

The stability and unexpected chemistry of oxide clusters

Xiaohu Yu^{1,2,*}, Artem R.Oganov^{3,1,5}, Qiang Zhu⁴, Fei Qi^{1,6} and Guangrui Qian⁴

¹Moscow Institute of Physics and Technology, 9 Institutskiy Lane, Dolgoprudny, Moscow Region, 141700, Russia

²Institute of Theoretical and Computational Chemistry, Shaanxi Key Laboratory of Catalysis, School of Chemical & Environment Sciences, Shaanxi University of Technology, Hanzhong 723000, China

³Skolkovo Institute of Science and Technology, 3 Nobel St., 143026 Moscow, Russia.

⁴Department of Geosciences, Stony Brook University, Stony Brook, New York 11794, USA

⁵International Center for Materials Discovery, Northwestern Polytechnical University, Xi'an 710072, China

⁶School of Electronic Engineering, Xidian University, Xi'an, Shaanxi, 710071, China

E-mail: yuxiaohu950203@126.com.

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$$F(\text{M}_m\text{O}_n) = E(\text{M}_m\text{O}_n) - mE(\text{M}) - 1/2nE(\text{O}_2)$$

Average formation energy:

$$\Delta F(\text{M}_m\text{O}_n) = F(\text{M}_m\text{O}_n)/(m+n)$$

Total oxygen binding energy:

$$\Delta E_n = E(\text{M}_m\text{O}_n) - E(\text{M}_m) - 1/2nE(\text{O}_2)$$

Stepwise oxygen binding energy:

$$\Delta \Delta E = \Delta E_n - \Delta E_{n-1}$$

Average oxygen binding energy:

$$\Delta E = \Delta E_n/n$$

Table S1. The effect of different methods on Fe magnetic moments of Fe₄O_n (n = 1-14) clusters.

	DFT+U (U = 4 eV)				Hybrid functional (HSE06)			
	Fe ₁	Fe ₂	Fe ₃	Fe ₄	Fe ₁	Fe ₂	Fe ₃	Fe ₄
Fe ₄ O ₁	3.42	3.45	3.45	-3.48	3.6	3.54	3.54	-3.51
Fe ₄ O ₂	3.39	3.64	-3.52	-3.5	3.56	3.55	-3.56	-3.54
Fe ₄ O ₃	3.58	-3.48	3.44	-3.73	3.61	-3.47	3.47	-3.57
Fe ₄ O ₄	3.48	-3.54	-3.48	3.54	3.48	-3.48	3.48	-3.48
Fe ₄ O ₅	3.97	-3.54	-3.97	3.54	3.99	-3.58	-3.99	3.58
Fe ₄ O ₆	3.95	3.95	-3.95	-3.95	3.97	3.97	-3.97	-3.97
Fe ₄ O ₇	2.68	3.93	-3.94	-3.95	2.64	3.93	-3.96	-3.97
Fe ₄ O ₈	4.02	-3.92	-3.5	4.03	4.03	-3.95	-3.49	4.04
Fe ₄ O ₉	3.9	4	-2.69	-3.98	3.79	4.01	-2.69	-3.98
Fe ₄ O ₁₀	4.05	-3.91	4.04	-4.89	4.06	-3.93	4.05	-3.88
Fe ₄ O ₁₁	4.06	-4.07	3.94	-3.47	4.03	-4.09	3.98	-3.27
Fe ₄ O ₁₂	3.09	-3.59	3.97	-3.67	2.05	-3.64	3.91	-3.55
Fe ₄ O ₁₃	-1.62	3.89	-3.68	-3.65	1.72	3.89	-3.5	-3.49
Fe ₄ O ₁₄	3.52	3.55	-3.65	-3.58	3.56	3.52	-3.54	-3.45

Table S2. The effect of different methods on Ce magnetic moments of Ce_4O_n ($n = 1-14$) clusters.

	DFT+U (U = 5 eV)				Hybrid functional (HSE06)			
	Ce ₁	Ce ₂	Ce ₃	Ce ₄	Ce ₁	Ce ₂	Ce ₃	Ce ₄
Ce ₄ O ₁	1.37	1.03	1.37	0.96	0.44	1.03	0.54	0.25
Ce ₄ O ₂	1.06	1.02	1.53	1.06	0.76	0.72	0.43	1.01
Ce ₄ O ₃	1.28	1.29	0.96	1.28	0.92	1.08	0.01	1.07
Ce ₄ O ₄	0.98	0.98	0.98	0.98	0.99	0.99	0.99	0.99
Ce ₄ O ₅	0.99	0.97	0.99	0.98	0.99	0.97	0.98	0.98
Ce ₄ O ₆	0.98	0.98	0.98	0.98	0.97	0.97	0.98	0.98
Ce ₄ O ₇	0.01	0.98	0.01	0.98	0	0.97	0	0.97
Ce ₄ O ₈	0.01	0.01	0	0	0.01	0.22	0	0
Ce ₄ O ₉	-0.92	0	0	0	0.54	0	0.27	0
Ce ₄ O ₁₀	0	0	0	0.95	0	0.26	0.26	0.35
Ce ₄ O ₁₁	0.93	0	0.94	0	0.91	0	0.93	0
Ce ₄ O ₁₂	-0.07	0	0	0.1	0.04	0	0.01	0.04
Ce ₄ O ₁₃	0.01	0	0	0.95	0	0	0	0.77
Ce ₄ O ₁₄	0.11	0.11	0.11	0.11	0.11	0.11	0.37	0.37

Figure S1. The effect of different methods on HOMO-LUMO gaps of Fe_4O_n ($n = 1-14$) clusters.

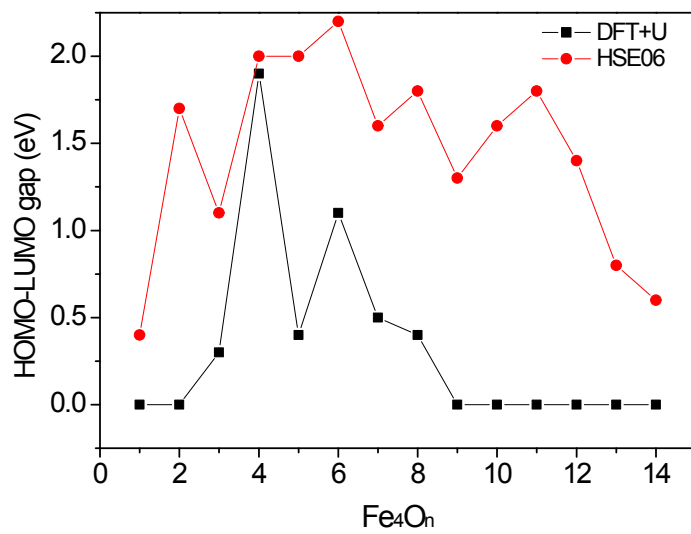


Figure S2. The effect of different methods on HOMO-LUMO gaps of Ce_4O_n ($n = 1-14$) clusters.

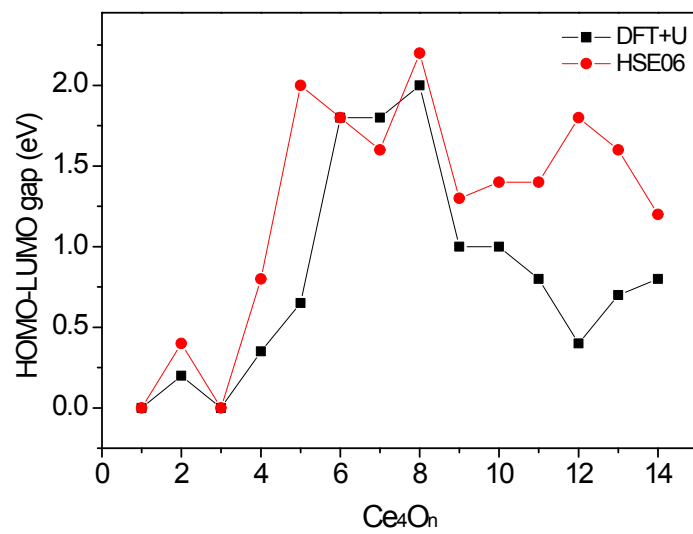


Figure S3. Free energy of formation of the most stable nonstoichiometric (a) Ce_mO_n ($n \neq 2m$) (b) Fe_mO_n ($n \neq m$) clusters, relative to stoichiometric (a) Ce_mO_n ($n = 2m$) (b) Fe_mO_n ($n = m$) clusters at several (T, p_{O_2}) conditions. The label of the horizontal axis shows the amount m of Ce and Fe atoms, and the amount n of O atoms and spin multiplicity M for the nonstoichiometric Ce_mO_n and Fe_mO_n clusters thermodynamically most stable at $p_{\text{O}_2} = 1$ atm and $T = 300$ K. The structures of stoichiometric clusters are also shown as a reference.

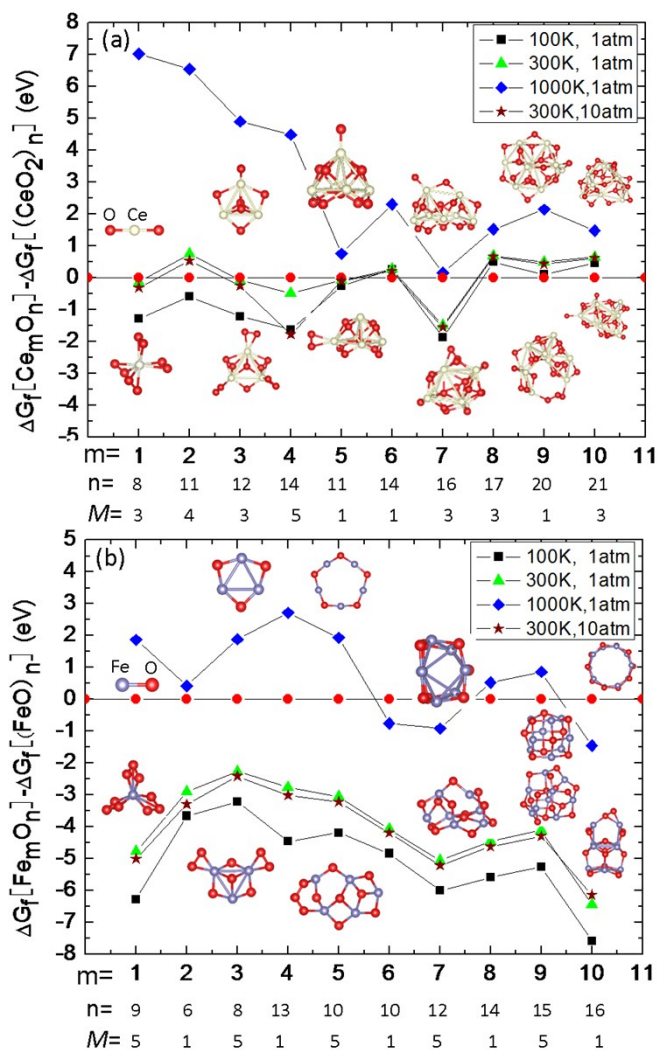


Figure S4. Spin density distribution in Ce_4O_n clusters (cerium in white ball, oxygen in red, spin down in light blue shell, spin up in yellow shell)

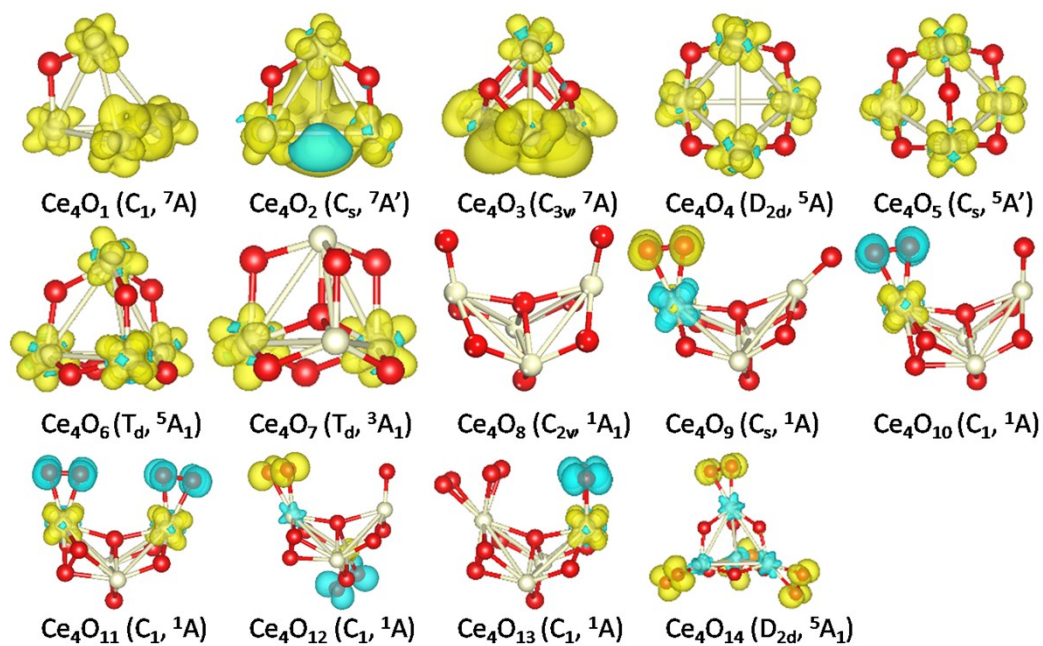


Figure S5. Spin density distribution in Fe_4O_n clusters (iron in blue ball, oxygen in red, spin down in light blue shell, spin up in yellow shell)

