573791750	8.5925352150
O	9.7229938970	1.9573791750	8.5925352150
O	5.8337972100	1.9573791750	8.5925352150
O	13.6121887180	1.9573791750	8.5925352150
O	1.9493701100	4.5639286330	9.5205713580
O	9.7271015300	4.5705311580	9.5148366280
O	5.8285736770	4.5659642710	9.5224702520
O	13.6085282480	4.5685010870	9.5146558510
O	-0.0003075540	10.3499724230	9.5876502300
O	7.7775259690	10.3511218610	9.5863274980
O	3.8910340200	10.3565025660	9.5812649770
O	11.6656349250	10.3528353040	9.5813733500
O	0.0086344420	1.3035011840	10.4281701110
O	7.7709127800	1.3081075450	10.4284397940
O	3.8916310270	1.3020566020	10.4126286790
O	11.6679919080	1.3078431900	10.4157552920
O	-1.9453609760	7.1515739210	10.5203380030
O	5.8384124430	7.1532952210	10.5148972020
O	1.9420513900	7.1507360010	10.5154691940
O	9.7197918190	7.1541988640	10.5188318970

O	-1.9549568660	9.7418614840	11.4359368860
O	5.8319650940	9.7382490280	11.4418002720
O	-0.0137239900	3.8739214470	11.2785372110
O	7.7936589150	3.8767170450	11.2794991630
O	3.8868262480	3.8568338220	11.3174287890
O	11.6662050570	3.8687071610	11.2923829800
O	1.9559258110	9.7382679220	11.4352128280
O	9.7233323170	9.7400068850	11.4410144540
O	-0.0013112960	6.3824039460	12.2975814490
O	7.7799850660	6.3848169670	12.2985377210
O	1.9662599190	0.6942257980	12.2440356920
O	9.7286214650	0.6959083370	12.2075748540
O	3.8912262010	6.3805578460	12.2873319400
O	11.6657546420	6.3754034840	12.2926888200
O	5.8203813990	0.6887338300	12.2425870380
O	13.6065952270	0.6968387070	12.2077216270
O	1.8958180380	3.3098596200	13.1404054960
O	9.7207633030	3.2977151100	13.1666505090
O	3.8864219370	9.3196157270	13.3222123300
O	11.6695398310	9.3205098430	13.3187581560
O	-0.0021153020	9.3214956000	13.2978722780
O	7.7779556970	9.3456332740	13.3223280690
O	5.8749324500	3.3022305740	13.1309630010
O	13.6134402730	3.2987196850	13.1648977890
O	3.8959870090	0.1361239530	14.1312093580
O	11.6687314300	0.2495760730	14.0906596030
O	-0.0237890580	0.2225187320	14.0825544770
O	7.8061863210	0.2222820910	14.0864790060
O	3.7122744960	2.4213371340	15.2711678870
O	4.8152445670	2.8401590090	15.9719594690
H	4.5313545590	2.7283628840	16.9063591190

221-Ce2-HOOH

Ce	1.9445951940	2.4093844220	2.8000527150
Ce	9.7229868580	2.4093844220	2.8000527150
Ce	5.8337906370	2.4093844220	2.8000527150
Ce	13.6121826120	2.4093844220	2.8000527150
Ce	0.0000208070	10.9489391440	3.6444218520
Ce	7.7784124720	10.9489391440	3.6444218520
Ce	3.8892167170	10.9489391440	3.6444218520
Ce	11.6676082260	10.9489391440	3.6444218520
Ce	1.9445888540	7.8041438960	4.5298469320
Ce	9.7229803630	7.8041438960	4.5298469320
Ce	-1.9446067450	7.8041438960	4.5298469320
Ce	5.8337846090	7.8041438960	4.5298469320
Ce	0.0000089450	4.6047904270	5.2434760540

Ce	7.7784006100	4.6047904270	5.2434760540
Ce	3.8892043880	4.6047904270	5.2434760540
Ce	11.6675954310	4.6047904270	5.2434760540
Ce	5.8337863200	1.3053169250	6.3566574820
Ce	13.6121782950	1.3053169250	6.3566574820
Ce	1.9445902540	1.3053169250	6.3566574820
Ce	9.7229816080	1.3053169250	6.3566574820
Ce	3.8891978160	9.7009476410	7.3076483830
Ce	11.6675893240	9.7009476410	7.3076483830
Ce	0.0000019060	9.7009476410	7.3076483830
Ce	7.7783935700	9.7009476410	7.3076483830
Ce	-1.9445979550	6.4819932090	8.1585764310
Ce	5.8337937090	6.4819932090	8.1585764310
Ce	1.9445979550	6.4819932090	8.1585764310
Ce	9.7229894640	6.4819932090	8.1585764310
Ce	-0.0005379240	3.2672308900	9.0108842660
Ce	7.7801687890	3.2667184460	9.0126745450
Ce	3.8890845340	3.2611020720	9.0250888190
Ce	11.6674119370	3.2668351780	9.0095417680
Ce	1.9514149880	0.0104901280	9.9704321010
Ce	5.8365855110	11.6645007760	9.9613850240
Ce	5.8343683710	0.0015508580	9.9654013310
Ce	9.7239847530	11.6657201140	9.9618027710
Ce	-0.0002416560	8.3848506460	11.0811471620
Ce	7.7794682440	8.3723528380	11.0834740340
Ce	3.8935836350	8.3714434520	11.0756660970
Ce	11.6674384440	8.3796141040	11.0804510850
Ce	1.9293620720	5.1978740850	11.7997745600
Ce	9.7267151570	5.1801904060	11.7989930390
Ce	5.8384036460	5.1771425380	11.8077090760
Ce	13.6092806770	5.1826256890	11.7960882210
Ce	-0.0236648790	2.0392684930	12.6779438460
Ce	7.7972273540	2.0364103580	12.6750542840
Ce	3.9386153800	2.0285059720	12.7333583750
Ce	11.6667228830	2.0371547180	12.6766405860
Ce	1.9583947270	10.5643781340	13.5266174890
Ce	9.7236960280	10.5814422250	13.5291528500
Ce	-1.9404997670	10.5852651520	13.5210190500
Ce	5.8372231940	10.5816102060	13.5296609080
O	0.0000278850	1.0936971120	2.2401547390
O	7.7784193940	1.0936971120	2.2401547390
O	3.8892236400	1.0936971120	2.2401547390
O	11.6676151490	1.0936971120	2.2401547390
O	0.0000530100	3.6598501530	3.0304604640
O	7.7784442070	3.6598501530	3.0304604640
O	3.8892489200	3.6598501530	3.0304604640
O	11.6676399620	3.6598501530	3.0304604640
O	1.9445652470	9.6970730690	3.1665399670

