

NiFe-Mixed Metal Porphyrin Aerogels as Oxygen Evolution Reaction Catalysts in Alkaline Electrolysers

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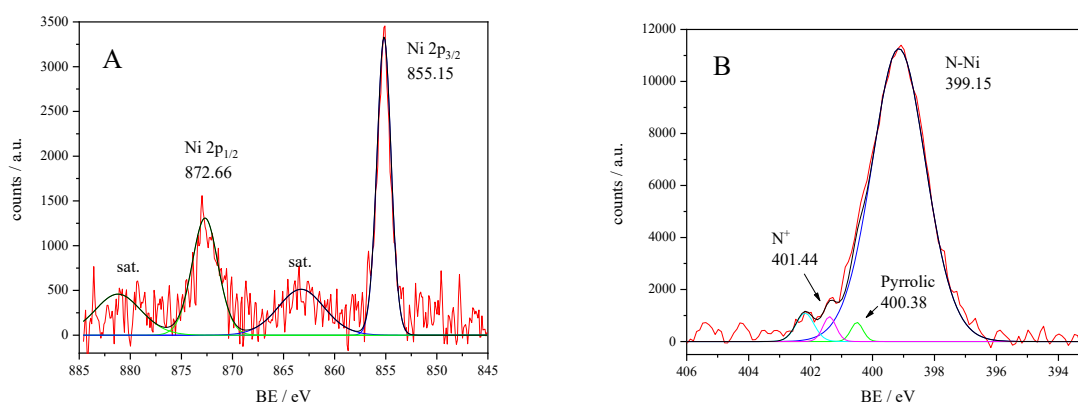


Figure S1: XPS spectra of NiTAPP AG. A: Ni2p, B: N1s

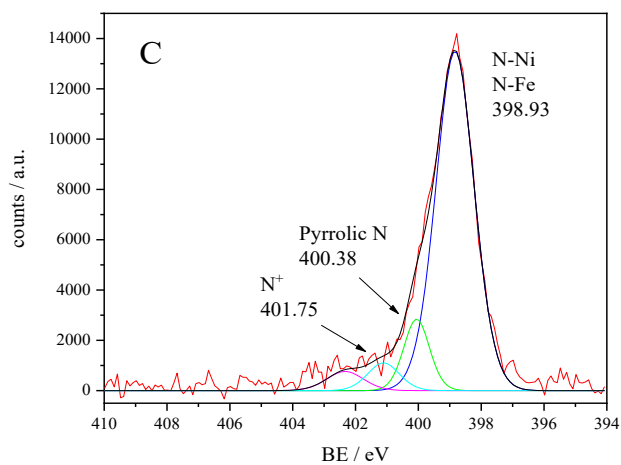
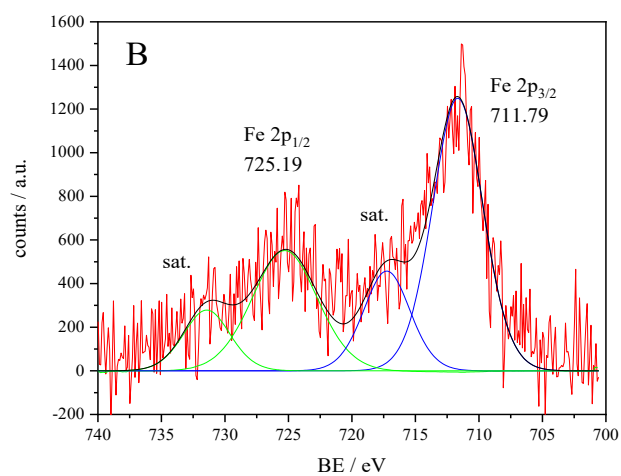
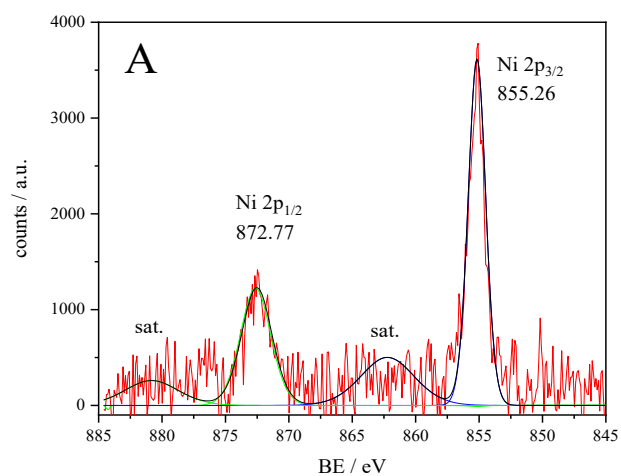