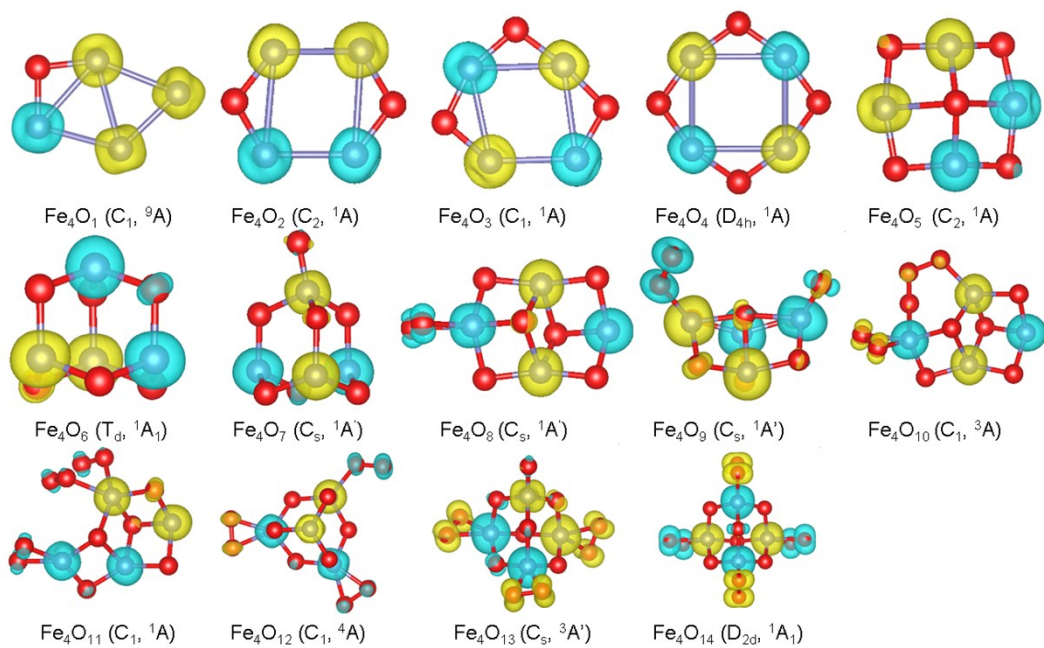


Figure S6. Energy difference between different spin states of Fe_4O_n clusters (iron in blue ball, oxygen in red, spin down in light blue shell, spin up in yellow shell). For Fe_4O_n clusters, ferromagnetic state is defined by four iron atoms with same spin up or spin down, ferrimagnetic state is defined by three iron atom with spin up and one iron atom with spin down, antiferromagnetic state is defined by two iron atoms with spin up and other two iron atoms with spin down.

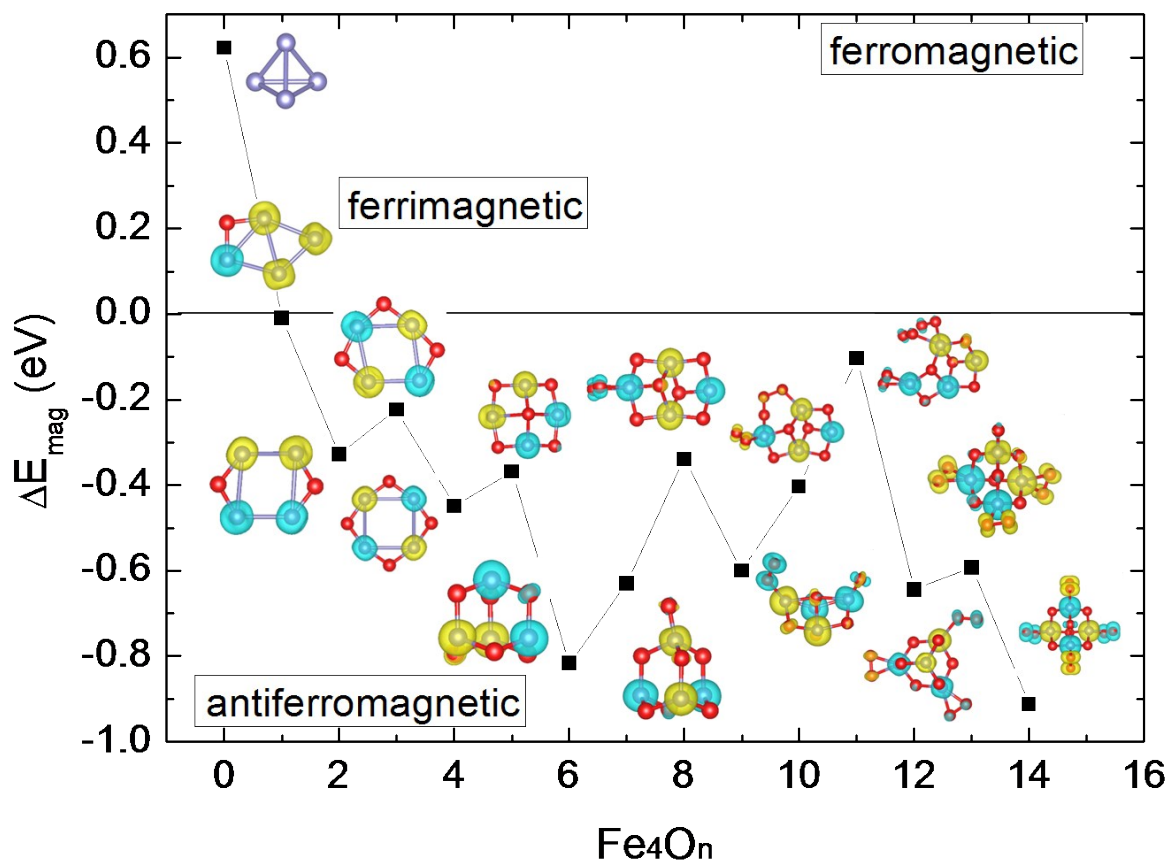


Figure S7. Magic Fe_mO_n clusters

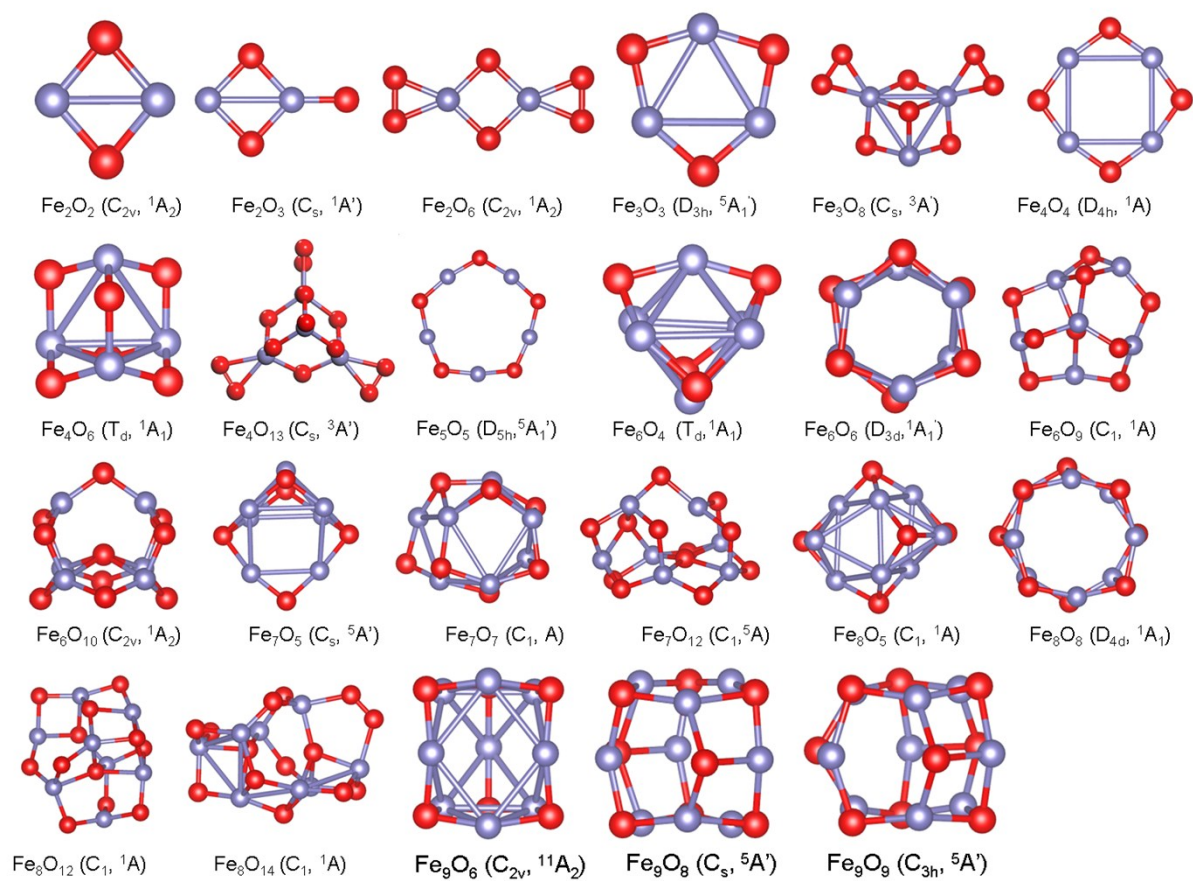


Figure S8. Magic Ce_mO_n clusters

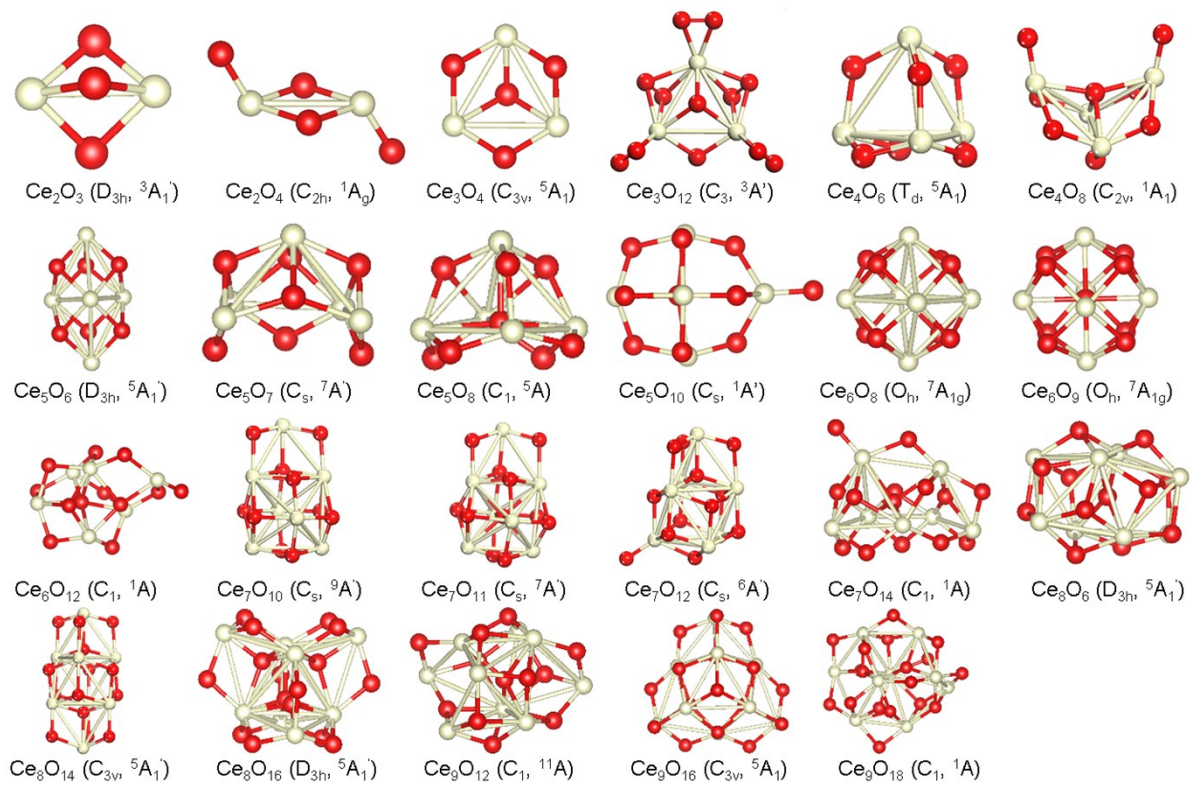


Figure S9. (a) Stepwise oxygen binding energy and (b) average binding energy of Ce_mO_n .