O	9.7229567560	9.6970730690	3.1665399670
O	-1.9446308190	9.6970730690	3.1665399670
O	5.8337610010	9.6970730690	3.1665399670
O	1.9445956990	0.6173987810	4.1099962430
O	9.7229875190	0.6173987810	4.1099962430
O	5.8337917650	0.6173987810	4.1099962430
O	13.6121832740	0.6173987810	4.1099962430
O	3.8892287350	6.6033288830	4.0372105540
O	11.6676205550	6.6033288830	4.0372105540
O	0.0000329800	6.6033288830	4.0372105540
O	7.7784249560	6.6033288830	4.0372105540
O	1.9446021160	3.2313913800	4.8946937290
O	9.7229937810	3.2313913800	4.8946937290
O	5.8337975600	3.2313913800	4.8946937290
O	13.6121886020	3.2313913800	4.8946937290
O	0.0000032280	9.1016627900	5.0340550170
O	7.7783944260	9.1016627900	5.0340550170
O	3.8891991380	9.1016627900	5.0340550170
O	11.6675911140	9.1016627900	5.0340550170
O	0.0000087900	11.6608973020	5.8961619820
O	7.7784002980	11.6608973020	5.8961619820
O	13.6122023700	5.8211656850	5.8086849850
O	5.8338108610	5.8211656850	5.8086849850
O	1.9446152620	5.8211656850	5.8086849850
O	9.7230066150	5.8211656850	5.8086849850
O	11.6675960530	11.6608973020	5.8961619820
O	3.8892045440	11.6608973020	5.8961619820
O	-0.0000275740	2.6100309870	6.7405680980
O	7.7783636230	2.6100309870	6.7405680980
O	-1.9446299240	8.4026813220	6.8008587780
O	5.8337614290	8.4026813220	6.8008587780
O	3.8891683360	2.6100309870	6.7405680980
O	11.6675603110	2.6100309870	6.7405680980
O	1.9445656750	8.4026813220	6.8008587780
O	9.7229571830	8.4026813220	6.8008587780
O	0.0000562380	5.2025083220	7.6500997840
O	7.7784479020	5.2025083220	7.6500997840
O	3.8892516810	5.2025083220	7.6500997840
O	11.6676427230	5.2025083220	7.6500997840
O	1.9445942210	11.0066060770	7.7246176470
O	9.7229852630	11.0066060770	7.7246176470
O	-1.9446015330	11.0066060770	7.7246176470
O	5.8337895090	11.0066060770	7.7246176470
O	-0.0011775670	7.7626718630	8.6665375520
O	7.7787946020	7.7626718630	8.6677461180
O	3.8930920070	7.7594895080	8.6698363030
O	11.6675958960	7.7620771990	8.6709023440
O	1.9446019220	1.9573791750	8.5925352150

O	9.7229938970	1.9573791750	8.5925352150
O	5.8337972100	1.9573791750	8.5925352150
O	13.6121887180	1.9573791750	8.5925352150
O	1.9539913870	4.5705832570	9.5246967990
O	9.7277642040	4.5727388920	9.5133344080
O	5.8191091270	4.5622869090	9.5360076980
O	13.6107260170	4.5749014610	9.5169624460
O	0.0008590100	10.3578128290	9.5838711000
O	7.7796612890	10.3550550190	9.5824169110
O	3.8899857430	10.3545265230	9.5818255540
O	11.6683579730	10.3590447260	9.5833286470
O	0.0023570620	1.3096994850	10.4215788700
O	7.7806144320	1.3104331490	10.4169699330
O	3.9028664850	1.3105210150	10.4225844910
O	11.6696750670	1.3139241920	10.4130766910
O	-1.9439071160	7.1651009180	10.5237052430
O	5.8418236160	7.1512133290	10.5185872480
O	1.9375464600	7.1630520450	10.5138490170
O	9.7235717860	7.1574907100	10.5224265370
O	-1.9467388220	9.7646568640	11.4333764580
O	5.8364004330	9.7399277340	11.4358480280
O	-0.0045577820	3.8760121330	11.2786853690
O	7.7975812700	3.8799398580	11.2796377980
O	3.8622368070	3.8446697640	11.3484421300
O	11.6688750180	3.8742701460	11.2886593870
O	1.9484424870	9.7447048880	11.4337792990
O	9.7258766150	9.7431808240	11.4379753670
O	0.0027925130	6.3829171460	12.2959686240
O	7.7774422000	6.3812010270	12.2992998280
O	1.9620867000	0.7346685200	12.2324835080
O	9.7332552070	0.6963752330	12.2052120460
O	3.8859335910	6.3855867630	12.2683332640
O	11.6728988310	6.3823190570	12.2953002070
O	5.8439267560	0.6939913870	12.2237007310
O	13.6046781670	0.6960994510	12.2072138910
O	1.8284990610	3.3613375150	13.2451346380
O	9.7309367290	3.3007568060	13.1634549870
O	3.8885329710	9.3303111250	13.3108387890
O	11.6755963210	9.3399902500	13.3098841670
O	-0.0032653520	9.3229806330	13.3000332660
O	7.7811744860	9.3394117810	13.3166713150
O	5.8865693810	3.2877712320	13.1307370420
O	13.6065618720	3.3001908550	13.1605486160
O	3.9130264850	0.2012886360	14.0734588560
O	11.6703961970	0.2441010650	14.0837879370
O	-0.0092716810	0.2406275260	14.0796805570
O	7.8050965980	0.2310814100	14.0829127790
O	3.2957652920	3.1130701850	15.2622691650

O	3.8841110820	4.4293404340	15.5262437550
H	3.5475602970	4.5811899530	16.4302704320
H	2.5321596890	3.3579318430	14.6029274320

221-Ce3-OOH

Ce	1.9445951940	2.4093844220	2.8000527150
Ce	9.7229868580	2.4093844220	2.8000527150
Ce	5.8337906370	2.4093844220	2.8000527150
Ce	13.6121826120	2.4093844220	2.8000527150
Ce	0.0000208070	10.9489391440	3.6444218520
Ce	7.7784124720	10.9489391440	3.6444218520
Ce	3.8892167170	10.9489391440	3.6444218520
Ce	11.6676082260	10.9489391440	3.6444218520
Ce	1.9445888540	7.8041438960	4.5298469320
Ce	9.7229803630	7.8041438960	4.5298469320
Ce	-1.9446067450	7.8041438960	4.5298469320
Ce	5.8337846090	7.8041438960	4.5298469320
Ce	0.0000089450	4.6047904270	5.2434760540
Ce	7.7784006100	4.6047904270	5.2434760540
Ce	3.8892043880	4.6047904270	5.2434760540
Ce	11.6675954310	4.6047904270	5.2434760540
Ce	5.8337863200	1.3053169250	6.3566574820
Ce	13.6121782950	1.3053169250	6.3566574820
Ce	1.9445902540	1.3053169250	6.3566574820
Ce	9.7229816080	1.3053169250	6.3566574820
Ce	3.8891978160	9.7009476410	7.3076483830
Ce	11.6675893240	9.7009476410	7.3076483830
Ce	0.0000019060	9.7009476410	7.3076483830
Ce	7.7783935700	9.7009476410	7.3076483830
Ce	-1.9445979550	6.4819932090	8.1585764310
Ce	5.8337937090	6.4819932090	8.1585764310
Ce	1.9445979550	6.4819932090	8.1585764310
Ce	9.7229894640	6.4819932090	8.1585764310
Ce	0.0018504530	3.2644661460	9.0109610870
Ce	7.7708677210	3.2723177050	9.0177161710
Ce	3.8986920260	3.2726851080	9.0197473380
Ce	11.6664841290	3.2651426800	9.0107474440
Ce	1.9437973100	-0.0003572710	9.9623424270
Ce	5.8364464450	11.6673810250	9.9626110120
Ce	5.8335943460	0.0011837920	9.9632867530
Ce	9.7241781700	11.6662564250	9.9621963770
Ce	-0.0029070850	8.3728326740	11.0783722690
Ce	7.7818620610	8.3730187750	11.0734294430
Ce	3.8832338780	8.3774715470	11.0737973340
Ce	11.6680930740	8.3717600920	11.0786364400
Ce	1.9372985610	5.1774747580	11.7999983950

