

Supporting Information

**GUEST-DEPENDENT SPIN TRANSITIONS IN HOFMANN-LIKE FEII SCO METAL-ORGANIC
FRAMEWORKS: HINTS FROM QUANTUM CHEMISTRY CALCULATIONS**

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Table S1. (a) Selected bond lengths (Å) and cell volume (Å³) for Ni-naph and Ni-nitro in the optimized HSHS, HSLs and LSLs electronic configurations. (b) Selected information for Pd-naph and Pd-nitro. Available experimental data in parentheses.

Table S2. Optimized cell parameters for M-naph and M-nitro, for M=Pd, Ni.

Table S3. . Transition electronic energy (kJ/mol) and zero-point corrections (ZPE) for M-naph and M-nitro systems.

Figure S1. Transition enthalpy and entropy calculated at 298K for all considered systems

Table S4. Optimized coordinates for Pd-nitro, Pd-naph, Ni-nitro and Ni-naph systems

Table S1. Selected bond lengths (Å) and cell volume (Å³) for (a) Ni-naph and Ni-nitro and (b) Pd-naph and Pd-nitro in the optimized HSHS, HSLs and LSLs electronic configurations. Available experimental data in parentheses. Labelling as in Figure 3 in main text.

(a)

	Ni-naph			Ni-nitro		
	HSHS	HSLs	LSLS	HSHS	HSLs model	LSLS
Volume	1592 (1639)	1531 (1575)	1488 (1519)	1554 (1595)	1507	1450 (1473)
Fe ₂ - N _{3,4}	2.06 (2.14)	1.89 (1.94)	1.89 (1.94)	2.09 (2.15)	1.89	1.89 (1.94)
Fe ₂ - N _{11,12}	2.11 (2.15)	1.89 (1.95)	1.90 (1.95)	2.09 (2.15)	1.89	1.89 (1.94)
Fe ₂ - N _{1,2}	2.21 (2.20)	1.96 (2.00)	1.96 (2.00)	2.15 (2.21)	1.96	1.96 (2.00)
Fe ₁ - N _{5,6}	2.06 (2.14)	2.08 (2.14)	1.89 (1.94)	2.09 (2.14)	2.09	1.90 (1.94)
Fe ₁ - N _{7,8}	2.11 (2.14)	2.10 (2.13)	1.90 (1.95)	2.09 (2.14)	2.09	1.90 (1.94)
Fe ₁ - N _{9,10}	2.16 (2.22)	2.17 (2.23)	1.97 (2.00)	2.14 (2.22)	2.14	1.96 (2.00)
Fe ₂ - N aver	2.13 (2.16)	1.91 (1.96)	1.92 (1.96)	2.11 (2.17)	1.91	1.91 (1.96)
Fe ₁ - N aver	2.11 (2.17)	2.12 (2.17)	1.92 (1.96)	2.11 (2.17)	2.11	1.92 (1.96)

(b)

	Pd-naph			Pd-nitro		
	HSHS	HSLs	LSLS	HSHS	HSLs model	LSLS
Volume	1634 (1693)	1588 (1635)	1538 (1568)	1534 (1592)	1521	1489(1517)
Fe ₂ - N _{3,4}	2.09 (2.14)	1.89(1.95)	1.88 (1.94)	2.10 (2.15)	2.09	1.89 (1.93)
Fe ₂ - N _{11,12}	2.11 (2.15)	1.90 (1.94)	1.89 (1.95)	2.10 (2.16)	2.08	1.89 (1.93)
Fe ₂ - N _{1,2}	2.15 (2.2)	1.97 (2.01)	1.96 (2.00)	2.15 (2.19)	2.15	1.96 (1.99)
Fe ₁ - N _{5,6}	2.08 (2.13)	2.10 (2.12)	1.89 (1.93)	2.09 (2.14)	1.89	1.89 (1.93)
Fe ₁ - N _{7,8}	2.12 (2.13)	2.07 (2.13)	1.90 (1.94)	2.10 (2.14)	1.89	1.89 (1.94)
Fe ₁ - N _{9,10}	2.14 (2.22)	2.17 (2.22)	1.97 (2.00)	2.16 (2.21)	1.96	1.96 (1.99)
Fe ₂ - N aver	2.12 (2.16)	1.92 (1.97)	1.91 (1.96)	2.12 (2.17)	2.11	1.91 (1.95)
Fe ₁ - N aver	2.11 (2.16)	2.11 (2.16)	1.92 (1.96)	2.12 (2.16)	1.91	1.91 (1.95)

Table S2. Optimized cell parameters for M-naph and M-nitro, for M=Pd, Ni. In parenthesis, the available experimental data.