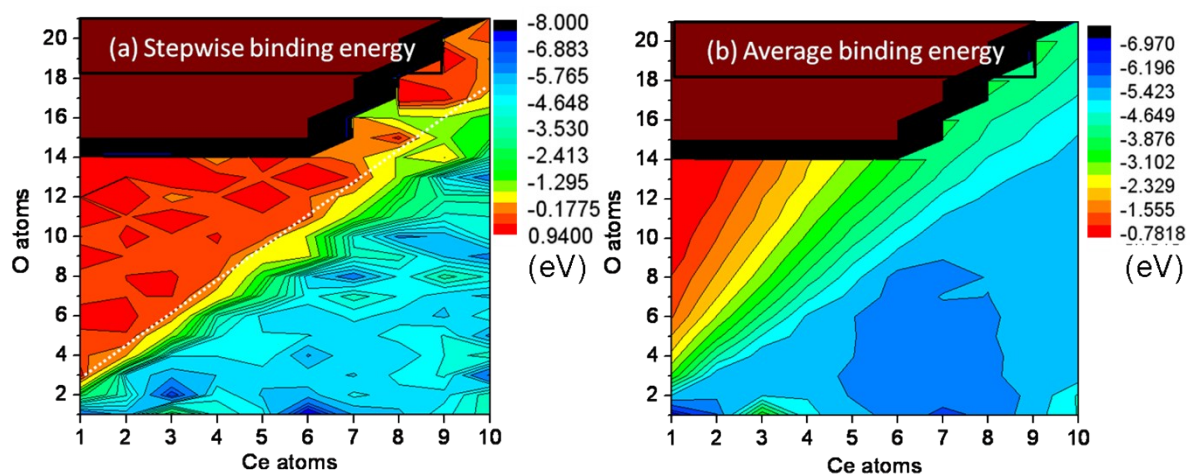


Figure S10. (a) Total formation energy and (b) average formation energy of Ce_mO_n

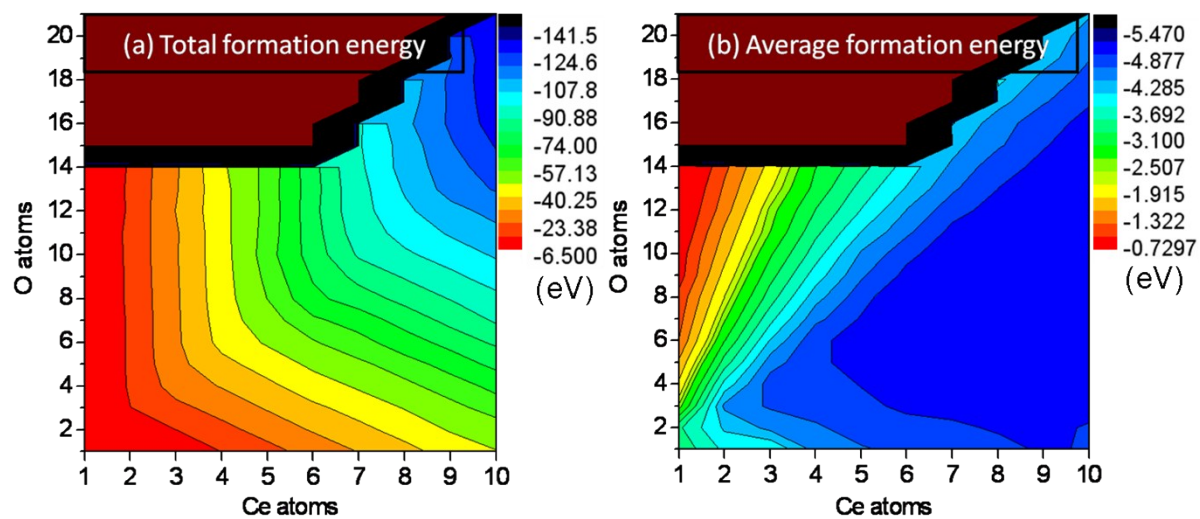


Figure S11. (a) Stepwise oxygen binding energy and (b) average binding energy of Fe_mO_n

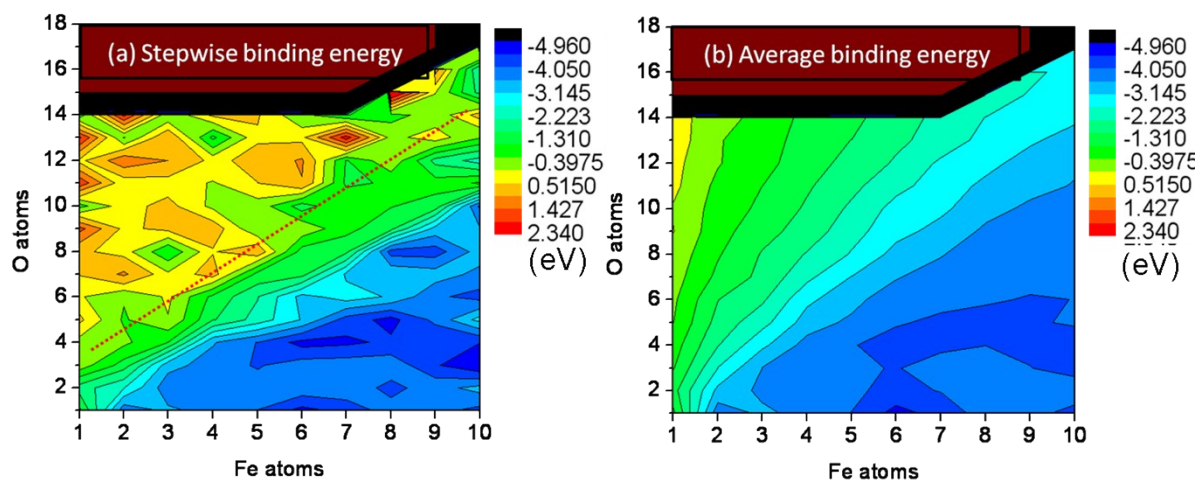
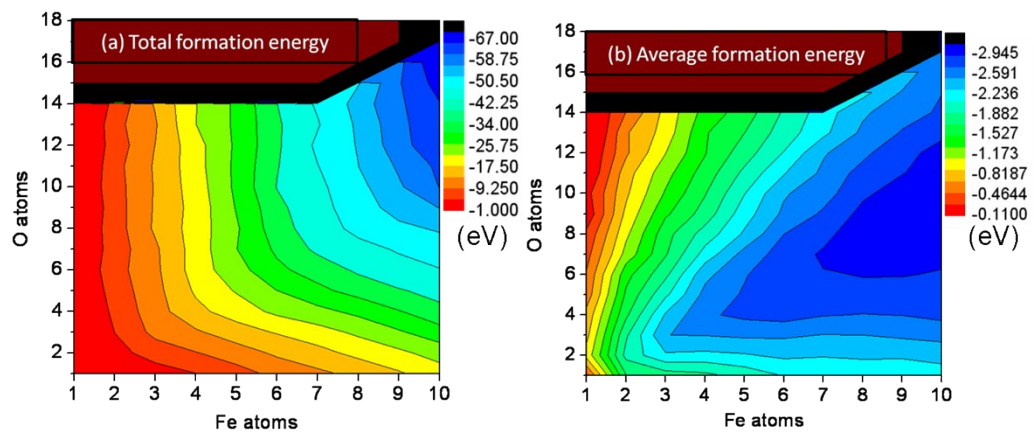


Figure S12. (a) Total formation energy and (b) average formation energy of Fe_mO_n



Coordinate of double magic clusters:

Ce2O3 cluster

Structure_186 Sym.group: 0
1.0000000000000000
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0.0000000000000000 13.269201999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 12.2037270000000007
Ce O
2 3

Direct

0.39207199999999989 0.50189499999999975 0.52687699999999989
0.60721300000000016 0.49766400000000003 0.47271500000000009
0.50414899999999982 0.38408600000000035 0.52558100000000025
0.47095000000000020 0.53740100000000027 0.38356699999999993
0.52561500000000019 0.57895299999999985 0.59125900000000009

Ce2O4 cluster

Structure_27 Sym.group: 0
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0.00000000000000000 13.26345300000000002 0.00000000000000000
0.00000000000000000 0.00000000000000000 11.54277899999999995
Ce O
2 4

Direct

0.3960017252383525 0.4987978931242522 0.4404841262642924
0.6035924016242699 0.4982184701557607 0.5601204052977964
0.7066650762578212 0.5019222303585936 0.4681497004508424
0.2933217633997539 0.5046048141901935 0.5332276357272957
0.5003053221893669 0.5980705765160875 0.4998078851332480
0.5001127112904310 0.3983860156551126 0.4982092471265277

Ce3O4 cluster

Structure_39 Sym.group: 0
1.0000000000000000
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0.00000000000000000 12.83163599999999996 0.00000000000000000
0.00000000000000000 0.00000000000000000 12.47959400000000005
Ce O
3 4

Direct

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0.4599170470942922 0.3526895650182953 0.5135348384507893

0.6389723724431852	0.5366392429445890	0.5174668726266201
0.6001383663452863	0.3892044473801517	0.4483447326667639
0.3583768034819015	0.4637543589769296	0.4505334228652835
0.5407570236035537	0.6453971421268203	0.4454830649843949
0.5000924152173469	0.5001134382927942	0.6090987393520798

Ce3O5 cluster

Structure_2 Sym.group: 0

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0.0000000000000000	12.7728819999999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.3337380000000003

Ce O
3 5

Direct

0.4090180321103481	0.6043217386987615	0.5000000000000000
0.6411540312008649	0.5269156129829251	0.5000000000000000
0.4597341992978893	0.3579110119505273	0.5000000000000000
0.3198583019338883	0.4739751546917138	0.5000000000000000
0.6245092254986880	0.3569164645426255	0.5000000000000000
0.5437868308455479	0.6824028111502826	0.5000000000000000
0.5009701895563888	0.4987786029915784	0.6005400497644269
0.5009701895563888	0.4987786029915784	0.3994599502355731

Ce3O6 cluster

Structure_559 Sym.group: 0

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0.0000000000000000	13.9011479999999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.7129169999999991

Ce O
3 6

Direct

0.5896330441179879	0.3892251015267434	0.5114531665065191
0.3914230502961242	0.4975911355214472	0.4685314257874788
0.5836256712307277	0.6153438463756010	0.5172293546406975
0.4563775595756481	0.6550399765926910	0.4812524006485270
0.6832695771769762	0.5043814418403757	0.5468950860493416
0.5071869307063289	0.4980580190024941	0.5992441421017565
0.2680580742803780	0.4925960863386798	0.5045495227493564
0.4648780253635955	0.3436332342974007	0.4724056714091045
0.5555480672522329	0.5041301585045777	0.3984392301072118

Ce3O12 cluster

Structure_34 Sym.group: 0
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0.0000000000000000 15.8059080000000005 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.1965330000000005
Ce O
3 12

Direct

0.4053950914032529 0.5828763469877632 0.4949409586829414
0.4827787562143133 0.3882190470084044 0.4347194209541307
0.6210113521379946 0.5504554458336891 0.4986697479811855
0.5159801758712791 0.6407104716833202 0.4172478456247298
0.5177187667791161 0.6654197495805935 0.5254588407093163
0.7092356832182124 0.5741195701357135 0.6398229709773837
0.5799284652817813 0.4630229924993360 0.3499973873496720
0.6194071453163323 0.4074644994216761 0.4260720245338794
0.4979160808333812 0.4887637787204221 0.5486818699559436
0.7310793478963266 0.4990241606386369 0.5982410799167256
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0.2688894369753890 0.6362828773478538 0.5203560262019290
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0.4343513635977063 0.2488265096014139 0.4796856829125843
0.3874993540218425 0.4752669331952503 0.4013569556508218

Ce4O6 cluster

Structure_73 Sym.group: 0
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0.0000000000000000 14.7021470000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.2258440000000004
Ce O
4 6

Direct

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0.4389305092484793 0.3828281551963744 0.6025112408449079
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0.3460793182901968 0.4510996757902841 0.4993949209043224
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0.5000000000000000 0.5000000000000000 0.6757756928509695

Ce4O7 cluster

Structure_294 Sym.group: 0
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0.0000000000000000 14.1401699999999995 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.2801399999999994
Ce O
4 7