Ce	9.7279842480	5.1797291920	11.7974193020
Ce	5.8408435340	5.2012408850	11.8583435370
Ce	13.6116420370	5.1753599490	11.7987994360
Ce	-0.0002671390	2.0350349000	12.6809008790
Ce	7.8007702600	2.0239827870	12.6837958940
Ce	3.8763866560	2.0270531320	12.6857083340
Ce	11.6743127540	2.0367249040	12.6821181550
Ce	1.9461015790	10.5709130630	13.5225781090
Ce	9.7244082670	10.5832330950	13.5288388450
Ce	-1.9466944270	10.5741566470	13.5281429230
Ce	5.8393597840	10.5724219390	13.5234506270
O	0.0000278850	1.0936971120	2.2401547390
O	7.7784193940	1.0936971120	2.2401547390
O	3.8892236400	1.0936971120	2.2401547390
O	11.6676151490	1.0936971120	2.2401547390
O	0.0000530100	3.6598501530	3.0304604640
O	7.7784442070	3.6598501530	3.0304604640
O	3.8892489200	3.6598501530	3.0304604640
O	11.6676399620	3.6598501530	3.0304604640
O	1.9445652470	9.6970730690	3.1665399670
O	9.7229567560	9.6970730690	3.1665399670
O	-1.9446308190	9.6970730690	3.1665399670
O	5.8337610010	9.6970730690	3.1665399670
O	1.9445956990	0.6173987810	4.1099962430
O	9.7229875190	0.6173987810	4.1099962430
O	5.8337917650	0.6173987810	4.1099962430
O	13.6121832740	0.6173987810	4.1099962430
O	3.8892287350	6.6033288830	4.0372105540
O	11.6676205550	6.6033288830	4.0372105540
O	0.0000329800	6.6033288830	4.0372105540
O	7.7784249560	6.6033288830	4.0372105540
O	1.9446021160	3.2313913800	4.8946937290
O	9.7229937810	3.2313913800	4.8946937290
O	5.8337975600	3.2313913800	4.8946937290
O	13.6121886020	3.2313913800	4.8946937290
O	0.0000032280	9.1016627900	5.0340550170
O	7.7783944260	9.1016627900	5.0340550170
O	3.8891991380	9.1016627900	5.0340550170
O	11.6675911140	9.1016627900	5.0340550170
O	0.0000087900	11.6608973020	5.8961619820
O	7.7784002980	11.6608973020	5.8961619820
O	13.6122023700	5.8211656850	5.8086849850
O	5.8338108610	5.8211656850	5.8086849850
O	1.9446152620	5.8211656850	5.8086849850
O	9.7230066150	5.8211656850	5.8086849850
O	11.6675960530	11.6608973020	5.8961619820
O	3.8892045440	11.6608973020	5.8961619820
O	-0.0000275740	2.6100309870	6.7405680980

O	7.7783636230	2.6100309870	6.7405680980
O	-1.9446299240	8.4026813220	6.8008587780
O	5.8337614290	8.4026813220	6.8008587780
O	3.8891683360	2.6100309870	6.7405680980
O	11.6675603110	2.6100309870	6.7405680980
O	1.9445656750	8.4026813220	6.8008587780
O	9.7229571830	8.4026813220	6.8008587780
O	0.0000562380	5.2025083220	7.6500997840
O	7.7784479020	5.2025083220	7.6500997840
O	3.8892516810	5.2025083220	7.6500997840
O	11.6676427230	5.2025083220	7.6500997840
O	1.9445942210	11.0066060770	7.7246176470
O	9.7229852630	11.0066060770	7.7246176470
O	-1.9446015330	11.0066060770	7.7246176470
O	5.8337895090	11.0066060770	7.7246176470
O	-0.0039183490	7.7630878820	8.6641398790
O	7.7731118120	7.7617784110	8.6716438760
O	3.8927381190	7.7620390060	8.6708952740
O	11.6733523550	7.7636928610	8.6620563950
O	1.9446019220	1.9573791750	8.5925352150
O	9.7229938970	1.9573791750	8.5925352150
O	5.8337972100	1.9573791750	8.5925352150
O	13.6121887180	1.9573791750	8.5925352150
O	1.9530822820	4.5658378560	9.5266560130
O	9.7163646660	4.5659369760	9.5235418760
O	5.8355999830	4.5701426020	9.5147173700
O	13.6122497940	4.5660442280	9.5179418070
O	-0.0020690170	10.3576441890	9.5816113450
O	7.7809657940	10.3548538010	9.5818991000
O	3.8868133720	10.3591130480	9.5802204840
O	11.6672583730	10.3529412110	9.5838022490
O	0.0012159530	1.3098207720	10.4157001350
O	7.7840871110	1.3133105760	10.4212863820
O	3.8869865770	1.3151564900	10.4224345850
O	11.6709544440	1.3111779100	10.4162586530
O	-1.9468551140	7.1519386210	10.5168660860
O	5.8309803020	7.1521739190	10.5426604710
O	1.9291709600	7.1599368540	10.5057981240
O	9.7398250120	7.1603784490	10.5019725500
O	-1.9446367350	9.7368925220	11.4372253250
O	5.8329612830	9.7441331460	11.4325787200
O	-0.0012490010	3.8691197020	11.2901381560
O	7.7644845750	3.8715715160	11.3175293330
O	3.9132935290	3.8737520500	11.3204092610
O	11.6689549830	3.8715861270	11.2912568650
O	1.9402452930	9.7434634690	11.4305139530
O	9.7249709150	9.7419870630	11.4399520650
O	-0.0047395440	6.3759013240	12.2952736800

O	7.8196876530	6.3940425770	12.2611859570
O	1.9410455240	0.6873308310	12.2098888470
O	9.7345283600	0.6902908250	12.2086573770
O	3.8415738520	6.3956588460	12.2704976360
O	11.6684962790	6.3789510110	12.2981071010
O	5.8369335790	0.6862719670	12.2114220440
O	13.6157398680	0.6947673750	12.2073861650
O	1.9379118560	3.2899358520	13.1646578030
O	9.7318577400	3.2901255280	13.1696965780
O	3.8782884550	9.3387804260	13.3064490350
O	11.6702889220	9.3397659800	13.3201713260
O	0.0049580960	9.3349235990	13.3129840410
O	7.7730659130	9.3425233830	13.3152621710
O	5.8435982570	3.2351609800	13.1983768060
O	13.6131400270	3.2993713460	13.1664711420
O	3.8808916490	0.2393874190	14.0892759620
O	11.6843507660	0.2461208130	14.0896627780
O	-0.0010785740	0.2465922380	14.0898335710
O	7.8003556600	0.2376631340	14.0902025490
O	5.6452173470	5.5454915830	14.4096644150
O	6.7324966910	5.9844538670	15.1122181160
H	6.4718347890	5.8188821580	16.0466436060

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Ce	1.9445951940	2.4093844220	2.8000527150
Ce	9.7229868580	2.4093844220	2.8000527150
Ce	5.8337906370	2.4093844220	2.8000527150
Ce	13.6121826120	2.4093844220	2.8000527150
Ce	0.0000208070	10.9489391440	3.6444218520
Ce	7.7784124720	10.9489391440	3.6444218520
Ce	3.8892167170	10.9489391440	3.6444218520
Ce	11.6676082260	10.9489391440	3.6444218520
Ce	1.9445888540	7.8041438960	4.5298469320
Ce	9.7229803630	7.8041438960	4.5298469320
Ce	-1.9446067450	7.8041438960	4.5298469320
Ce	5.8337846090	7.8041438960	4.5298469320
Ce	0.0000089450	4.6047904270	5.2434760540
Ce	7.7784006100	4.6047904270	5.2434760540
Ce	3.8892043880	4.6047904270	5.2434760540
Ce	11.6675954310	4.6047904270	5.2434760540
Ce	5.8337863200	1.3053169250	6.3566574820
Ce	13.6121782950	1.3053169250	6.3566574820
Ce	1.9445902540	1.3053169250	6.3566574820
Ce	9.7229816080	1.3053169250	6.3566574820
Ce	3.8891978160	9.7009476410	7.3076483830
Ce	11.6675893240	9.7009476410	7.3076483830