	Ni-naph			Ni-nitro		
	HSHS	HSLs	LSLS	HSHS	HSLs model	LSLS
a(Å)	7.40 (7.33)	7.26 (7.82)	7.14 (7.04)	13.42 (14.02)	13.24	13.08 (13.56)
b (Å)	13.49 (14.14)	13.49 (13.93)	13.35 (13.77)	7.50 (7.32)	7.39	7.24 (7.06)
c (Å)	16.41 (16.39)	16.41 (16.47)	16.39 (16.49)	15.56 (5.70)	15.62	15.57 (15.66)
α (°)	77.03 (76.39)	74.84 (74.78)	106.36 (106.95)	90.00 (90.00)	90.00	90.00 (90.00)
β (°)	86.37 (83.50)	80.89 (82.11)	96.30 (96.41)	97.43 (98.41)	99.24	100.18 (100.70)
γ (°)	91.17 (89.94)	90.18 (89.881)	90.23 (90.01)	90.00 (90.00)	90.00	90.00 (90.00)
V (Å ³)	1592 (1639)	1531 (1575)	1488 (1519)	1554 (1595)	1508	1450 (1473)

	Pd-naph			Pd-nitro		
	HSHS	HSLs	LSLS	HSHS	HSLs model	LSLS
a(Å)	7.53 (7.51)	7.42 (7.38)	7.31 (7.23)	7.55 (7.49)	7.42	7.36 (7.23)
b (Å)	13.95 (14.33)	13.73 (14.14)	13.55 (13.94)	13.85 (14.27)	13.58	13.36 (13.80)
c (Å)	15.97 (16.19)	16.27 (16.39)	16.24 (16.33)	14.68 (15.03)	15.18	15.33 (15.43)
α (°)	101.56 (102.72)	75.70 (74.81)	105.68 (106.29)	89.28 (86.07)	83.86	81.55 (80.62)
β (°)	95.85(95.11)	81.46 (82.40)	96.65 (96.50)	80.03 (84.01)	91.50	89.24 (86.87)
γ (°)	90.61 (90.03)	90.08 (89.90)	90.12 (89.90)	88.46 (89.60)	90.94	90.00 (89.87)
V (Å ³)	1634 (1693)	1588 (1635)	1538 (1568)	1534 (1592)	1521	1489(1517)

Table S3. Transition electronic energy (kJ/mol) and zero-point corrections (ZPE) for M-naph and M-nitro systems.

		Pd-nitro 1 step	Pt-nitro 1 step	Ni-nitro 2 steps	Pd-naph 2 steps	Pt-naph 2 steps	Ni-naph 2 steps
ΔE_{elec}	HSLs-LSLS	37.8	37.4	37.1	34.7	33.7	31.1
	HSHS-HSLS	35.8	33.8	36.5	42.5	39.9	35.2
	barycentre	36.8	35.6	36.8	38.6	36.8	33.2
ΔZPE	HSLs-LSLS	-7.73	-6.22	-8.61	-8.27	-6.75	-7.35
	HSHS-HSLS	-7.80	-8.82	-6.28	-8.54	-9.28	-7.42

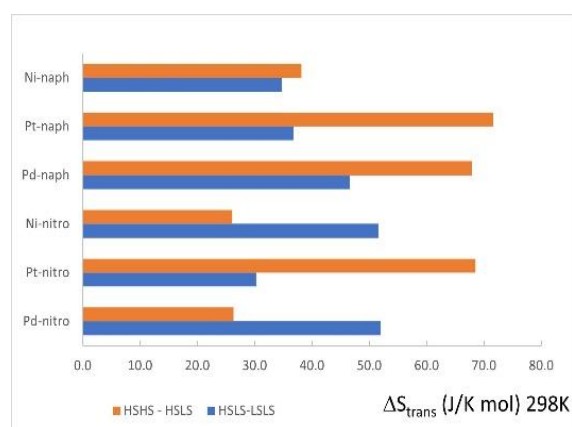
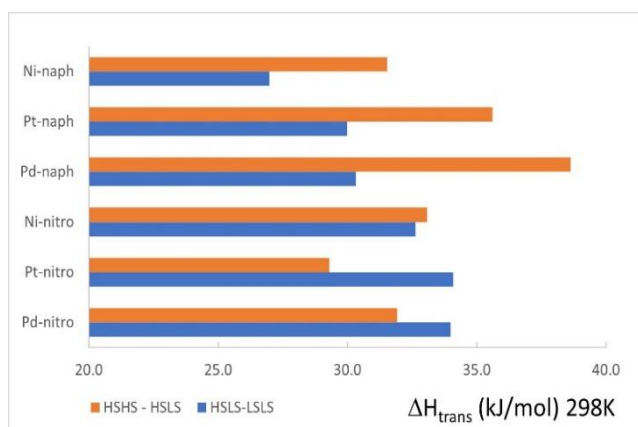


Figure S1. Transition enthalpy and entropy calculated at 298K for all considered systems.