Direct

0.4262205551826529 0.4133507885049210 0.6082233365480627
0.3975936633978697 0.5932708090485495 0.4208970158363544
0.5737794448173473 0.4133507885049210 0.3917766634519372
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0.5000000000000000 0.6843266383982926 0.5000000000000000
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0.5000000000000000 0.5010159687328697 0.5000000000000000
0.5213452225596146 0.4945372260630648 0.6915673500691514
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0.4786547774403855 0.4945372260630648 0.3084326499308488
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Ce4O8 cluster

Structure_319 Sym.group: 0
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0.0000000000000000 15.6131209999999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.7736040000000006
Ce O
4 8

Direct

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0.6542712114287974 0.5456305920868425 0.4843007162162637
0.4807109350482884 0.4304150828161623 0.3639351313607984
0.5114799112893409 0.4049523905146531 0.6148880431664514
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0.3902527640841336 0.4618100391940184 0.6480281887657783
0.3341956755971514 0.6717774758496442 0.5320660748609217
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0.3550487906444793 0.4825822949178827 0.3849820754331500
0.6082340513924069 0.4798127098238145 0.3460677996758458
0.6400725127368481 0.4529997587079281 0.6092849701940773
0.5001358297156275 0.5165055333408805 0.5011064889843633

Ce5O6 cluster

Structure_300 Sym.group: 0
1.0000000000000000
14.7041170000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.213824999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.6401760000000003
Ce O
5 6

Direct

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0.2976228593913193 0.5003823862929277 0.5000503753354774
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0.4999056405842885 0.4546170358022680 0.6299802299525447
0.4998138977581781 0.6236201058013799 0.4781010233622732
0.6046645960312895 0.5696870341327535 0.5949003487112949
0.6046472342008268 0.5393564566629367 0.3854562750121301
0.6062371909157982 0.3914573751925354 0.5194336868810366
0.3944232600984450 0.3911753635473603 0.5193075610213987
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0.3952095735182607 0.5389180053359771 0.3857120189297525

Ce5O7 cluster

Structure_218 Sym.group: 0
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0.0000000000000000 14.4151609999999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 12.5638539999999992
Ce O
5 7

Direct

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0.6098628550845044 0.3784833900561416 0.4882977266887811
0.3765283751604599 0.3912510719184544 0.4824912370441880
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0.6508086438275072 0.4670324176390592 0.6250552495983163
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0.5082685549822048 0.6439321262707037 0.5249848756601040
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0.6430475372645413 0.5397394367350222 0.4164178661456036
0.3638755040849648 0.5552332053997260 0.4167631257142290
0.4964693686231736 0.4228588853571809 0.3697789988495910

Ce5O8 cluster

Structure_143 Sym.group: 0
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 0.0000000000000000 14.0676039999999993 0.0000000000000000
 0.0000000000000000 0.0000000000000000 14.6388079999999992

Ce O
 5 8

Direct

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 0.3381154711586269 0.4433807747886342 0.4818031483152560
 0.5128135857167277 0.4769724606780215 0.6538048460179434
 0.5479268920511770 0.3392598912584016 0.4398143128769615
 0.6613245910425088 0.5637389255273195 0.4724750126798579
 0.4079181295247552 0.3522968933089504 0.3809080153305638
 0.5091002161235539 0.5077269222305270 0.4824021213205882
 0.5838179769191434 0.6909065697065294 0.4622516142024650
 0.3225010208406069 0.5836696249052087 0.4196360471635804
 0.3893320785366424 0.5681729459693901 0.6153363456433582
 0.4661365470993144 0.3498312100501706 0.5767270009310216
 0.6579558169075839 0.5268918783939145 0.6130450245513377
 0.6771507434141975 0.4331575582331487 0.4058529561724304

Ce5O9 cluster

Structure_289 Sym.group: 0
 1.0000000000000000
 13.3338599999999996 0.0000000000000000 0.0000000000000000
 0.0000000000000000 13.7973140000000001 0.0000000000000000
 0.0000000000000000 0.0000000000000000 14.0012070000000008

Ce O
 5 9

Direct

0.4133315042681125 0.3453697935244304 0.4766441997532931
 0.3467289720793629 0.5794299686022613 0.4750517574313555
 0.5023243234696000 0.5020483840689109 0.6516268019171311
 0.5857477373763140 0.6538580727532814 0.47018444842768261
 0.6524094000109436 0.4197377721974155 0.4729230308541921
 0.4357377354882884 0.6741752600661958 0.3968097314111241
 0.5464339447761405 0.3616529104675737 0.5969135658307523
 0.6465538433868775 0.5413381603122490 0.5937398000305725
 0.6859367137370536 0.5450122191585155 0.3966776270238358
 0.5610918181412097 0.3231654725883031 0.3996676266058738
 0.3112197740998123 0.4521503315918637 0.4029466305606605
 0.3563717009322273 0.4614334806857336 0.5987302546311744
 0.4564904523010860 0.6409896282887206 0.5944423886770059
 0.4996230799329688 0.4996375456945474 0.4736441009961973

Ce5O10 cluster

Structure_314 Sym.group: 0
1.000000000000000
16.2911870000000008 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.7980560000000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 13.2106610000000000
Ce O
5 10

Direct

0.3317605008442607 0.4965962921921017 0.5035448594137145
0.6732782124058225 0.4930312980223114 0.5603497489124777
0.5347581414853474 0.5235947610094068 0.3552526425089466
0.5084127612214258 0.6354086306324657 0.5832479499631871
0.5137844685770735 0.3480692910225726 0.5164118588112236
0.3901127376799857 0.5999884224399935 0.6039326885391396
0.6673526875283076 0.5189832044986383 0.4088349418824085
0.4084291557004463 0.5167987159115738 0.3637062016006534
0.6292684752027178 0.5987733078875759 0.6425212994950779
0.2172871225579094 0.5011789303682951 0.4929483539609284
0.5288986501167422 0.6505285249030144 0.4302047051528720
0.3945643022564779 0.3709639715690986 0.5513452830692680
0.6332640961884023 0.3681287826392416 0.5899726560641479
0.5381985205284733 0.3823023950666595 0.3689816448691425
0.5306281677066137 0.4956534718370586 0.5287441657568220

Ce6O7 cluster

Structure_549 Sym.group: 0
1.000000000000000
14.6205449999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.0429469999999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.7941040000000008
Ce O
6 7

Direct

0.5107755988607345 0.6343093093775619 0.4210456668949210
0.6102876541631050 0.4268128628976298 0.4124610191688247
0.6308914964363098 0.5548868105382563 0.6076991089440323
0.4890686673850542 0.3590392494095772 0.6030741167681737
0.3847116858933591 0.5761030136254445 0.6118340315778314
0.3753533856624683 0.4469054706395857 0.4164945255705781
0.4977872885511179 0.5051717784992574 0.3372644566549358
0.5153133287189848 0.6534779195163526 0.5789236076033312
0.3545985733052830 0.4318306499330801 0.5738225084441341
0.3633331750704870 0.5942195063817176 0.4610517328390659

0.4844318365142549	0.3404304235513756	0.4509958736494430
0.6502131700869439	0.5695096474735328	0.4566508711749230
0.6332351393518882	0.4073033581566355	0.5686794807097998

Ce6O8 cluster

Structure_364 Sym.group: 0

1.0000000000000000		
18.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	18.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	18.0000000000000000

Ce O
6 8

Direct

0.4999157817680238	0.5003495589045222	0.3626994425722269
0.5000842182319762	0.4996504410954777	0.6373005574277733
0.5274825006341591	0.3653005680411471	0.4998444528866988
0.4725174993658408	0.6346994319588529	0.5001555471133012
0.6351874721465015	0.5273263346430516	0.5000275087475037
0.3648125278534986	0.4726736653569484	0.4999724912524963
0.4033842378709332	0.5638064410300722	0.5818213329574676
0.4030598809838151	0.5638834333591428	0.4181536299839613
0.4361637691109105	0.4035030207678023	0.5815908909122863
0.4363446928785444	0.4039366984788826	0.4186158485619054
0.5636553071214555	0.5960633015211173	0.5813841514380947
0.5638362308890894	0.5964969792321975	0.4184091090877209
0.5969401190161850	0.4361165666408571	0.5818463700160386
0.5966157621290669	0.4361935589699278	0.4181786670425322

Ce6O9 cluster

Structure_296 Sym.group: 0

1.0000000000000000		
14.7851440000000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.7755749999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	14.8168220000000002

Ce O
6 9

Direct

0.3634612706543112	0.5936942381121535	0.5001075477618036
0.4062808596592431	0.3637617510023073	0.4999649012588138
0.6365387293456889	0.4063057618878465	0.5001075477618036
0.5937191403407568	0.6362382489976928	0.4999649012588138
0.5000000000000000	0.5000000000000000	0.3358513845069863
0.5000000000000000	0.5000000000000000	0.6641577859798089
0.6433368239143308	0.5271461279575428	0.6027549764813692
0.4728995249646868	0.6434513592554135	0.3973150391076236

0.3566631760856693	0.4728538720424574	0.6027549764813692
0.5271004750353130	0.3565486407445865	0.3973150391076236
0.6438842272520722	0.5267696261333271	0.3975171413339009
0.4731264022335074	0.6434061889974332	0.6024549672371984
0.3561157727479277	0.4732303738666729	0.3975171413339009
0.5268735977664926	0.3565938110025669	0.6024549672371984
0.5000000000000000	0.5000000000000000	0.4997636831517949

Ce6O10 cluster

Structure_490 Sym.group: 0

1.0000000000000000		
16.5376800000000017	0.0000000000000000	0.0000000000000000
0.0000000000000000	13.8861209999999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	13.9391020000000001

Ce O

6	10
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Direct

0.3353858733691566	0.4880143845801029	0.4812769663466590
0.4993303639745104	0.4744317911979773	0.3262333192582572
0.4758859534169353	0.6711947746993833	0.4708886595836084
0.6401077715733996	0.5148870384881908	0.5147404240505300
0.4689372200876458	0.5281582772204410	0.6705916779681023
0.4918992855603178	0.3353749347062535	0.5252015195972025
0.5841910390123355	0.3783817955902762	0.4227801001732427
0.3948074500353421	0.5801897842775235	0.3627078757874574
0.5771034555350013	0.5970816702865861	0.3834480230963367
0.5579552948298205	0.6305899743984296	0.5992022109544549
0.5655639592412450	0.4111689580847754	0.6300683770585698
0.3907012389358592	0.3947355853571272	0.6102604928428907
0.4090049392217587	0.3625640430144394	0.4028706128243301
0.4798203758483989	0.4988462959965881	0.4977899554776788
0.7534909656535581	0.5208731029568988	0.5227804201049001
0.3758168137047249	0.6135065891450027	0.5791593648757727

Ce6O11 cluster

Structure_262 Sym.group: 0

1.0000000000000000		
17.8585139999999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.2144589999999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	14.4108900000000002

Ce O

6	11
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Direct

0.4939145644178788	0.4043780814124334	0.6369536019983897
0.5060854355821214	0.5956219185875670	0.3630463980016104

0.4927427246689975	0.6213032156900352	0.5937644006266912
0.5072572753310026	0.3786967843099646	0.4062355993733091
0.3532471595584914	0.4967689861478600	0.4882096086990003
0.6467528404415088	0.5032310138521401	0.5117903913009999
0.5720573831947625	0.5266886040825915	0.6538821776964766
0.4279426168052375	0.4733113959174088	0.3461178223035234
0.5796561956016674	0.6420438099546348	0.4878539789116751
0.4203438043983327	0.3579561900453655	0.5121460210883249
0.2486032331128402	0.4955202675613161	0.4863691729651717
0.7513967668871600	0.5044797324386844	0.5136308270348284
0.5897210802723840	0.4770537259506655	0.3607520993578101
0.4102789197276160	0.5229462740493345	0.6392479006421898
0.4179455050876881	0.6386561052515365	0.4739943017505838
0.5820544949123120	0.3613438947484633	0.5260056982494160
0.5000000000000000	0.5000000000000000	0.5000000000000000

Ce6O12 cluster

Structure_103 Sym.group: 0

1.0000000000000000		
16.8859449999999995	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.2684709999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.5771180000000005