Ce	0.0000019060	9.7009476410	7.3076483830
Ce	7.7783935700	9.7009476410	7.3076483830
Ce	-1.9445979550	6.4819932090	8.1585764310
Ce	5.8337937090	6.4819932090	8.1585764310
Ce	1.9445979550	6.4819932090	8.1585764310
Ce	9.7229894640	6.4819932090	8.1585764310
Ce	-0.0028354720	3.2721464050	9.0112917140
Ce	7.7741814030	3.2658427830	9.0119660010
Ce	3.8859507900	3.2690614630	9.0069443710
Ce	11.6617573540	3.2705631090	9.0104433150
Ce	1.9408396820	0.0089038470	9.9665598760
Ce	9.7151832130	0.0030249280	9.9847768050
Ce	5.8282864510	0.0003862990	9.9811406660
Ce	13.6110177560	0.0054905030	9.9626583050
Ce	0.0018480450	8.3912829890	11.0813255170
Ce	7.7917057830	8.3764480120	11.0609264900
Ce	3.8990701420	8.3950953810	11.0924451700
Ce	11.6707451360	8.3832331820	11.0734021540
Ce	1.9356465740	5.2063369050	11.7979703640
Ce	9.7176728010	5.1849094360	11.8014724520
Ce	5.8258528730	5.1989217190	11.7972461160
Ce	13.6025151540	5.1937960880	11.8030562180
Ce	-0.0166211250	2.0625150270	12.6756668770
Ce	7.7382768640	2.0616536610	12.6932261250
Ce	3.8613397450	2.0794719330	12.6725371500
Ce	11.6472886000	2.0495629870	12.6768923900
Ce	1.8184543100	10.6540971410	13.5903742720
Ce	9.7414455440	10.5891019180	13.5310767030
Ce	-1.9839352670	10.6089810950	13.5414509960
Ce	5.9436397220	10.5299528300	13.5545218410
O	0.0000278850	1.0936971120	2.2401547390
O	7.7784193940	1.0936971120	2.2401547390
O	3.8892236400	1.0936971120	2.2401547390
O	11.6676151490	1.0936971120	2.2401547390
O	0.0000530100	3.6598501530	3.0304604640
O	7.7784442070	3.6598501530	3.0304604640
O	3.8892489200	3.6598501530	3.0304604640
O	11.6676399620	3.6598501530	3.0304604640
O	1.9445652470	9.6970730690	3.1665399670
O	9.7229567560	9.6970730690	3.1665399670
O	-1.9446308190	9.6970730690	3.1665399670
O	5.8337610010	9.6970730690	3.1665399670
O	1.9445956990	0.6173987810	4.1099962430
O	9.7229875190	0.6173987810	4.1099962430
O	5.8337917650	0.6173987810	4.1099962430
O	13.6121832740	0.6173987810	4.1099962430
O	3.8892287350	6.6033288830	4.0372105540
O	11.6676205550	6.6033288830	4.0372105540

O	0.0000329800	6.6033288830	4.0372105540
O	7.7784249560	6.6033288830	4.0372105540
O	1.9446021160	3.2313913800	4.8946937290
O	9.7229937810	3.2313913800	4.8946937290
O	5.8337975600	3.2313913800	4.8946937290
O	13.6121886020	3.2313913800	4.8946937290
O	0.0000032280	9.1016627900	5.0340550170
O	7.7783944260	9.1016627900	5.0340550170
O	3.8891991380	9.1016627900	5.0340550170
O	11.6675911140	9.1016627900	5.0340550170
O	0.0000087900	11.6608973020	5.8961619820
O	7.7784002980	11.6608973020	5.8961619820
O	13.6122023700	5.8211656850	5.8086849850
O	5.8338108610	5.8211656850	5.8086849850
O	1.9446152620	5.8211656850	5.8086849850
O	9.7230066150	5.8211656850	5.8086849850
O	11.6675960530	11.6608973020	5.8961619820
O	3.8892045440	11.6608973020	5.8961619820
O	-0.0000275740	2.6100309870	6.7405680980
O	7.7783636230	2.6100309870	6.7405680980
O	-1.9446299240	8.4026813220	6.8008587780
O	5.8337614290	8.4026813220	6.8008587780
O	3.8891683360	2.6100309870	6.7405680980
O	11.6675603110	2.6100309870	6.7405680980
O	1.9445656750	8.4026813220	6.8008587780
O	9.7229571830	8.4026813220	6.8008587780
O	0.0000562380	5.2025083220	7.6500997840
O	7.7784479020	5.2025083220	7.6500997840
O	3.8892516810	5.2025083220	7.6500997840
O	11.6676427230	5.2025083220	7.6500997840
O	1.9445942210	11.0066060770	7.7246176470
O	9.7229852630	11.0066060770	7.7246176470
O	-1.9446015330	11.0066060770	7.7246176470
O	5.8337895090	11.0066060770	7.7246176470
O	-0.0010374290	7.7657830360	8.6729251060
O	7.7822215110	7.7621769430	8.6702406060
O	3.8892671260	7.7668231460	8.6645348570
O	11.6714790130	7.7674527440	8.6713243550
O	1.9446019220	1.9573791750	8.5925352150
O	9.7229938970	1.9573791750	8.5925352150
O	5.8337972100	1.9573791750	8.5925352150
O	13.6121887180	1.9573791750	8.5925352150
O	1.9347225710	4.5785228020	9.5166629490
O	9.7206057850	4.5717127140	9.5185215230
O	5.8301463980	4.5734286830	9.5176436100
O	13.6065572250	4.5746731420	9.5206234130
O	0.0022789780	10.3570676420	9.5948388180
O	7.7909201040	10.3682003610	9.5728882300

O	3.8855803270	10.3576609760	9.6052256980
O	11.6700072260	10.3676298760	9.5821222950
O	-0.0048431940	1.3303334640	10.4199173010
O	7.7741452690	1.3162015540	10.4302627290
O	3.8705523010	1.3277315890	10.4125718660
O	11.6433230980	1.3162415790	10.4411987880
O	-1.9426648080	7.1667657930	10.5212526640
O	5.8314186250	7.1635978080	10.5175767140
O	1.9426180150	7.1788068800	10.5235089870
O	9.7305553510	7.1621108210	10.5108909760
O	-1.9536920130	9.7573586360	11.4482258890
O	5.8908510020	9.7497507310	11.4196454530
O	-0.0124513210	3.8945010860	11.2950968930
O	7.7685735220	3.8827047620	11.2941838630
O	3.8726491170	3.8949796340	11.2849484250
O	11.6610681550	3.8822989650	11.2908439570
O	1.9377807970	9.7585266580	11.4951050290
O	9.7320721360	9.7565770440	11.4323472900
O	-0.0006119370	6.4110263900	12.2991919430
O	7.7863540540	6.3916351830	12.2854284990
O	1.9254626270	0.7196433030	12.2131636160
O	9.6796933920	0.6817897520	12.2721629180
O	3.8824837810	6.3982583620	12.2975314240
O	11.6687767640	6.3944799310	12.2913869690
O	5.7782037060	0.7341041930	12.1996573190
O	13.6095555080	0.7130639350	12.2106447960
O	1.9288312900	3.3245069900	13.1615894120
O	9.7221744900	3.3124104190	13.1627088240
O	4.0220860130	9.3146287150	13.2821716070
O	11.6581573350	9.3486935960	13.3242463080
O	-0.0342524250	9.3840938780	13.3488134910
O	7.8173098570	9.3166497120	13.3257788420
O	5.8099663680	3.3404180520	13.1577162920
O	13.5946886340	3.3128552930	13.1628697000
O	3.8526577590	0.2841880200	14.1021220030
O	11.6810764480	0.2224817560	14.0769639490
O	-0.0081480080	0.2560430410	14.0888843010
O	7.5519008320	0.3808914620	14.1773495490
O	3.3352347730	9.5151940590	15.6638283760
O	4.4512262400	10.4396098650	15.9070755670
H	4.0856518670	11.2791598850	15.3925441110
H	3.6616031330	9.1322406520	14.7461366310