Figure S2: XPS spectra of NiFeTAPP AG 3565. A: Ni2p, B: Fe2p, C: N1s

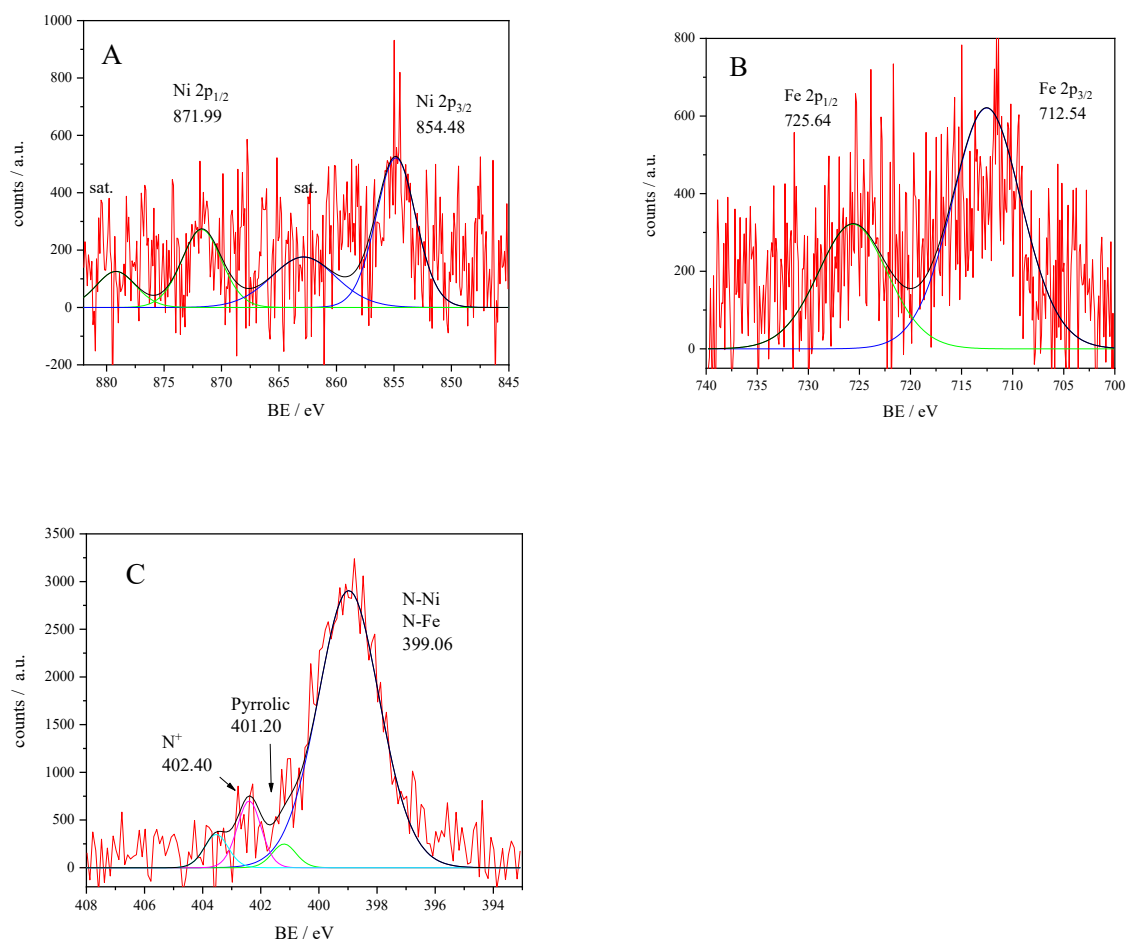


Figure S3: XPS spectra of NiFeTAPP AG 2377. A: Ni2p, B: Fe2p, C: N1s

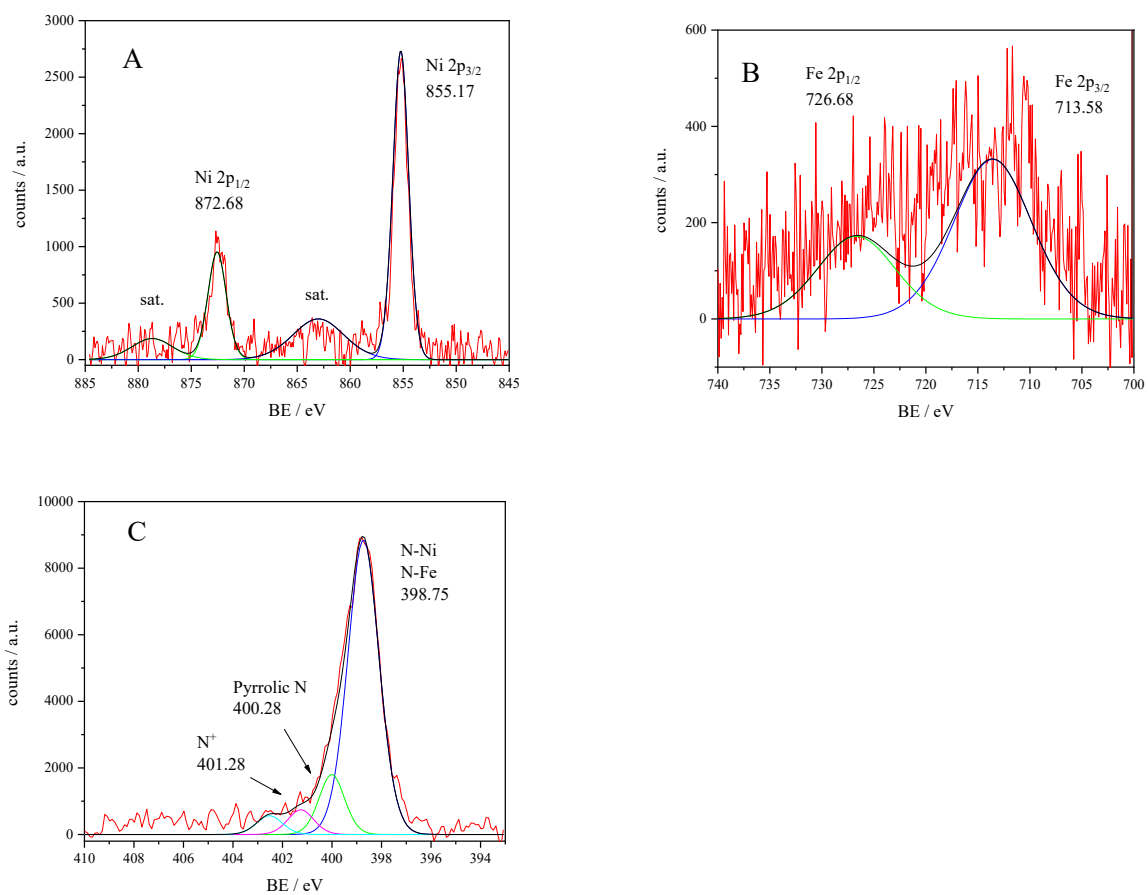


Figure S4: XPS spectra of NiFeTAPP AG 6139. A: Ni2p, B: Fe2p, C: N1s

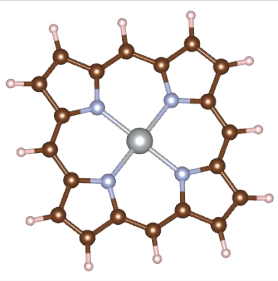
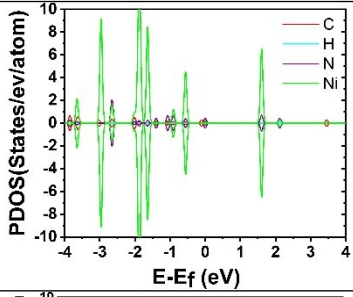
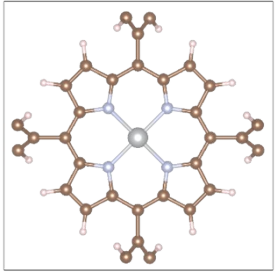
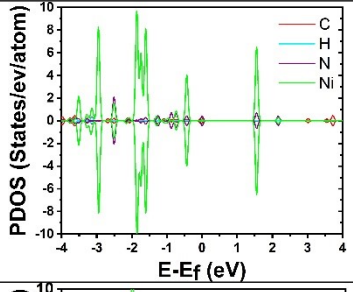
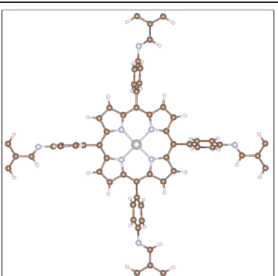