Ce O
6 12

Direct

0.3017008022968746	0.5231784850286033	0.4403649250833324
0.6718791682585694	0.4191259465320505	0.4869796249493584
0.5008068888788731	0.3601777922979835	0.5719115911120063
0.5039150870796373	0.4903048548707214	0.3830696180644371
0.6184722825396202	0.6326614887336792	0.5086753235084192
0.4433874148274598	0.5668001410492945	0.6078389780612498
0.5586181302781241	0.5010112702461740	0.5333605349601938
0.2058161575348212	0.4616667515645438	0.4376464740773813
0.5453535395794971	0.3557093937540805	0.4422993366768773
0.3904830163350197	0.5135284828651636	0.3342532867529230
0.6375891022642083	0.4872308244659428	0.3760756598168735
0.6261002840587641	0.3467100738438052	0.5922310178123389
0.4134507384566445	0.4565945703039545	0.5019325653102752
0.7139525026789723	0.5456403585554970	0.5312749710959415
0.4618492797435808	0.4406713764699315	0.6721575989276345
0.3388901456218978	0.6085155631320018	0.5545097086728532
0.5389504652611223	0.6624250535778649	0.6091851459063170
0.5287839943063299	0.6280465727087040	0.4162346392115923

Ce7O10 cluster

Structure_158 Sym.group: 0
 1.0000000000000000
 16.2318530000000010 0.0000000000000000 0.0000000000000000
 0.0000000000000000 16.0629470000000012 0.0000000000000000
 0.0000000000000000 0.0000000000000000 13.1829739999999997
 Ce O
 7 10

Direct

0.5879242744588142 0.4901006703651082 0.6838393824886471
 0.4329357494076329 0.3832967891215601 0.5269072696392898
 0.6517293728159426 0.3889042786855528 0.4569027671369988
 0.6531085661219468 0.6135331620421403 0.4747282973093057
 0.5102498938544814 0.5099600715204821 0.3115647961527404
 0.2580871781409465 0.5029686283525511 0.4562362531639353
 0.4335869181771699 0.6135183555509152 0.5450516055523728
 0.5748059200502899 0.6208891184293241 0.6156495890410729
 0.6906791397526441 0.4958973027851565 0.5627379982372928
 0.5731479939170401 0.3674982256729069 0.5957462761097989
 0.4546210978106174 0.4933010067292873 0.6354932147651929
 0.2925706354895932 0.3892704319785997 0.5254010764505608
 0.5241436971742007 0.3821198480965645 0.3853801732635115
 0.6462028156402574 0.5071766513255880 0.3559901760144323
 0.5250540546460533 0.6287239228159667 0.4050911417235047
 0.2935656524588584 0.6084928932965777 0.5421920618580638
 0.3975870400835046 0.5043486432317189 0.4210879210932796

Ce7O12 cluster

Structure_352 Sym.group: 0
 1.0000000000000000
 17.0291810000000012 0.0000000000000000 0.0000000000000000
 0.0000000000000000 14.4387869999999996 0.0000000000000000
 0.0000000000000000 0.0000000000000000 14.7189599999999992
 Ce O
 7 11

Direct

0.4405516687835807 0.6290082331577712 0.5200919231333649
 0.6373793768427518 0.3768263525276902 0.4801018244443201
 0.4406559640562063 0.3842230103275979 0.5337477746892034
 0.2690596370041490 0.5009924009388574 0.4644824649354127
 0.6403841696052711 0.6161788859140774 0.4683280287082950
 0.5735574691090610 0.5094067104738724 0.6603419528534628
 0.5136140051544089 0.4930869498582051 0.3364962919485381
 0.6459560404000499 0.4882200250682407 0.3653679060304987
 0.4409277762992113 0.5043757060780764 0.6287472112200395
 0.3031921009851408 0.6263846190837834 0.5223538949609131
 0.3137127172779768 0.3780882712197486 0.5353822688018002

0.6835636301465811	0.4981134377715122	0.5672311001573401
0.5153544760864024	0.3458488091384080	0.4099688627213836
0.5555179741013468	0.3540824378689655	0.6072859538137556
0.3949146988956192	0.4979016696323454	0.4195754956520756
0.5402174486967406	0.5001340423268097	0.4969480015925192
0.5668019428552259	0.6539815461687069	0.5954922793319897
0.5246379037002709	0.6431458924453277	0.3880567650050952

Ce7O12 cluster

Structure_81 Sym.group: 0

1.0000000000000000

17.617640999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.617129999999995	0.0000000000000000
0.0000000000000000	0.0000000000000000	14.040635000000000

Ce O

7 12

Direct

0.4637965196327415	0.5471465304864025	0.3546375133670053
0.4150206757139399	0.3701656746873151	0.5271435756685474
0.5916170647554048	0.3677990541882619	0.3902966666434615
0.6002551974053797	0.4059777745564156	0.6418783733285263
0.6507850565832570	0.5791147170877070	0.4733125141281275
0.2976035933695455	0.5566579043205450	0.5037290922473928
0.4764114751085096	0.5862609453639256	0.6141255476581327
0.4188170718758591	0.5129172258101163	0.5009825144668981
0.4658712296721264	0.3963308266616384	0.3741674263647762
0.5432105618255747	0.3190282358346695	0.5330654928179892
0.6645375359780724	0.4310737638162815	0.5059213796489153
0.4763211574277016	0.4442193844263848	0.6561295829249207
0.2901272467679017	0.4273220255182365	0.5300950660658114
0.7356592573303904	0.6517440446290071	0.4559859159692023
0.3601200640382551	0.6263990496119124	0.6176505973077480
0.5247546822914972	0.6294183443475259	0.4749686370767749
0.5983539884693668	0.5538250056327755	0.6312775481624463
0.5933190571388364	0.5067474124184953	0.3455101421949192
0.3334185646156548	0.5878530806023826	0.3691214139584086

Ce7O13 cluster

Structure_148 Sym.group: 0

1.0000000000000000

18.2575970000000005	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.6540740000000014	0.0000000000000000
0.0000000000000000	0.0000000000000000	14.3448429999999991

Ce O

7 13

Direct

0.6293312155958534	0.3671349155082019	0.5037747359739385
0.5112333533720345	0.4852572365180673	0.3729236176238589
0.3721722732981538	0.5866836021883495	0.6029227502037076
0.6564683997966090	0.5583977014343204	0.4947737420458559
0.3249905778623504	0.4537672485656957	0.4220802627212359
0.5347890917827314	0.7196924853168264	0.4842476319051794
0.4608361460131666	0.3970717244438896	0.5868599506685861
0.4407454023871685	0.6928017993068855	0.5627097554674614
0.4258722639610180	0.5059002328492476	0.4883865126535569
0.5652449655253132	0.4843598036228494	0.5426572756660630
0.5643192849934054	0.3274126111719167	0.6133387425899358
0.5586324569588829	0.6100992184280970	0.3994058839935950
0.4036647484827942	0.4690533745696462	0.3097232209388469
0.6334201043301142	0.6732573505599067	0.5529859354104188
0.6335359154932082	0.4597309522604299	0.3818651654495973
0.4192073365323194	0.4814527332324490	0.6805680093618195
0.5166706496155958	0.3665129864525095	0.4374046258195153
0.2816367200286577	0.5456960920498605	0.5023341080837020
0.3563954546776420	0.3627444389998982	0.5137699238282263
0.7108366392929870	0.4529734925209453	0.5472681495948922

Ce7O14 cluster

Structure_220 Sym.group: 0
1.0000000000000000
16.9900340000000014 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.4840969999999984 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.7362219999999997
Ce O
7 14

Direct

0.4980165856349262	0.5284790267130440	0.3497262657378274
0.4489899535921165	0.3139498592039791	0.4844765166307988
0.6761823583095762	0.5748325192040307	0.5280366618172510
0.4697987894111185	0.4893101946208616	0.6483880779850998
0.4676910650708298	0.6709639148697932	0.5223472702527533
0.3266693478629447	0.5160869377427917	0.4802750193538433
0.6349570555143577	0.3925116247109876	0.4744983486521447
0.5988879854307793	0.4767087401807658	0.5873041280277601
0.4781307014327613	0.6164140906617726	0.6577501688052462
0.3466652533983082	0.6472101163881211	0.5017762935074949
0.3743664056886060	0.5193107742278407	0.3428997711878611
0.5180685611066315	0.3954366483485069	0.3936557890781842
0.4969062270436415	0.6534698156158323	0.3806811432790191
0.3476660154281953	0.3755452152847912	0.4626467946985204
0.7410117895729459	0.4661579668202185	0.5095603588886556

~ S29 ~

0.5775971583317073	0.2826657492742083	0.5017435384059070
0.6062755244348498	0.6729257619745402	0.5369496267098705
0.3447087866506795	0.4943150953272708	0.6194201323704019
0.4608411452547876	0.5308480535895918	0.4989089415473386
0.4628444667780552	0.3623259744519922	0.6154212632360634
0.6237218240521840	0.5205309207890628	0.4035328898279603

Ce8O12 cluster

Structure_358 Sym.group: 0
 1.0000000000000000
 16.3907589999999992 0.0000000000000000 0.0000000000000000
 0.0000000000000000 15.1201399999999992 0.0000000000000000
 0.0000000000000000 0.0000000000000000 14.6253860000000007
 Ce O
 8 12

Direct

0.5486343730898273	0.6463648817294182	0.4534832548103304
0.6874087971547972	0.4444407805070741	0.3648782571603968
0.3314896734124463	0.6219580170123119	0.4614162381269741
0.4460852324640301	0.4520400133635042	0.3538517015756086
0.5354533923558732	0.3535505929589702	0.5628578780085739
0.4669122293004044	0.5526181915220129	0.6449607860031153
0.3217638097590217	0.3975006318678877	0.5445438019368404
0.6819163325940434	0.5224018543912301	0.5943775035349448
0.4270146020362842	0.3364733946238398	0.4596697046443493
0.3120866809560616	0.4794612063323380	0.4129571239497135
0.4387576919324173	0.6071361449463005	0.3593322186278751
0.6803911024286429	0.5724512319437235	0.4373213448508462
0.6712782068628141	0.3890769747175254	0.5039226091136245
0.4238396546006863	0.3966136742988732	0.6448067815626858
0.3260761658060901	0.5408593881242522	0.5921010723441054
0.5860087278006704	0.4538449725885631	0.6696700316310896
0.5092837610646480	0.4980437148687474	0.4966813912724237
0.5938123048246335	0.6304043306219504	0.6042420952840426
0.5754514441355150	0.4297790398923705	0.2972189602806316
0.4363358174210945	0.6749809636891071	0.5417052452818252

Ce8O14 cluster

Structure_422 Sym.group: 0
 1.0000000000000000
 18.59227299999999987 0.0000000000000000 0.0000000000000000
 0.0000000000000000 14.4039859999999997 0.0000000000000000
 0.0000000000000000 0.0000000000000000 14.6788380000000007
 Ce O
 8 14

Direct

0.7318355213705714	0.5003054121327131	0.4998605434789181
0.2684110522249765	0.5005326229030191	0.5007176452409225
0.4200186587081207	0.3644727831098378	0.4313525161589375
0.5791609960693644	0.3742589707280006	0.5776933993119281
0.4205347732096992	0.5064483432401017	0.6495978804413368
0.5790230938893767	0.6312884442534399	0.5672361892455052
0.4202742434677284	0.6282356868569732	0.4193991112447937
0.5790270544722633	0.4936089529956751	0.3542469072877681
0.6092797419568631	0.4997169622716816	0.4999178115100971
0.3919547038394279	0.5000749490714228	0.4999796893168348
0.2962047467220355	0.6183490762816561	0.4241774338204506
0.6926155399923912	0.4953573923458265	0.3532263967986655
0.2960332485753969	0.3741675529186940	0.4389781829857823
0.6926585017339369	0.3731120020319350	0.5778512549324479
0.2967212006944937	0.5097759862278610	0.6386157708433181
0.6926209912309707	0.6323935180850716	0.5683165603852335
0.5492783467937720	0.5063750263999128	0.6582554319362837
0.4622207352072886	0.6474377673575301	0.5752823122625306
0.5492638627313858	0.6360891533329994	0.4145466270418642
0.4619131378327654	0.4925970303875327	0.3364633713319089
0.5490003542336447	0.3564106391743675	0.4266202043440165
0.4619484950435219	0.3589917278937411	0.5876647600804703

Ce8O15 cluster

Structure_259 Sym.group: 0
1.0000000000000000
17.2198659999999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 15.9964879999999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.1095599999999995

Ce O
8 15

Direct

0.4414933027627375	0.5912370525846581	0.6138433815870628
0.5199659272381603	0.6335264636700406	0.4085633359663393
0.6976500042433830	0.6059395942118017	0.5202261833685696
0.2733949522624227	0.4869301122822631	0.5365402664593419
0.6194243495617316	0.4623118481672527	0.6418983876769573
0.6040286080266094	0.3841380043444854	0.4157633589702214
0.4075210616103825	0.4669553696821147	0.3573175995949783
0.4409425015489702	0.3625474445774784	0.5706837642733239
0.2853395740388461	0.4660840739522772	0.3989505573679032
0.4606183848694567	0.3570212522228227	0.4188418852533349
0.5673442037335691	0.5796801287322129	0.5512230530836437
0.7058778896474570	0.5777770499041069	0.6505944702555491
0.6420642389199309	0.6719377007193047	0.4160422452531479