331-Ce1-OOH

Ce	-0.0000000020	6.9507133630	2.3670970170
Ce	3.8891956530	6.9507207260	2.3670759380

Ce	1.9445977200	15.4270460790	2.3670955860
Ce	-1.9445979550	15.4270460790	2.3670955860
Ce	-0.0000000020	12.4228856140	3.5203780730
Ce	3.8891961160	12.4228886680	3.5203753370
Ce	1.9445982560	3.9465691430	3.5203870530
Ce	5.8337936290	3.9465691430	3.5203870530
Ce	-1.9445991460	9.3609901900	4.5898474610
Ce	1.9445994620	9.3609901900	4.5898474610
Ce	-0.0000000020	0.8846764880	4.5898703710
Ce	3.8891960310	0.8846819140	4.5898688270
Ce	1.9445974610	14.7231392280	6.0359420990
Ce	-1.9445975780	14.7231392280	6.0359420990
Ce	3.8891960020	6.2468290920	6.0359347630
Ce	-0.0000000000	6.2468342360	6.0359376290
Ce	3.8891958870	11.5628706430	7.2731916820
Ce	0.0000000000	11.5628681570	7.2731922510
Ce	5.8337918010	3.0865645100	7.2732007650
Ce	1.9446000880	3.0865645100	7.2732007650
Ce	-1.9479292680	8.5141432230	8.4977807740
Ce	1.9466983210	8.5139431000	8.4990033500
Ce	0.0001506330	0.0374451790	8.5003084350
Ce	3.8892976350	0.0364803390	8.4989984060
Ce	1.9448013860	13.8343838260	9.7367828650
Ce	3.8873830310	5.3539990550	9.7628581980
Ce	-1.9447460450	13.8336043160	9.7365941570
Ce	-0.0001568290	5.3572068840	9.7367505000
Ce	-0.000099960	10.7154445430	11.1770460270
Ce	1.9498206420	2.2555958370	11.1695400480
Ce	3.8884264940	10.7152149080	11.1808631390
Ce	5.8299339100	2.2563600060	11.1689717310
Ce	3.8911417680	16.1387333790	12.2593689540
Ce	1.9447080890	7.6475529060	12.2448833630
Ce	-0.0009608690	16.1370584960	12.2577212010
Ce	5.8314622210	7.6474578840	12.2382645720
Ce	1.9433939390	13.1337930640	13.4032313800
Ce	-1.9444601030	13.1321616220	13.4033920180
Ce	0.0011486030	4.6603246910	13.4126449430
Ce	3.8822114310	4.6219201300	13.5070305740
O	1.9445887870	5.5490558700	1.9335942950
O	3.8891958830	14.0253876620	1.9336029210
O	-0.0000000030	14.0253887860	1.9336008020
O	5.8338029790	5.5490558700	1.9335942950
O	1.9445908170	8.1935857730	2.4635064340
O	5.8338009510	8.1935857730	2.4635064340
O	-0.0000000030	16.6699198080	2.4635100400
O	3.8891958840	16.6699191890	2.4635187780
O	1.9445985820	11.1825729010	3.1763256020
O	-1.9445985870	11.1825729010	3.1763256020

O	3.8891958840	2.7062566780	3.1763346120
O	-0.0000000030	2.7062551340	3.1763349690
O	1.9445949560	13.8336284430	3.8696194020
O	-1.9445949580	13.8336284430	3.8696194020
O	3.8891958860	5.3573044120	3.8696200540
O	-0.0000000010	5.3573111040	3.8696153590
O	1.9445953790	16.4701576290	4.3638358960
O	-1.9445952660	16.4701576290	4.3638358960
O	3.8891957690	7.9938543410	4.3638299020
O	-0.0000000020	7.9938460830	4.3638247910
O	5.8337950840	2.1685343300	5.0305281930
O	1.9445964570	2.1685343300	5.0305281930
O	-0.0000000010	10.6448420120	5.0305093800
O	3.8891958860	10.6448400810	5.0305102620
O	1.9446010490	4.8520739810	5.6962716020
O	5.8337907230	4.8520739810	5.6962716020
O	3.8891956540	13.3283842090	5.6962689610
O	-0.0000000020	13.3283816710	5.6962746390
O	3.8891956540	16.0624346680	6.2752528180
O	-0.0000000000	16.0624317930	6.2752523580
O	5.8337916220	7.5861299260	6.2752432660
O	1.9446001510	7.5861299260	6.2752432660
O	1.9445965700	10.2543739410	6.9222146910
O	-1.9445968610	10.2543739410	6.9222146910
O	3.8891957130	1.7780622010	6.9222298330
O	-0.0000000000	1.7780609630	6.9222314740
O	1.9445987410	12.9360348810	7.5912439110
O	-1.9445989730	12.9360348810	7.5912439110
O	3.8891956550	4.4597271670	7.5912502650
O	0.0000000000	4.4597250260	7.5912453510
O	3.8885596110	7.1407187480	8.1831225120
O	1.9446140680	15.6171285240	8.1816098310
O	-1.9444757450	15.6172629480	8.1817272100
O	-0.0011419750	7.1393509420	8.1823999170
O	3.8886932890	9.8284831200	8.8493791170
O	-0.0001799520	9.8251023070	8.8474183910
O	5.8350074840	1.3486021340	8.8504570990
O	1.9439336630	1.3494665290	8.8520323840
O	3.8894943550	12.4987211000	9.4961972660
O	-0.0004087150	12.4952810140	9.4953535110
O	1.9445768980	4.0176473920	9.4987628290
O	5.8329155970	4.0181947450	9.4994368220
O	0.0000587780	15.2274648220	10.0785693390
O	5.8222760520	6.7524003620	10.0789031340
O	1.9535576220	6.7534817050	10.0775518520
O	3.8893503300	15.2325583510	10.0804063270
O	1.9439202310	9.4361463460	10.7359160230
O	3.8899656570	0.9401547580	10.7416107710

O	0.0001392400	0.9485508110	10.7466950050
O	-1.9451074980	9.4349571500	10.7334502730
O	3.8874715720	3.5906635640	11.4078016600
O	0.0028351270	3.6120763000	11.4001699270
O	1.9447040130	12.0923462880	11.4077372920
O	-1.9450193370	12.0891636200	11.4088220690
O	-1.9443396740	14.7336341480	11.9049277430
O	1.9444922210	14.7372710670	11.9055173240
O	3.8833247690	6.2390128820	11.9403529280
O	0.0023995560	6.2504610760	11.8727827510
O	-0.0019273010	8.8990376360	12.5873252850
O	5.8330818730	0.4341893590	12.6196877120
O	1.9464825030	0.4324066860	12.6160637860
O	3.8893602590	8.9048454320	12.5893713740
O	3.8883026200	11.8982051630	13.3092881150
O	0.0008861180	11.8941830720	13.3078173950
O	5.8452789670	3.3727205500	13.2824217390
O	1.9391624040	3.3819209160	13.2967911000
O	0.0001009040	14.5377455390	13.8367405090
O	3.8904581120	14.5418461480	13.8367595760
O	5.8914404500	6.0151520310	13.7876729080
O	1.8803630200	6.0313588060	13.8135447550
O	3.9183465100	4.4774768680	15.9628543840
O	4.7313005650	5.3883124000	16.6410021960
H	4.4324782940	5.2762549100	17.5681101950