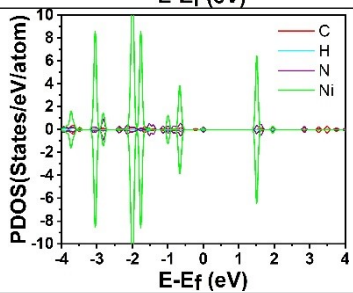
System	Aerogel	PDOS	Mag	Ox
Porphyrin (Ni)			0.00	Ni(+4)
Porphyrin (Ni) with small ligand			0.00	Ni(+4)
Porphyrin (Ni) with big ligand			0.00	Ni(+4)

Figure S5: Unit cell of the aerogel with different size of the ligand and the corresponding PDOS. Mag represents the magnetization value from the OUTCAR and ox is the predicted oxidation state of the metal ions

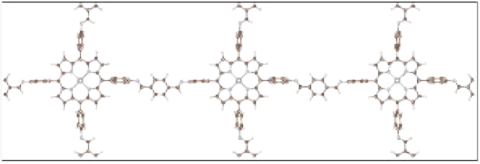
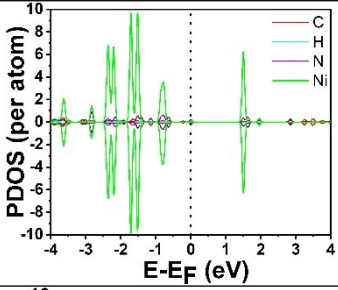