~ S31 ~

0.4475512087540955	0.6825940205555937	0.5142982390749775
0.3071268907851712	0.3765878569388196	0.5900757516084011
0.5375384458960030	0.5022063083001503	0.3691039625642595
0.6524977578160958	0.3227790311835189	0.3250729161633266
0.6865371840445866	0.4739847269671541	0.4994655253471877
0.3164334948825542	0.5785746494764401	0.6269083552239860
0.4867786590098308	0.4721237382401963	0.6703547948338999
0.4065962123833001	0.4969847760684999	0.5081293944423204
0.4179216442243101	0.5968388727736487	0.3325379123155116
0.5753555037404045	0.3512379244451655	0.5635646593157650

Ce8O16 cluster

EA109 18.822 20.429 20.429 90.00 90.00

1.0000000000000000

18.822493999999989	0.0000000000000000	0.0000000000000000
0.0000000000000000	20.429497999999988	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.429497999999988

Ce O

8 16

Direct

0.5742559999999983	0.4687950000000001	0.5904870000000031
0.4257440000000017	0.4095129999999969	0.4687950000000001
0.5742559999999983	0.5312049999999999	0.4095129999999969
0.4257440000000017	0.5904870000000031	0.5312049999999999
0.3902629999999974	0.4537679999999966	0.6361059999999981
0.6097370000000026	0.3638940000000019	0.4537679999999966
0.3902629999999974	0.5462320000000034	0.3638940000000019
0.6097370000000026	0.6361059999999981	0.5462320000000034
0.4532979999999966	0.4805350000000033	0.5568570000000008
0.5467020000000034	0.4431429999999992	0.4805350000000033
0.4532979999999966	0.5194649999999967	0.4431429999999992
0.5467020000000034	0.5568570000000008	0.5194649999999967
0.3612699999999975	0.6099019999999982	0.4417809999999989
0.6387300000000025	0.5582190000000011	0.6099019999999982
0.3612699999999975	0.3900980000000018	0.5582190000000011
0.6387300000000025	0.4417809999999989	0.3900980000000018
0.4988999999999990	0.4413010000000028	0.6671479999999974
0.5011000000000010	0.3328520000000026	0.4413010000000028
0.4988999999999990	0.5586989999999972	0.3328520000000026
0.5011000000000010	0.6671479999999974	0.5586989999999972
0.3650340000000014	0.5543029999999973	0.6154900000000012
0.6349659999999986	0.3845099999999988	0.5543029999999973
0.3650340000000014	0.4456970000000027	0.3845099999999988
0.6349659999999986	0.6154900000000012	0.4456970000000027

Ce9O12 cluster

Structure_19 Sym.group: 0
1.0000000000000000
16.7154039999999995 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.3090070000000011 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.7136530000000008

Ce O
9 12

Direct

0.5027721787375481 0.2823194465719007 0.5578421551342584
0.6935581250868136 0.6293261868501990 0.4794735276563456
0.2758960372484572 0.5954767030847375 0.4576144913927854
0.4026941943747374 0.3806243313976447 0.3587500048618261
0.4953036993316800 0.5770182765976997 0.3956144636166696
0.6079826804248364 0.4038605963211548 0.4083255777264777
0.4890448565922327 0.6879116511445657 0.5963394458573958
0.3961505720588339 0.4837424475784197 0.5916872737231661
0.5938470009514510 0.4684569558142078 0.6328276211000807
0.6429225344573893 0.5427985403829239 0.3890571388715406
0.5036408187472382 0.3048262705556279 0.4156178840610584
0.3594871572255602 0.5117555202614470 0.3886489245299432
0.6189169243223839 0.3522783929533005 0.5469374848985910
0.4751537975433482 0.3793794270320339 0.6499680984751163
0.5695648622658412 0.6818425530133606 0.4841151435829560
0.6890364571325843 0.5578219667645740 0.5916183779306616
0.2667665293509235 0.5231427843710672 0.5651495542254645
0.4000207539228228 0.6328356268226359 0.5084122324707591
0.4920238715050975 0.5688326878283892 0.6612882663351239
0.5070904098908945 0.4523365685769545 0.3200103251717728
0.5181225388293424 0.4834140660771455 0.5007010083779939

Ce9O13 cluster

Structure_455 Sym.group: 0
1.0000000000000000
16.6462029999999999 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.3726540000000007 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0536849999999998

Ce O
9 13

Direct

0.4641491736032773 0.7354018196611738 0.4733860196048945
0.4851153443940029 0.5460909193760863 0.6179636074308560
0.4780904230544157 0.3581674048223130 0.4857340167408778
0.2712326660294455 0.3929653216086281 0.5896638045153452
0.3212836243498399 0.5745288706619505 0.4903330754914167
0.6886440338448672 0.5918110006508499 0.4980081348398297

0.5136145810276531	0.5519123268914716	0.3557231801796258
0.6705245074661086	0.4010347383939228	0.3777404259842974
0.6570996319014558	0.4043736866012352	0.6153115938235985
0.2327358418509580	0.4737522518170087	0.4848123096007725
0.4058185098445032	0.6524235401057569	0.3801922526409439
0.3563505802451177	0.3141007091675875	0.5273731810554890
0.5227001748508662	0.4096940235566310	0.6222330034505384
0.4446566874068186	0.5007522646054828	0.4745515056863915
0.4051808047504015	0.6684402788947175	0.5762199629582583
0.6309006278976990	0.5424633299558520	0.6235151031936290
0.5592086233948375	0.6405135542507865	0.4760876417560511
0.6220550765619688	0.3291856104215838	0.4944882938863665
0.7323884893770725	0.4593713453071375	0.5017635992172156
0.3469684412697644	0.5018832608495332	0.6238278490504072
0.6530328062426007	0.5397394491513470	0.3617234879751292
0.5382473506363236	0.4113972932489367	0.3493479509180603

Ce9O16 cluster

Structure_471 Sym.group: 0
 1.0000000000000000
 17.297807999999999 0.0000000000000000 0.0000000000000000
 0.0000000000000000 16.135107999999989 0.0000000000000000
 0.0000000000000000 0.0000000000000000 17.753502999999985

Ce O
 9 16

Direct

0.3514945589515360	0.4965718771046269	0.5635963525194115
0.6087465393936857	0.5052810577948325	0.3742229842985931
0.3926930835816924	0.2777886773756089	0.5629648359810215
0.3887317730413369	0.7162186681019148	0.5735611982183672
0.5791921996942012	0.3586094852243123	0.5302507889501428
0.4258833059416992	0.3894281444913088	0.3916292620521333
0.4241078872485888	0.6140915885468552	0.3989314186045620
0.7360592249203054	0.5010842516943986	0.5338305928199175
0.5777587144369375	0.6416350134477288	0.5370702701691619
0.3252240823532314	0.3658542930185852	0.6137663156630317
0.6975289385727195	0.3816748896801897	0.5697966697277855
0.5135859578788743	0.7384439998132295	0.5894516679125655
0.3704296203448810	0.2734591888366272	0.4495151657400400
0.6051780458019494	0.5009768216551407	0.5107596151560788
0.6967291569457178	0.6174654630415827	0.5754865030949504
0.4826594843581152	0.5048017359629566	0.3325176355585371
0.3499148707945829	0.4996920641791292	0.4343359016996492
0.4527231215003607	0.3988726840939040	0.5257535305417137
0.4513617533628852	0.5984731497565859	0.5306070465705514
0.3666204534785921	0.7264627988132113	0.4604284495339168

0.5642539092905727	0.3705832636710876	0.4091422029053721
0.5631674656269714	0.6367008020825501	0.4162096204972152
0.3213240833505067	0.6238488038097285	0.6182697051747729
0.5170691652611907	0.2577638409706245	0.5784860614191704
0.7375616038688487	0.5042194368332749	0.4194162051913528

Ce9O17 cluster

Structure_61 Sym.group: 0

1.0000000000000000		
15.6465630000000004	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.6465630000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.6465630000000004

Ce O

9 17

Direct

0.6501132510569452	0.4400562040636996	0.6051675914748684
0.3531577501658860	0.5578428025390870	0.4101206035027868
0.5802492942945036	0.5440573780733012	0.3692827063356348
0.2614461573473073	0.3840437994446921	0.5287387096613818
0.4224105336084047	0.5001214352765891	0.6356149098112807
0.6422107944313649	0.6584731755346608	0.5866297811003455
0.4783058867420044	0.3326874298582486	0.4850899477928728
0.6910267306331797	0.3476917103564144	0.4008597220643531
0.4229095029784406	0.7318925211609241	0.5004959727567926
0.3549946073883998	0.2803465577027770	0.4957341443991132
0.6708027490169944	0.4603252203478060	0.3150122999562717
0.3225103822888822	0.7021841775086070	0.4213450364177326
0.5542057510918126	0.5563291244072017	0.6325152868604930
0.5924369767389009	0.4394753594848443	0.4714723649349644
0.3810197534753998	0.6142772493295421	0.5617997726368882
0.3950278842439819	0.4507742107808230	0.5054632698590302
0.4550838304216943	0.4904724558788937	0.3403091344471715
0.3053132989266799	0.4413111770864558	0.6556229064791647
0.7325038981955131	0.3599499488293760	0.5402285853202492
0.6579807448856871	0.6235448098572062	0.4617257748473545
0.5737470820759264	0.2687612141575682	0.4148840099062756
0.5387579311935847	0.7508857058599727	0.5730923500939396
0.4827595050576645	0.6435565492674884	0.4131723888473675
0.5155102980630034	0.3811244172721846	0.6198384053494650
0.2426778039588831	0.4831614699134077	0.4271933476897744
0.7228356017189608	0.5566548960082317	0.6285919774544337

Ce9O18 cluster

Structure_14 Sym.group: 0

1.0000000000000000

16.1337560000000018	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.979113999999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.9813980000000004

Ce O
9 18

Direct

0.4670679934081354	0.5130733914659401	0.6730738443290373
0.4875977967529553	0.5044136317699577	0.3612952467196622
0.2869455138412026	0.5701916082630115	0.4072055897374285
0.6876519281092618	0.3999078755968074	0.3697423997135059
0.5059207026600294	0.3013598167764685	0.4794245317539995
0.4427937090575666	0.6945637488170925	0.5190131532652885
0.3316239412841860	0.3797400023690173	0.5572841077887447
0.6775121926808672	0.4675856423697823	0.6194534999224158
0.6416226569728102	0.6363384154180334	0.4606654390251765
0.5648387299467738	0.3624520648664700	0.3329802614849702
0.3731933021908158	0.5412275566415022	0.2893212141425066
0.3425784258873818	0.4582610703630683	0.6869423834272356
0.5928272866811709	0.4809851925399340	0.7380512159745252
0.4475162661221330	0.6458572226028823	0.6700239992934103
0.7165841377975438	0.5933896523681581	0.5824942584075875
0.4720677553475187	0.3833238457589906	0.6046954914448657
0.4012564896046755	0.5504878209828136	0.5011338413310887
0.4163909422563247	0.3930591086994005	0.4165073118062070
0.6379756822178548	0.5232627261060365	0.3396451007639204
0.5136932063155019	0.6402262832489048	0.3835956723650606
0.5738440141338101	0.7331706808563803	0.5305485416032198
0.3173438437139968	0.6949504366134442	0.4530075724157597
0.6359597509269150	0.3486758749061357	0.5192143612401063
0.7652755253830461	0.4455224248298968	0.4785805612763492
0.2423517671645315	0.4581607066664400	0.4704883555284680
0.3884241584157829	0.2541160601385819	0.5234838445047800
0.5691422811271801	0.5256981389648405	0.5321292007346993

Fe2O2 cluster

Structure_59 Sym.group: 0
1.0000000000000000
12.9868620000000004 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.425648999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.3468420000000005

Fe O
2 2

Direct

0.5022270280186268	0.6043866272847208	0.5013092204963612
0.4977512051928780	0.3949380791275894	0.5013977477819727
0.6092634350216684	0.4973089941936157	0.4986297386141943

0.3907583317668267 0.5033652993940766 0.4986632931074648

Fe2O3 cluster

Structure_10 Sym.group: 0
1.0000000000000000
13.9161750000000008 0.0000000000000000 0.0000000000000000
0.0000000000000000 13.9161750000000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.1965160000000008
Fe O
2 3

Direct

0.5477605351133239 0.4998086036593233 0.4986553831168558
0.3661709212394158 0.5002048446646229 0.5020535805431734
0.4591133376913311 0.4045034492045761 0.4988527282771655
0.6673565098870633 0.5000196824070364 0.5016801336735932
0.4595996960688705 0.5954624200644367 0.4987571743892074

Fe2O6 cluster

Structure_166 Sym.group: 0
1.0000000000000000
16.2243430000000011 0.0000000000000000 0.0000000000000000
0.0000000000000000 12.4991099999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.1374990000000000
Fe O
2 6