331-Ce1-HOOH

Ce	-0.0000000000	6.9507100000	2.3671000000
Ce	3.8892000000	6.9507200000	2.3670800000
Ce	1.9446000000	15.4270500000	2.3671000000
Ce	-1.9446000000	15.4270500000	2.3671000000
Ce	0.0000000000	12.4228900000	3.5203800000
Ce	3.8892000000	12.4228900000	3.5203800000
Ce	1.9446000000	3.9465700000	3.5203900000
Ce	5.8337900000	3.9465700000	3.5203900000
Ce	-1.9446000000	9.3609900000	4.5898500000
Ce	1.9446000000	9.3609900000	4.5898500000
Ce	-0.0000000000	0.8846800000	4.5898700000
Ce	3.8892000000	0.8846800000	4.5898700000
Ce	1.9446000000	14.7231400000	6.0359400000
Ce	-1.9446000000	14.7231400000	6.0359400000
Ce	3.8892000000	6.2468300000	6.0359300000
Ce	0.0000000000	6.2468300000	6.0359400000
Ce	3.8892000000	11.5628700000	7.2731900000
Ce	-0.0000000000	11.5628700000	7.2731900000
Ce	5.8337900000	3.0865600000	7.2732000000

Ce	1.944600000	3.086560000	7.273200000
Ce	-1.9491216610	8.5120332150	8.4966403250
Ce	1.9438939410	8.5096864380	8.4999714580
Ce	0.0015653970	0.0319169810	8.4948148900
Ce	3.8889701010	0.0317127240	8.4975636160
Ce	1.9477856410	13.8298086600	9.7351852060
Ce	3.8838203020	5.3501589050	9.7516518700
Ce	-1.9433446680	13.8286222870	9.7355220940
Ce	-0.0023403210	5.3446238720	9.7373670110
Ce	0.0032140370	10.7191496020	11.1726573910
Ce	1.9441242000	2.2319287590	11.1656010040
Ce	3.8920113640	10.7182676730	11.1739738170
Ce	5.8427970420	2.2251224890	11.1595215320
Ce	3.8892674650	16.1272798300	12.2543876570
Ce	1.9283658550	7.6575302050	12.2586173930
Ce	-0.0003491300	16.1254158480	12.2485597140
Ce	5.8238738510	7.6582531540	12.2420770380
Ce	1.9509102650	13.1221592150	13.4044471380
Ce	-1.9365848250	13.1219377160	13.4058664300
Ce	0.0059017540	4.6728303850	13.4196059440
Ce	3.9232013410	4.5552667240	13.4255553590
O	1.9445900000	5.5490600000	1.9335900000
O	3.8892000000	14.0253900000	1.9336000000
O	-0.0000000000	14.0253900000	1.9336000000
O	5.8338000000	5.5490600000	1.9335900000
O	1.9445900000	8.1935900000	2.4635100000
O	5.8338000000	8.1935900000	2.4635100000
O	-0.0000000000	16.6699200000	2.4635100000
O	3.8892000000	16.6699200000	2.4635200000
O	1.9446000000	11.1825700000	3.1763300000
O	-1.9446000000	11.1825700000	3.1763300000
O	3.8892000000	2.7062600000	3.1763300000
O	-0.0000000000	2.7062600000	3.1763300000
O	1.9445900000	13.8336300000	3.8696200000
O	-1.9445900000	13.8336300000	3.8696200000
O	3.8892000000	5.3573000000	3.8696200000
O	0.0000000000	5.3573100000	3.8696200000
O	1.9446000000	16.4701600000	4.3638400000
O	-1.9446000000	16.4701600000	4.3638400000
O	3.8892000000	7.9938500000	4.3638300000
O	-0.0000000000	7.9938500000	4.3638200000
O	5.8338000000	2.1685300000	5.0305300000
O	1.9446000000	2.1685300000	5.0305300000
O	0.0000000000	10.6448400000	5.0305100000
O	3.8892000000	10.6448400000	5.0305100000
O	1.9446000000	4.8520700000	5.6962700000
O	5.8337900000	4.8520700000	5.6962700000
O	3.8892000000	13.3283800000	5.6962700000

O	0.000000000	13.328380000	5.696270000
O	3.889200000	16.062430000	6.275250000
O	-0.000000000	16.062430000	6.275250000
O	5.833790000	7.586130000	6.275240000
O	1.944600000	7.586130000	6.275240000
O	1.944600000	10.254370000	6.922210000
O	-1.944600000	10.254370000	6.922210000
O	3.889200000	1.778060000	6.922230000
O	-0.000000000	1.778060000	6.922230000
O	1.944600000	12.936030000	7.591240000
O	-1.944600000	12.936030000	7.591240000
O	3.889200000	4.459730000	7.591250000
O	-0.000000000	4.459730000	7.591250000
O	3.8837170580	7.1358195790	8.1849434260
O	1.9450834770	15.6157607390	8.1802748370
O	-1.9434959230	15.6157341270	8.1799103360
O	-0.0050650570	7.1312366680	8.1897685820
O	3.8884401420	9.8198291950	8.8495961630
O	-0.0003212990	9.8177795090	8.8477832690
O	5.8347126820	1.3471549660	8.8507910570
O	1.9453116130	1.3493593840	8.8501043910
O	3.8942132780	12.4904977840	9.4949811670
O	0.0025206500	12.4865996460	9.4931702210
O	1.9413900830	4.0178077400	9.4951130100
O	5.8410026240	4.0180677200	9.4924347840
O	-0.0000086290	15.2146021490	10.0737929400
O	5.8063611830	6.7507063390	10.0887033220
O	1.9519269600	6.7492018770	10.0913897900
O	3.8905482030	15.2204880550	10.0764084690
O	1.9439569520	9.4305708590	10.7413324480
O	3.8883610280	0.9289640110	10.7306846690
O	0.0028533720	0.9416970100	10.7310559390
O	-1.9466761890	9.4330804380	10.7350419570
O	3.9018648270	3.5611882590	11.3706954010
O	0.0053270910	3.5932933880	11.4124721480
O	1.9523406010	12.0819572920	11.4011526630
O	-1.9365561970	12.0822283840	11.4048791300
O	-1.9441623680	14.7183169690	11.9036057160
O	1.9439567140	14.7188018520	11.9011929420
O	3.8737608650	6.1964902670	11.9626196510
O	-0.0172370900	6.2353318860	11.8867670540
O	-0.0100642390	8.8901856660	12.5825590630
O	5.8352118450	0.4211430550	12.5919758580
O	1.9431919720	0.4253742470	12.5943427800
O	3.8891985040	8.8778203330	12.5826138090
O	3.8998211510	11.8804129160	13.2944860560
O	0.0131992050	11.8812810670	13.2946810600
O	5.8348477520	3.4102654610	13.2986705010