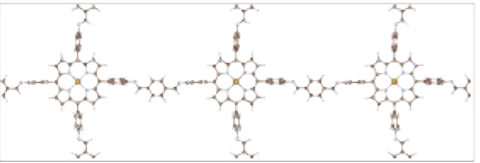
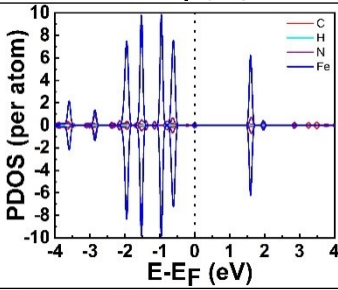
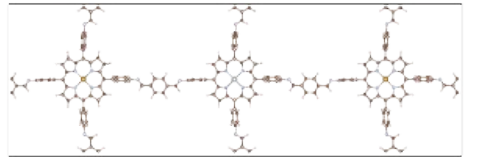
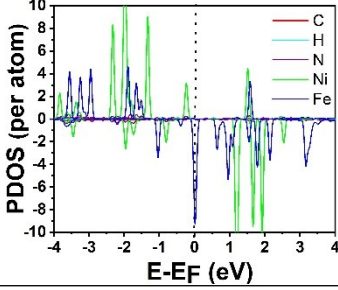
System	Aerogel	PDOS	Mag	Ox
NiTAPP			Ni=0.00	Ni(+4))
FeTAPP			Fe~3.7	Fe(+4))
NiFeTAPP P (33:67)			Ni=3.9 Fe=3.1,3.5	Ni(+4)) Fe(+2))

Figure S6: TAPP with three Ni, three Fe and two Fe and one Ni, respectively. Column 3, 4 and 5 shows the respective PDOS, magnetization value and oxidation state of the metal ions.