Direct

0.5810416904993667 0.5003569650394331 0.5006247144605809
0.4189583095006333 0.4996430349605667 0.4993752855394191
0.4997701459324022 0.6011063061101763 0.4958495132920778
0.5002298540675979 0.3988936938898234 0.5041504867079224
0.6867550801850041 0.5557500459942537 0.5031942196541335
0.3136403926618214 0.5559057835649891 0.5035373142200823
0.6863596073381785 0.4440942164350109 0.4964626857799175
0.3132449198149959 0.4442499540057463 0.4968057803458666

Fe3O3 cluster

Structure_168 Sym.group: 0
1.0000000000000000
13.7988610000000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 13.3596120000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.2005429999999997
Fe O
3 3

Direct

0.4179074776746620	0.4138016450485608	0.4982712740307154
0.4721930351881706	0.6155375161100824	0.5021989488722501
0.6070151508227029	0.4704500701025090	0.4990235473016271
0.3604359965216940	0.5389065998324911	0.4998472466663894
0.6047946730476634	0.6071419364002091	0.4994600199116843
0.5376546667451115	0.3541612325061493	0.5012009632173361

Fe3O4 cluster

Structure_187 Sym.group: 0

1.0000000000000000		
13.2990250000000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	13.1052750000000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	10.7006940000000004

Fe O

3	4
---	---

Direct

0.4738592238369064	0.6096936852244556	0.5047175164838342
0.6060944944590749	0.4707418227327313	0.4908614968458535
0.4173654427734559	0.4216378943738084	0.4835349990562297
0.6135955871007343	0.6015911734955671	0.5464279227466955
0.5300945653093206	0.3660500422462121	0.5592365963073429
0.3576833980736783	0.5346847829358394	0.5477899191237861
0.5013082884468274	0.4956005989913789	0.3674325494362557

Fe3O8 cluster

Structure_117 Sym.group: 0

1.0000000000000000		
16.5468599999999988	0.0000000000000000	0.0000000000000000
0.0000000000000000	13.8280320000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.6214350000000000

Fe O

3	8
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Direct

0.4139144915322070	0.4925671212522910	0.5142631654186034
0.5855221806491139	0.4881104714758066	0.5196428031874665
0.5040829319650411	0.6447922754528157	0.4662382689818798
0.3504552914069254	0.3780407614012763	0.4960957820133766
0.3068391888693803	0.4566890933878167	0.4670656069375159
0.5029916458409454	0.5183618883153599	0.4051129092496060
0.6899816238961007	0.4508649345366694	0.4656685682035006
0.4977788378348417	0.4545942083244549	0.6000541404092429
0.4070357086743934	0.6246787493214015	0.5303427758327911
0.5951362173869997	0.6192414054750474	0.5422365667773010
0.6462618819440519	0.3720590910570609	0.4932784129887255

Fe4O4 cluster

EA229 16.858 16.858 12.978 90.00 90.00

1.0000000000000000

16.8581029999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.8581029999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.9775849999999995

Fe O

4 4

Direct

0.5663456489299897	0.3959475027387624	0.4994565787789471
0.3949126299544267	0.4352846541208468	0.4994124044095584
0.4336543510700106	0.6040524972612377	0.4994565787789471
0.6050873700455733	0.5647153458791531	0.4994124044095584
0.5333883710768004	0.6466613340186029	0.5005969600043072
0.6481535533747746	0.4662762384397051	0.5005340568071873
0.4666116289231996	0.3533386659813972	0.5005969600043072
0.3518464466252254	0.5337237615602947	0.5005340568071873

Fe4O6 cluster

EA98 16.579 16.810 16.612 90.00 90.00

1.0000000000000000

16.5794390000000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.8101200000000013	0.0000000000000000
0.0000000000000000	0.0000000000000000	16.6123350000000016

Fe O

4 6

Direct

0.5644186782559614	0.4381648748720177	0.4372288742679992
0.4355813217440387	0.4381648748720177	0.5627711257320008
0.4355813217440387	0.5618351251279824	0.4372288742679992
0.5644186782559614	0.5618351251279824	0.5627711257320008
0.5000000000000000	0.5000000000000000	0.3730963319572165
0.5000000000000000	0.5000000000000000	0.6269036680427834
0.629799895994656	0.5000000000000000	0.5000000000000000
0.3702000104005345	0.5000000000000000	0.5000000000000000
0.5000000000000000	0.3726461310405669	0.5000000000000000
0.5000000000000000	0.6273538689594331	0.5000000000000000

Fe4O13 cluster

EA174 18.932 18.803 17.976 90.00 90.00

1.0000000000000000

18.9315199999999990	0.0000000000000000	0.0000000000000000
0.0000000000000000	18.8029240000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9762400000000007

Fe O
4 13

Direct

0.4808590986770799	0.4878904419399202	0.6146640771777343
0.5696302058717103	0.5701803281948120	0.4917051720976683
0.5304689037055803	0.4110068314157048	0.4665760067126014
0.4114278714531736	0.5305034539836816	0.4613938134467729
0.4660177260236900	0.4784280607636133	0.7013636021743668
0.6354065275445221	0.6398112837214871	0.4338487124893774
0.6518151656181885	0.6380561092111352	0.5049588549723696
0.5416886765491740	0.3180144238559655	0.4161647237675316
0.3254285270561222	0.5847824324491011	0.4378916634023347
0.3113031296913721	0.5157511144164130	0.4351607323952094
0.5916546985543240	0.3272482107705886	0.4669213392372485
0.4079170366794114	0.5145731749278039	0.5671432389433915
0.5922834185891176	0.4818215910608031	0.4569487087464396
0.4515369529302462	0.4488611300865594	0.4275657004857384
0.5440813309614467	0.5490825526219516	0.5927496381872751
0.4810222838864083	0.5918530091324133	0.4539872423796306
0.5074584462084247	0.4121358514480332	0.5709557733843056

Fe5O5 cluster

Structure_199 Sym.group: 0

1.0000000000000000

18.7103800000000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	18.5905179999999994	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.0000000000000000

Fe O

5 5

Direct

0.4590535504062288	0.3634616966447741	0.5000000000000000
0.6168471409348925	0.4184157952295119	0.5000000000000000
0.6135846400097380	0.5856911331553889	0.5000000000000000
0.4536402809822001	0.6345405219609879	0.5000000000000000
0.3569087192994619	0.4979016263653496	0.5000000000000000
0.3686944723755758	0.4007720962671300	0.5000000000000000
0.5538825427001557	0.3450159307868201	0.5000000000000000
0.6643422412646037	0.5030132025137984	0.5000000000000000
0.5476173425040537	0.6566338075160133	0.5000000000000000
0.3654290695231110	0.5945551895602301	0.5000000000000000

Fe5O7 cluster

EA595 18.655 17.480 14.950 90.00 90.00

1.0000000000000000

18.6552709999999990	0.0000000000000000	0.0000000000000000
---------------------	--------------------	--------------------

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0.0000000000000000	17.480219999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	14.950222999999994

Fe O
5 7

Direct

0.6465127511211632	0.5291835319623210	0.5132767636593536
0.5482959026704646	0.4181639342019211	0.5102539757557119
0.5129328014948507	0.5810296458985856	0.4955655469074008
0.3578700224831081	0.5664093357923188	0.5126940461441204
0.4092375486622933	0.4159443979609139	0.4706253642192159
0.6447811266635161	0.4297347266446264	0.4751565961442077
0.5600860082867621	0.5112059683085448	0.5848946670432618
0.6058496841468030	0.6096712925090075	0.4577536526143515
0.4838971310599797	0.4845371258597558	0.4323128243238754
0.4312501468220687	0.6340138914753771	0.5209606451274554
0.3279384243017241	0.4672970794005324	0.4969079883702078
0.4713484522872740	0.3528080699861049	0.5295979296908451

Fe6O4 cluster

EA604 16.680 16.708 16.166 90.00 90.00

1.0000000000000000		
16.680212999999998	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.708252000000017	0.0000000000000000
0.0000000000000000	0.0000000000000000	16.165673999999992

Fe O
6 4

Direct

0.6121281621563430	0.5292539217965977	0.4961804067090603
0.4703457716174555	0.6119782194118456	0.5008122620999913
0.5004374615560470	0.5021134798910023	0.6088611376635619
0.5296630553355250	0.3881266717444297	0.5048591233605342
0.3879705738868298	0.4702625249799763	0.4983465982410042
0.4994977234262923	0.4981301420295134	0.3911036235249544
0.4043643102730043	0.5573978512983994	0.4210459602966470
0.5593260465546993	0.5965433450593937	0.5761112829944454
0.4414829391500374	0.4064639712702868	0.5805404266486539
0.5947839560437663	0.4397298725185406	0.4221391784611478

Fe6O6 cluster

Structure_48 Sym.group: 0

1.0000000000000000		
12.2996160000000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	12.442403999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.7027850000000004

Fe O

6 6

Direct

0.3737355021311605	0.5749353011590177	0.5765669404406432
0.4988155295701601	0.6299064227404735	0.4108674107807909
0.5057350272626844	0.3649650016933493	0.5829723159553596
0.6266118629682366	0.4245274714465493	0.4239974157798447
0.6206652704526807	0.5781910848962748	0.5728942948278193
0.3725496684009857	0.4241121451840953	0.4327884206637613
0.3520438836428101	0.5756880794273870	0.4136799305914348
0.3589231781047737	0.4210103280235752	0.5941537186354923
0.6449539329151512	0.5773911648188270	0.4095109359034609
0.6489241104118751	0.4262513725136430	0.5863874743750985
0.5002006670277377	0.3324546760443362	0.4243974950086979
0.4968423671117563	0.6705659520524886	0.5717846470376018

Fe6O9 cluster

EA124 18.230 17.475 16.449 90.00 90.00

1.0000000000000000

18.2298049999999989	0.0000000000000000	0.0000000000000000
0.0000000000000000	17.4748820000000009	0.0000000000000000
0.0000000000000000	0.0000000000000000	16.4494569999999989

Fe O

6 9

Direct

0.3690392927578218	0.4370342328514127	0.4994315130169454
0.4963436298992742	0.4743244693140306	0.3796062132780520
0.5092633557804312	0.4237692666067067	0.5994046790965433
0.6368286522966276	0.4546348146936868	0.4893122298248197
0.4281865766092453	0.5952733472972409	0.5171886922032606
0.5625823259593085	0.6047971075449934	0.5108992267255951
0.4911285848159126	0.5739945679950857	0.4191566325303594
0.5860855180011243	0.4332247092654882	0.3962956773825844
0.4112809632670965	0.4247401369634843	0.3996826335628629
0.5001053280047492	0.5271702353758302	0.5745457885218194
0.4200655042058162	0.3838529175559002	0.5768379766022106
0.6023563446116208	0.3975666995929318	0.5746038573746149
0.3432224691247310	0.5372093519675671	0.5195350200309229
0.4923355434048260	0.6754207433081978	0.5400737370454955
0.6511769112614058	0.5569873996674646	0.5034261228039281

Fe6O10 cluster

EA307 16.192 16.299 15.050 90.00 90.00

1.0000000000000000

16.1918679999999995	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.2986770000000014	0.0000000000000000

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0.0000000000000000 0.0000000000000000 15.0502109999999991

Fe O
6 10

Direct

0.5869733943603014	0.4283904238349758	0.5765003706162228
0.5874760832719834	0.4753313846640934	0.3928590140600772
0.5909745284214658	0.6008680315785351	0.5268852991886045
0.4130266056396987	0.4283904238349758	0.5765003706162228
0.4125239167280167	0.4753313846640934	0.3928590140600772
0.4090254715785344	0.6008680315785351	0.5268852991886045
0.5000000000000000	0.3819134954875265	0.6342932759151870
0.5000000000000000	0.4562392118812835	0.3189853211658438
0.5000000000000000	0.6617134046264443	0.5526338324561463
0.3725729379902799	0.5782073962280009	0.4153623000402125
0.3700310513810485	0.5221677048152916	0.6107489379679419
0.3633160709909191	0.3991227816604375	0.4765160805953386
0.6274270620097199	0.5782073962280009	0.4153623000402125
0.6299689486189515	0.5221677048152916	0.6107489379679419
0.6366839290090812	0.3991227816604375	0.4765160805953386
0.5000000000000000	0.4919574424420870	0.4963435655260433

Fe7O5 cluster

EA658 16.501 16.558 17.898 90.00 90.00

1.0000000000000000

16.5009470000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.5576170000000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.8979430000000015