O	1.9696924060	3.4463293570	13.2920031530
O	-0.0025340700	14.5193110470	13.8314707770
O	3.8838852870	14.5221381890	13.8339331700
O	5.8949017370	6.0841092070	13.8985165940
O	1.7901175590	6.1400464120	13.9247943700
O	3.5309105640	5.5940611710	15.7615027650
O	4.5254830620	6.6062479130	16.1204547730
H	5.1680653200	6.5009369690	15.3383680700
H	2.7793067200	6.1078948400	15.3055030620

331-Ce2-OOH

Ce	-0.0000000020	6.9507133630	2.3670970170
Ce	3.8891956530	6.9507207260	2.3670759380
Ce	1.9445977200	15.4270460790	2.3670955860
Ce	-1.9445979550	15.4270460790	2.3670955860
Ce	-0.0000000020	12.4228856140	3.5203780730
Ce	3.8891961160	12.4228886680	3.5203753370
Ce	1.9445982560	3.9465691430	3.5203870530
Ce	5.8337936290	3.9465691430	3.5203870530
Ce	-1.9445991460	9.3609901900	4.5898474610
Ce	1.9445994620	9.3609901900	4.5898474610
Ce	-0.0000000020	0.8846764880	4.5898703710
Ce	3.8891960310	0.8846819140	4.5898688270
Ce	1.9445974610	14.7231392280	6.0359420990
Ce	-1.9445975780	14.7231392280	6.0359420990
Ce	3.8891960020	6.2468290920	6.0359347630
Ce	-0.0000000000	6.2468342360	6.0359376290
Ce	3.8891958870	11.5628706430	7.2731916820
Ce	0.0000000000	11.5628681570	7.2731922510
Ce	5.8337918010	3.0865645100	7.2732007650
Ce	1.9446000880	3.0865645100	7.2732007650
Ce	-1.9460959600	8.5116619990	8.4997417180
Ce	1.9429439320	8.5064362620	8.5074486830
Ce	0.0015098410	0.0320604950	8.4963363160
Ce	3.8879338540	0.0322420790	8.4966160050
Ce	1.9437719620	13.8246450490	9.7334851630
Ce	3.8815528980	5.3552264820	9.7410125130
Ce	-1.9451486290	13.8263552350	9.7333178510
Ce	0.0059729730	5.3546906380	9.7419571500
Ce	-0.0061631210	10.7067974910	11.1670900510
Ce	1.9455696780	2.2285082530	11.1747216170
Ce	3.8878767710	10.7065604410	11.1660226750
Ce	5.8361742930	2.2176401000	11.1594422940
Ce	3.8895589910	16.1151913920	12.2506992970
Ce	1.9427619780	7.6683092150	12.3165664400
Ce	0.0004281710	16.1153852230	12.2507477690

Ce	5.8277825810	7.6450138120	12.2423367220
Ce	1.9432926090	13.1025695460	13.3953497570
Ce	-1.9460473520	13.1095193140	13.3978940120
Ce	-0.0237273500	4.6133779440	13.4053817480
Ce	3.9225770600	4.6044846510	13.4019392360
O	1.9445887870	5.5490558700	1.9335942950
O	3.8891958830	14.0253876620	1.9336029210
O	-0.0000000030	14.0253887860	1.9336008020
O	5.8338029790	5.5490558700	1.9335942950
O	1.9445908170	8.1935857730	2.4635064340
O	5.8338009510	8.1935857730	2.4635064340
O	-0.0000000030	16.6699198080	2.4635100400
O	3.8891958840	16.6699191890	2.4635187780
O	1.9445985820	11.1825729010	3.1763256020
O	-1.9445985870	11.1825729010	3.1763256020
O	3.8891958840	2.7062566780	3.1763346120
O	-0.0000000030	2.7062551340	3.1763349690
O	1.9445949560	13.8336284430	3.8696194020
O	-1.9445949580	13.8336284430	3.8696194020
O	3.8891958860	5.3573044120	3.8696200540
O	-0.0000000010	5.3573111040	3.8696153590
O	1.9445953790	16.4701576290	4.3638358960
O	-1.9445952660	16.4701576290	4.3638358960
O	3.8891957690	7.9938543410	4.3638299020
O	-0.0000000020	7.9938460830	4.3638247910
O	5.8337950840	2.1685343300	5.0305281930
O	1.9445964570	2.1685343300	5.0305281930
O	-0.0000000010	10.6448420120	5.0305093800
O	3.8891958860	10.6448400810	5.0305102620
O	1.9446010490	4.8520739810	5.6962716020
O	5.8337907230	4.8520739810	5.6962716020
O	3.8891956540	13.3283842090	5.6962689610
O	-0.0000000020	13.3283816710	5.6962746390
O	3.8891956540	16.0624346680	6.2752528180
O	-0.0000000000	16.0624317930	6.2752523580
O	5.8337916220	7.5861299260	6.2752432660
O	1.9446001510	7.5861299260	6.2752432660
O	1.9445965700	10.2543739410	6.9222146910
O	-1.9445968610	10.2543739410	6.9222146910
O	3.8891957130	1.7780622010	6.9222298330
O	-0.0000000000	1.7780609630	6.9222314740
O	1.9445987410	12.9360348810	7.5912439110
O	-1.9445989730	12.9360348810	7.5912439110
O	3.8891956550	4.4597271670	7.5912502650
O	0.0000000000	4.4597250260	7.5912453510
O	3.8953500610	7.1369281740	8.1821107670
O	1.9444931950	15.6142194490	8.1779965970
O	-1.9446802110	15.6135618570	8.1781798240

O	-0.0089587860	7.1363754350	8.1840188890
O	3.8765294480	9.8198541220	8.8499789830
O	0.0084544940	9.8198598300	8.8494792980
O	5.8342160490	1.3423587170	8.8486933470
O	1.9449662010	1.3445019060	8.8483308850
O	3.8897783270	12.4884810230	9.4883093100
O	-0.0030104450	12.4886448450	9.4881862440
O	1.9445374310	4.0109383670	9.4997487050
O	5.8355149910	4.0134061860	9.4891607420
O	-0.0003586160	15.2187098100	10.0736436210
O	5.8293822450	6.7405573090	10.0939532390
O	1.9445885690	6.7453741430	10.0716605320
O	3.8893175760	15.2185052520	10.0735285690
O	1.9389760540	9.4163772360	10.7692714480
O	3.8877443970	0.9402007100	10.7360535760
O	0.0031211840	0.9401424750	10.7356225300
O	-1.9481910960	9.4281829680	10.7108247650
O	3.9027824760	3.5927586840	11.3965741350
O	-0.0080300150	3.5937187400	11.4010266380
O	1.9417696220	12.0733530710	11.3944140020
O	-1.9469255820	12.0760169550	11.3968020390
O	-1.9443999630	14.7114229470	11.9004361430
O	1.9447469200	14.7050265750	11.8997853260
O	3.8623944650	6.2288552660	11.9298061450
O	0.0188140770	6.2325595920	11.9246180580
O	-0.0489590140	8.8814569880	12.5653174590
O	5.8346431220	0.3951316370	12.5873248940
O	1.9449969400	0.4126786570	12.5974693210
O	3.9212318270	8.8797702680	12.5599445850
O	3.8869804060	11.8683664210	13.2922705530
O	-0.0041093520	11.8683733420	13.2937868030
O	5.8348169150	3.3461208670	13.3056601630
O	1.9505053350	3.3795635200	13.2870608340
O	-0.0009639370	14.5093743570	13.8347375190
O	3.8918264490	14.5091269780	13.8350426310
O	5.8281171280	5.9823802100	13.8311618500
O	1.9292645860	5.9339653850	13.8900682500
O	1.7575268080	8.2482198780	14.8108390940
O	2.9080902460	8.5319335960	15.5093480360
H	2.6382704740	8.3638942370	16.4390003910