Table S1: The Magnetization and the oxidation state of the aerogel-type systems are represented below. System column represents the aerogel type used to study the particular ratio.

System	Magnetization	Oxidation State
Porphyrin (Ni)	0.000	4
Porphyrin (Ni) with small ligand	0.000	4
Porphyrin (Ni) with big ligand	0.000	4
NiTAPP (0 Fe)	0.000	4
FeTAPP (0 Ni)	~3.8	4
NiFeTAPP (33:67)	Ni1=3.945	4
	Fe1=3.189	2
	Fe2=3.519	2
NiFeTAPP (25:75)	Ni1=0.002	4
	Fe1=2.864	5
	Fe2=2.537	5
	Fe3=1.884	6
NiFeTAPP (50:50)	Ni1=0.006	4

	Ni2=0.000	4
	Fe1=2.879	5
	Fe2=2.798	5

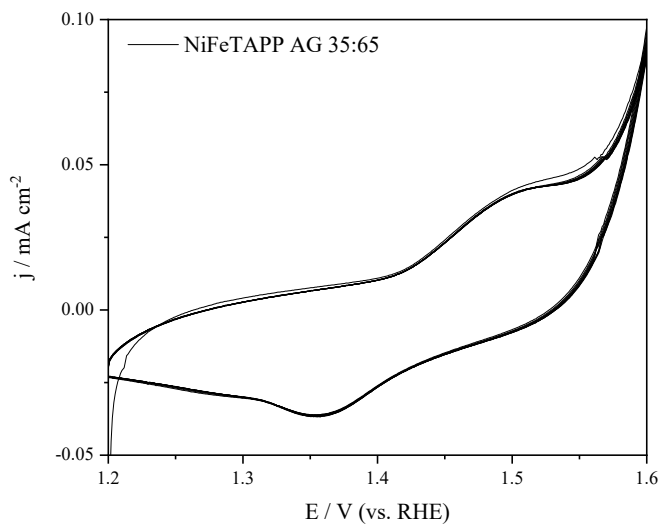


Figure S7: CVs of NiFeTAPP AG 3565 deaerated 1M KOH solution in DI water (scan rate 50 mV/s).

Sample INCAR

ICHARG = 2
 ISTART = 0
 IBRION = 2
 NSW = 0
 ISMEAR = 0
 SIGMA = 0.05
 NSIM= 3
 ISYM = 2
 NPAR = 9
 ALGO = Fast
 PREC = Accurate
 EDIFF = 1e-4
 EDIFFG = -0.03
 NELM=60
 POTIM = 0.5
 MAGMOM = 108*0 24*0 180*0 3*2
 GGA = PE
 ENCUT = 600
 LREAL = .FALSE.
 ISPIN=2
 ISIF=2

LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = -1 -1 -1 2
LDAUU = 0 0 0 4
LDAUJ = 0 0 0 0
LDAUPRINT = 1

OPTIMISED CONTCAR

1. Just Porphyrin Ring

Aerosol

1.0000000000000000
10.4448194504000007 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.4010038375999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.6836090088000013
H N C Ni
12 4 20 1