Fe O
7 5

Direct

0.4645869514263939	0.4149333790955976	0.5701073185695206
0.3669609123707868	0.5093773141574814	0.4979834884631602
0.4626549951797002	0.4134711993519165	0.4215022915397577
0.4741840312087869	0.5945873164098038	0.5736669441961453
0.6168470047826891	0.5726705376113923	0.5057644749974657
0.6113218115357636	0.4080905153926949	0.5074907942936974
0.4709690650406181	0.5891016554860300	0.4243152083238349
0.5133217801457155	0.3471028232905591	0.4960134567332259
0.3980210272737192	0.5045310588011513	0.3938556287351233
0.4034104813569513	0.5077968426806250	0.6011636234153287
0.5321623218262463	0.6501031688811063	0.4958804961625059
0.6855596178526292	0.4882361888416437	0.5122562745702345

Fe7O7 cluster

EA749 18.435 16.754 15.956 90.00 90.00

1.0000000000000000

18.4346759999999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	16.7540489999999984	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.9556129999999996

Fe O

7 7

Direct

0.4059691311117991	0.4144452645641872	0.4991610853732930
0.5684513500739344	0.4437418742532963	0.4062345485840798
0.4738595634343364	0.5539613466222696	0.5900415760789429
0.5410308178318812	0.3953966054510232	0.5605358149490137
0.5265997594261977	0.6213591285337325	0.4573606274372334
0.6329162169140834	0.5316177457680270	0.5193313060334452
0.3584125454433720	0.5568988598688520	0.4660003597656408
0.3196715705334374	0.4572693489524177	0.4608894134595333
0.6336438094033391	0.4180567273135880	0.5126814649238041
0.4927877162494332	0.3754986224425502	0.4476708552122466
0.4289754946929217	0.6297739773076066	0.4994165448325781
0.5682202092422756	0.6054911360558486	0.5731364541915019
0.5947834584450467	0.5548401016169527	0.3988106012381681
0.4546783571979351	0.4416512612496503	0.6087283479205152

Fe7O10 cluster

EA320 19.773 18.017 15.736 90.00 90.00

1.0000000000000000

19.7734890000000014	0.0000000000000000	0.0000000000000000
0.0000000000000000	18.0172820000000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.7360509999999998

Fe O

7 10

Direct

0.6565066751108876	0.4508031486434417	0.4816160847253723
0.3907520539283558	0.3901143590055898	0.4974081201050398
0.3524706446000277	0.5555006266140051	0.4828952882807583
0.4699601364700238	0.6083110138127434	0.5322350937750576
0.6022548699495736	0.5770972282483001	0.5133339360710338
0.5176414467292156	0.4050144324152219	0.5419367309473766
0.5059075423510947	0.5041846852897456	0.3982929286758031
0.6794334100515229	0.5284106587981584	0.5501258201805490
0.4394101974224459	0.3669885799229366	0.5918572290376153
0.3249337404403418	0.4597294941642956	0.4870754966451614
0.3815684784465172	0.6108777347962617	0.5723365746547533
0.5196186845318062	0.5144459930414568	0.5497674847514883
0.4683332869216705	0.4045641048337794	0.4298815324659429
0.4312431464647997	0.5727545983573620	0.4177709480854335
0.5497079270973421	0.6605052133255033	0.5217133416738091

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0.6040387261109695 0.5137274258410743 0.4065615601039583
0.6062180333734016 0.3769697028901399 0.5251928298208521

Fe8O5 cluster

EA564 17.980 17.490 16.244 90.00 90.00

1.0000000000000000

17.9799089999999993 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.4900100000000016 0.0000000000000000

0.0000000000000000 0.0000000000000000 16.2442819999999983

Fe O

8 5

Direct

0.4177519800160465 0.4174735666688157 0.4374295828636040

0.5717492562136635 0.4117698859903512 0.4538614607727796

0.6053761415983068 0.5675083804776101 0.4454782593111362

0.4533062565626748 0.5686981204990981 0.4165319027764252

0.3684631507547507 0.5255397792828194 0.5380339084267824

0.6283581004953609 0.4906361345100109 0.5808758726616677

0.5051678947958020 0.5878511370077022 0.5717569599492818

0.4805339099546769 0.4314361703619696 0.5842022163445955

0.3627715729983309 0.5091560470489424 0.4208194352271354

0.4887646053926303 0.3571968519822449 0.4926829922114851

0.6569757215417836 0.4744304527880986 0.4656220822491397

0.4343931392402466 0.5232861133563431 0.6293632887884971

0.5263882704357200 0.6350173600259937 0.4633410384174725

Fe8O8 cluster

EA245 17.851 17.875 17.827 90.00 90.00

1.0000000000000000

17.8510980000000004 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.8752549999999992 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.8268349999999991

Fe O

8 8

Direct

0.6259726287161216 0.4620417776101226 0.4426828014142665

0.5391876183529989 0.6186760089910301 0.4433690648518934

0.4375236280423429 0.6083960557505088 0.5571746570730657

0.6154163582457430 0.5609763748587693 0.5574800637033048

0.5616743502926295 0.3912866971649293 0.5568947302453726

0.4609882151797665 0.3800759741979773 0.4427010496225025

0.3858197837252348 0.4398471778023931 0.5566315899996170

0.3731173060372259 0.5388867907784761 0.4423787821635056

0.6323309392036993 0.5684863557735385 0.4400950634292790

0.4330640876081360 0.6259013230140764 0.4401037783504629

0.5403513446395845	0.6352002318145394	0.5608042814269605
0.6436364234493699	0.4582013892989479	0.5598962338546445
0.5672046110898519	0.3741924730019726	0.4398949659624727
0.4591137635285443	0.3635628639620683	0.5601249259594716
0.3554432882907276	0.5418651061756856	0.5599685779555768
0.3691566535980139	0.4324033998049643	0.4397984339875994

Fe8O10 cluster

EA671 18.121 18.180 17.298 90.00 90.00

1.0000000000000000

18.1209969999999991	0.0000000000000000	0.0000000000000000
0.0000000000000000	18.1798129999999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.2982000000000014

Fe O
8 10

Direct

0.3663394888467699	0.4942749958742110	0.5483499964618652
0.4348666002737807	0.6174139763192279	0.4696324361555683
0.4982918900436825	0.5387801111904591	0.6030937992443443
0.4814528624411942	0.3792445082023819	0.5527329857269361
0.6418658796468032	0.4656343393304926	0.5473447683130319
0.4219974724502676	0.4608560966885582	0.4113415838697759
0.5903223743183309	0.5875626363065107	0.4768822047448548
0.5726133573706889	0.4367923824959862	0.4187321236249184
0.3612597817631069	0.5410726825874330	0.4375341456312070
0.4113793786328170	0.5898330000124260	0.5837346381487882
0.3898980447894148	0.3985732668955699	0.4950377434509040
0.4595447068054713	0.4492022598808887	0.6312700227674519
0.6022518938448983	0.5558565028601123	0.5895075192146854
0.584085388959360	0.3798631411675911	0.5139014326845899
0.5292476441682872	0.6630196097453998	0.4599501968345156
0.6521541546213081	0.5062282411733466	0.4389503278676544
0.5057428146017132	0.5152621288267817	0.4700879961561187
0.4966882664855174	0.4205301204426236	0.3519180791027773

Fe8O12 cluster

Structure_427 Sym.group: 0

1.0000000000000000

14.6833200000000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	15.3921650000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.3921740000000007

Fe O
8 12

Direct

0.3022942798242501	0.4549682995195182	0.2012151963834138
--------------------	--------------------	--------------------

0.3022942798242501	0.2590080083834163	0.2808028784804820
0.3022942798242501	0.3385956334804833	0.4767624566165853
0.3022942798242501	0.5345559246165853	0.3971747745195172
0.5293952618373833	0.2592471201401401	0.2811997669682862
0.5293952618373833	0.4545716900317122	0.2014543231401424
0.5293952618373833	0.5343168128598546	0.3967778850317165
0.5293952618373833	0.3389922429682822	0.4765233298598568
0.5683521602595437	0.5278280342849577	0.2855094753604985
0.5683521602595437	0.3433024123605006	0.2079430257150401
0.5683521602595437	0.2657358987150441	0.3924681766394971
0.5683521602595437	0.4502615216394975	0.4700346272849590
0.2637043506632682	0.2652904865258618	0.3923840777785403
0.2637043506632682	0.3433868292214624	0.2074974555258660
0.2637043506632682	0.5282734464741325	0.2855935742214624
0.2637043506632682	0.4501771047785357	0.4704801974741331
0.4159376454155586	0.2172347159657193	0.2632163498428867
0.4159376454155586	0.3210092868428888	0.5185362720342795
0.4159376454155586	0.5763292170342752	0.4147613031571125
0.4159376454155586	0.4725546461571127	0.1594413809657198

Fe9O6 cluster

EA235 17.000000 17.000000 17.000000 90.

1.0000000000000000

17.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.0000000000000000

Fe O

9 6

Direct

0.5685813998713090	0.3754298702043216	0.5000000000000000
0.3578557685225273	0.5000000000000000	0.5000000000000000
0.5685813998713090	0.6245701297956784	0.5000000000000000
0.4553090206300896	0.4230397562806454	0.6079938920152530
0.4553090206300897	0.5769602437193543	0.6079938920152530
0.5946715639602614	0.5000000000000000	0.5960643258896591
0.4553090206300896	0.4230397562806454	0.3920061079847472
0.5946715639602614	0.5000000000000000	0.4039356741103409
0.4553090206300897	0.5769602437193543	0.3920061079847472
0.3716375710458628	0.5000000000000000	0.3905407977335522
0.5627817690505658	0.6096480072276538	0.3912165461885039
0.5627817690505658	0.3903519927723462	0.3912165461885039
0.5627817690505658	0.3903519927723462	0.6087834538114962
0.5627817690505658	0.6096480072276538	0.6087834538114962
0.3716375710458628	0.5000000000000000	0.6094592022664477

Fe9O9 cluster

EA115 17.030 16.772 15.643 90.00 90.00

1.0000000000000000

17.0296610000000008 0.0000000000000000 0.0000000000000000

0.0000000000000000 16.7724769999999985 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.6425640000000001

Fe O

9 9

Direct

0.4540706846754239 0.5905334421201933 0.3935090189169141

0.4314377450649941 0.4142825759325707 0.3998745451945885

0.5957437480347841 0.4763148654835599 0.3919454656179196

0.4695764939498598 0.6019608473390761 0.6042865376238098

0.4432075430273549 0.4255857316948505 0.6122687997170561

0.5397393592034671 0.3510332885378394 0.5070404634086638

0.6079415568143325 0.4915011519027936 0.6007659129079409

0.6063460542733862 0.6089909133175014 0.4822874781934021

0.3523478353538683 0.5393074066090007 0.5083827758346544

0.5646364446488255 0.5895525981718426 0.3685241128494444

0.3695716069513703 0.5092977318493384 0.3884365633923856

0.5408481357955577 0.3767784722881526 0.3847166022232523

0.5827107123116454 0.6074473605455765 0.6061310340770446

0.3858033228402009 0.5227809309367719 0.6271417410920326

0.5548106811990551 0.3926784198060223 0.6232887991766348

0.4227321529122527 0.3626466179182511 0.5113916813952918

0.6590757342382543 0.5017282254858539 0.4903482261273638

0.4194021887053552 0.6375784200608072 0.4996602422515862

Fe9O12 cluster

EA95 19.083 17.981 17.423 90.00 90.00

1.0000000000000000

19.0826439999999984 0.0000000000000000 0.0000000000000000

0.0000000000000000 17.9813960000000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 17.4232610000000001

Fe O

9 12

Direct

0.3532763393148775 0.5225801225569833 0.4430531060996710

0.4754062998319838 0.4630478139658946 0.6163443858519313

0.6563393717782565 0.4986042284658485 0.4472267893412677

0.5867289053883044 0.5505722408225601 0.5972042283067605

0.4400828971728752 0.6098417413243152 0.5484988195969775

0.5743258252247203 0.6208210459686309 0.4521871017514685

0.4943823365266865 0.4821241431270979 0.3998554015305449

0.4098203638684646 0.3869864698182409 0.5010255147499521

0.5798492329683994 0.3793427444280627 0.5067697261063366

0.6504428393608583	0.5817607170081553	0.5187904711758082
0.4896146960341123	0.5653029176066245	0.6394929311662659
0.3506291235890371	0.6003400956528063	0.5103103745138868
0.5736022925957877	0.4390164426546634	0.5972357486667961
0.4231379224054176	0.3794317101930113	0.6055304069560695
0.5782703271344384	0.5354398729485919	0.3818529266402945
0.6614518590497434	0.3962411038888539	0.4599749830023549
0.3295658564827919	0.4244839188831108	0.4631466292837886
0.4143988696054202	0.5194112400232498	0.3597795484221573
0.4993466900384779	0.3763296069120245	0.4426229385656791
0.5033324899535599	0.6698892238083597	0.5020899683277373
0.4559964616757918	0.4984345999429167	0.5070069999442257