331-Ce2-HOOH

Ce	-0.0000000020	6.9507133630	2.3670970170
Ce	3.8891956530	6.9507207260	2.3670759380
Ce	1.9445977200	15.4270460790	2.3670955860
Ce	-1.9445979550	15.4270460790	2.3670955860
Ce	-0.0000000020	12.4228856140	3.5203780730

Ce	3.8891961160	12.4228886680	3.5203753370
Ce	1.9445982560	3.9465691430	3.5203870530
Ce	5.8337936290	3.9465691430	3.5203870530
Ce	-1.9445991460	9.3609901900	4.5898474610
Ce	1.9445994620	9.3609901900	4.5898474610
Ce	-0.0000000020	0.8846764880	4.5898703710
Ce	3.8891960310	0.8846819140	4.5898688270
Ce	1.9445974610	14.7231392280	6.0359420990
Ce	-1.9445975780	14.7231392280	6.0359420990
Ce	3.8891960020	6.2468290920	6.0359347630
Ce	-0.0000000000	6.2468342360	6.0359376290
Ce	3.8891958870	11.5628706430	7.2731916820
Ce	0.0000000000	11.5628681570	7.2731922510
Ce	5.8337918010	3.0865645100	7.2732007650
Ce	1.9446000880	3.0865645100	7.2732007650
Ce	-1.9461030080	8.5138222370	8.4973090920
Ce	1.9450844140	8.5104161150	8.5054291260
Ce	0.0001679450	0.0393347080	8.5001887070
Ce	3.8895975380	0.0399282840	8.4995642290
Ce	1.9452760500	13.8356092340	9.7364119610
Ce	3.8837555710	5.3628304310	9.7439957470
Ce	-1.9431654250	13.8387067610	9.7353336720
Ce	0.0042015280	5.3575756150	9.7419922080
Ce	-0.0024042300	10.7262784990	11.1653246020
Ce	1.9463618690	2.2459655840	11.1827691680
Ce	3.9016176500	10.7346200750	11.1656792270
Ce	5.8367354910	2.2394615430	11.1775355560
Ce	3.8884042600	16.1324189530	12.2539661900
Ce	1.9157162180	7.6770162560	12.2880234820
Ce	-0.0017635820	16.1336297060	12.2557052270
Ce	5.8351407870	7.6599299660	12.2436988590
Ce	1.9460781400	13.1168519340	13.4043862150
Ce	-1.9407449020	13.1318017070	13.4053308230
Ce	-0.0122388160	4.6447011600	13.4200050040
Ce	3.9067401080	4.6419630120	13.4096523640
O	1.9445887870	5.5490558700	1.9335942950
O	3.8891958830	14.0253876620	1.9336029210
O	-0.0000000030	14.0253887860	1.9336008020
O	5.8338029790	5.5490558700	1.9335942950
O	1.9445908170	8.1935857730	2.4635064340
O	5.8338009510	8.1935857730	2.4635064340
O	-0.0000000030	16.6699198080	2.4635100400
O	3.8891958840	16.6699191890	2.4635187780
O	1.9445985820	11.1825729010	3.1763256020
O	-1.9445985870	11.1825729010	3.1763256020
O	3.8891958840	2.7062566780	3.1763346120
O	-0.0000000030	2.7062551340	3.1763349690
O	1.9445949560	13.8336284430	3.8696194020

O	-1.9445949580	13.8336284430	3.8696194020
O	3.8891958860	5.3573044120	3.8696200540
O	-0.0000000010	5.3573111040	3.8696153590
O	1.9445953790	16.4701576290	4.3638358960
O	-1.9445952660	16.4701576290	4.3638358960
O	3.8891957690	7.9938543410	4.3638299020
O	-0.0000000020	7.9938460830	4.3638247910
O	5.8337950840	2.1685343300	5.0305281930
O	1.9445964570	2.1685343300	5.0305281930
O	-0.0000000010	10.6448420120	5.0305093800
O	3.8891958860	10.6448400810	5.0305102620
O	1.9446010490	4.8520739810	5.6962716020
O	5.8337907230	4.8520739810	5.6962716020
O	3.8891956540	13.3283842090	5.6962689610
O	-0.0000000020	13.3283816710	5.6962746390
O	3.8891956540	16.0624346680	6.2752528180
O	-0.0000000000	16.0624317930	6.2752523580
O	5.8337916220	7.5861299260	6.2752432660
O	1.9446001510	7.5861299260	6.2752432660
O	1.9445965700	10.2543739410	6.9222146910
O	-1.9445968610	10.2543739410	6.9222146910
O	3.8891957130	1.7780622010	6.9222298330
O	-0.0000000000	1.7780609630	6.9222314740
O	1.9445987410	12.9360348810	7.5912439110
O	-1.9445989730	12.9360348810	7.5912439110
O	3.8891956550	4.4597271670	7.5912502650
O	0.0000000000	4.4597250260	7.5912453510
O	3.8953537770	7.1396312030	8.1871427450
O	1.9442405260	15.6170429790	8.1824438670
O	-1.9443995440	15.6201552610	8.1830869220
O	-0.0070912560	7.1400378020	8.1848039850
O	3.8795363170	9.8259348500	8.8448815220
O	0.0089004810	9.8232058490	8.8588809010
O	5.8340326340	1.3485149650	8.8534245850
O	1.9459198570	1.3529844800	8.8515052040
O	3.8943764840	12.4990682680	9.4940618020
O	-0.0005101320	12.4979384950	9.4911310380
O	1.9445175320	4.0202779630	9.5037130000
O	5.8364326570	4.0216209450	9.4952625960
O	-0.0003936420	15.2306696710	10.0791464410
O	5.8324258020	6.7463081410	10.0933508300
O	1.9401282870	6.7545908730	10.0702504370
O	3.8872417150	15.2303279040	10.0794655530
O	1.9633390720	9.4201303950	10.7735554010
O	3.8887874480	0.9612536740	10.7430509780
O	0.0037132090	0.9580707460	10.7404003390
O	-1.9571658570	9.4393678720	10.7100684180
O	3.9009440220	3.6184521690	11.4067054140

O	-0.0054836470	3.6074849350	11.4150484850
O	1.9488643450	12.0838448840	11.3915617870
O	-1.9400829970	12.0921604320	11.3983821260
O	-1.9466737510	14.7283921110	11.9021940720
O	1.9417800830	14.7187129650	11.9071584310
O	3.8487239640	6.2648179400	11.9291234900
O	0.0284954070	6.2450332280	11.9206164020
O	-0.0403416530	8.8981856160	12.5521733700
O	5.8361848430	0.4172372450	12.5928519230
O	1.9453180590	0.4307027070	12.6024729930
O	3.9619386220	8.9319366360	12.6426572970
O	3.8929321620	11.8826971290	13.2858543110
O	0.0042289730	11.8933420400	13.2774867250
O	5.8296921670	3.3876319520	13.3172173090
O	1.9566312670	3.4303182430	13.2984914770
O	-0.0140996430	14.5281634010	13.8384689680
O	3.8909800470	14.5208886380	13.8351945770
O	5.8358082640	6.0166840070	13.8178044320
O	1.9144819940	6.0648566590	13.9333945860
O	2.3377056870	8.9317954460	14.6983084710
O	2.6237792950	7.9112042260	15.7089031890
H	2.2966908220	7.0989788860	15.2001335360
H	3.2298250030	9.0908811330	14.2708988720