Direct

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0.8036930386060632 0.1004554050270485 0.0534289698612298
0.5616484980622474 0.0798512219701095 0.0813541087454652
0.3197628994219102 0.0534890864532329 0.1096615896315427
0.1143494167454904 0.2153996829501494 0.1113265346176675
0.0820816480662927 0.4595104577353624 0.0879082961316371
0.0449637648045353 0.7040036382202501 0.0662829923858936
0.1960252576020522 0.8992534536655938 0.0241437231838759
0.4381502417222123 0.9199479645103636 0.9962836092397609
0.6800831577892126 0.9462807365552095 0.9679449539290204
0.8855109911733905 0.7844053828521211 0.9664155093543201
0.9177361609267578 0.5402963425410832 0.9897596875947059
0.6496239417485512 0.3816792495960613 0.0371860464081877
0.3882704998194555 0.3556676062100763 0.0661629574064122
0.3501945105884730 0.6181341455694991 0.0404902345010996
0.6115268038730122 0.6441298285195458 0.0114662990999506
0.7735471211124789 0.4102979843642487 0.0198594865930062
0.8540060316577112 0.2978482593673490 0.0236304845440998
0.7783511613763352 0.2000590570076923 0.0444253827797993
0.6517194324040929 0.2528249479425924 0.0521843748982107
0.5466105242944437 0.1812678496189051 0.0709591422567684
0.4237814095985826 0.2299796200501163 0.0773345286576799
0.3155046074799728 0.1546859456478700 0.0973659960064026
0.2127521169806670 0.2356785731860995 0.0982236613736518
0.2590008587045460 0.3600535025165357 0.0790628897770063
0.1828634364440731 0.4691328816615083 0.0756717291673468
0.2262799263829720 0.5894993809910503 0.0578320974712909
0.1458153322183549 0.7019199197188826 0.0540214191136599
0.2214345789277772 0.7997042366036879 0.0331997026330910
0.3480667155181720 0.7469714609988429 0.0254346115137025
0.4531811233300971 0.8185134621521897 0.0066647601087908
0.5760235556482627 0.7698274449450011 0.0002989470962973
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0.7408073863304523 0.6397361149654799 0.9986018173735545
0.8169688240971027 0.5306655469570813 0.0020052718699475
0.4999119021389262 0.4998830733584469 0.0388220196323417

Energy: -.26005710E+03

2. Small Ligand

Aerosol

1.0000000000000000
13.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 13.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.1562156676999997
H N C Ni
16 4 32 1

Direct

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0.7014581177302475 0.1424867280770670 0.1176649884080021
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0.1478843736232207 0.2883137118956896 0.1197989599352525
0.1479807898765202 0.6965714581828593 0.1174676909959516
0.2942248068832427 0.8424134564409727 0.1177903398802371
0.7015885951260259 0.8423924154884332 0.1187643403336907
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0.9060142333477970 0.4093355859442340 0.0459607309765744
0.9021946757324599 0.5754280905060298 0.1882937016573507
0.5747675261515610 0.8968506641477489 0.0456016514754367
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0.0891998047568237 0.5754164971010880 0.1895664396069847
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0.6073352510412988 0.3828103046493894 0.1142520562505496
0.3880462753960856 0.3828088498780460 0.1177176165792986
0.3880643089733411 0.6020211106787414 0.1212823166463934
0.6073890282991385 0.6020589553861342 0.1177343671334512
0.7136589877254380 0.3974359622342902 0.1147737623299037
0.7649098190175820 0.2992567038454368 0.1159925788486333
0.6907939480252594 0.2251351575825211 0.1158900021095732
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0.3046700214401454 0.2251207498721541 0.1176213692682779
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0.2817194580387437 0.3974288502976506 0.1180732826362885
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0.6908457730497801 0.7597182899307953 0.1178977906818517
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0.4538817004112943 0.9394488073742835 0.1580360098368558
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0.4976951792544142 0.4924227240963006 0.1177501915124779
Energy: -.38211404E+03

3. Unit cell for the aerogels

Aerosol

1.0000000000000000

25.1964473724000015 0.0000000000000000 0.0000000000000000
0.0000000000000000 25.0620765685999984 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.1766090393000006

H N C Ni

36 8 60 1

Direct

0.6745599949210188 0.4018157216954350 0.1395379699178250
0.5987925217514984 0.3255826874867296 0.1444768127373663
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0.3160647722759364 0.3981888620784417 0.1138039264808981
0.3153678937132085 0.6053578416082743 0.0911871878869306
0.3907828592992928 0.6824521110626875 0.0901005666588190
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Energy: -.22190594E+04

6. 3 Ring, 2 Fe, 1 Ni

Aerosol

1.000000000000000

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Energy: -.22298618E+04

7. 4 Ring, 2 Fe, 2 Ni

Aerosol

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H N C Ni Fe

144 32 240 2 2

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Energy: -.29620800E+04

8. 4 Ring, 1 Ni, 3 Fe.

Aerosol

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H N C Ni Fe

144 32 240 1 3

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