Table S4. Optimized coordinates for Pd-nitro, Pd-naph, Ni-nitro and Ni-naph systems

2NiphNO2 HSHS

1.0000000000000000						
13.4205070581326780	0.0000000000000000	0.0885884002471205				
0.0000000000000000	7.5007842861084724	0.0000000000000000				
-2.1134339764031145	0.0000000000000000	15.4190133842251456				
Fe	N	C	H	Ni	O	
2	16	60	36	2	8	
Direct						
0.0000000000000000	0.0000000000000000	0.0000000000000000				
0.5000000000321023	0.0000000000000000	0.0000000000000000				
0.1024784538671284	0.0000000000000000	0.1183692918699180				
0.8975215162806904	0.0000000000000000	0.8816307304622271				
0.9137987168898576	0.2016680932386876	0.0465875378826723				
0.0862012756590573	0.7983319216848486	0.9534124770461858				
0.0862012756590573	0.2016680932386876	0.9534124770461858				
0.9137987168898576	0.7983319216848486	0.0465875378826723				
0.3900924285330518	0.1991449545962567	0.9955054182484631				
0.6099075714159596	0.8008550155430072	0.0044945817450852				
0.6099075714159596	0.1991449545962567	0.0044945817450852				
0.3900924285330518	0.8008550155430072	0.9955054182484631				
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0.5172476810911064	0.0000000000000000	0.1386996173110759				
0.3494835262377549	0.5000000000204778	0.2841252277599864				
0.6505164737388256	0.5000000000204778	0.7158748020397923				
0.1301766297743256	0.0000000000000000	0.5348188358648329				
0.8698233851556409	0.0000000000000000	0.4651811641287225				
0.2030534220246594	0.0000000000000000	0.1197215637492661				
0.7969466077626279	0.0000000000000000	0.8802784511795849				
0.2685356422460927	0.0000000000000000	0.1964002367127051				
0.7314643577466882	0.0000000000000000	0.8035997334746270				
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0.1432361108300029	0.3213744991686696	0.9572532876787747				
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0.3340145721371073	0.3200068812753472	0.9854376614035942				
0.6659854278394661	0.6799931187656156	0.0145623683961915				
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0.5250813488952417	0.1548346514477785	0.1832953963229400				
0.4749186510537626	0.8451653634757577	0.8167046036706225				
0.4553047239491761	0.1613048205216145	0.7270984862492966				
0.5446952462519477	0.8386951645002299	0.2729015137442730				
0.5446952462519477	0.1613048205216145	0.2729015137442730				

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0.4124756008733499	0.0000000000000000	0.5902597242551906
0.5875243991470072	0.0000000000000000	0.4097402757383719
0.3792788359982140	0.0000000000000000	0.5129636962706101
0.6207211639507904	0.0000000000000000	0.4870363037229595
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0.7608059030114234	0.5000000000204778	0.7235159536227442
0.1846881376502267	0.5000000000204778	0.1936862136944910
0.8153118325946593	0.5000000000204778	0.8063137564928553
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0.9197912108279453	0.5000000000204778	0.8139362795420624
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0.9679520588029575	0.5000000000204778	0.7393080978651980
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0.9121540879990917	0.5000000000204778	0.6568717751260849
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0.8250812290680045	0.1629579610120544	0.3277159771391283
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0.7944034475203878	0.1615882101925550	0.2386606598665608
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0.6108155502870716	0.5000000000204778	0.7842926897611591
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0.8816578139262390	0.1467886442245145	0.5028648606754729
0.1183422010037205	0.8532113706990359	0.4971351393180896

2NiphNO2 HSLs

1.0000000000000000							
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-2.7069581259491242	0.0000000000000000	15.3865804345564001					
Fe	N	C	H	Ni	O		
2	16	60	36	2	8		
Direct							
0.0000000000000000	0.0000000000000000	0.0000000000000000					
0.5000000000147509	0.0000000000000000	0.0000000000000000					
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0.5436860251897642	0.1642005611655577	0.2729839748119787
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Fe N C H Ni
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Direct

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0.4751685276844597	0.8167551143932741	0.2274193918507095
0.4423577429024093	0.2457113707771512	0.8215675080673535
0.5589181251750546	0.7548117012091353	0.1777076232094785
0.3858376806242418	0.3415460288089278	0.7857225484052393
0.6156534012028843	0.6590731766690539	0.2136410504533544
0.4118824956628799	0.3798028011408476	0.6978751975790303
0.5911880113069614	0.6213197221763380	0.3015910562440993
0.4940611505613433	0.3217568708531715	0.6476343295799794
0.5104302011956747	0.6798035313043087	0.3518346024016807
0.8166336996395032	0.9927199905531694	0.1710303131753932
0.1849529508988752	0.0099065206244617	0.8283720488833382
0.8057066215271078	0.8916151985478962	0.3181585026202001
0.1973214370883127	0.1106722407701781	0.6811201472659363
0.1447882222896908	0.6751076394066757	0.2295616440654413
0.8570395611782260	0.3275000942196371	0.7685448552420766
0.1349308455677800	0.7836496230967356	0.0856860678693536
0.8653024694562319	0.2192294536489854	0.9126224344592941
0.7286391198580304	0.4748589273756352	0.8714541964401121
0.2718387544366578	0.5283226485512884	0.1268893126282507
0.7077055753970072	0.5102318836443445	0.7163334520091240
0.2942906859084999	0.4925555144632270	0.2819294324798349
0.2647666398680570	0.6228790581721313	0.6898784107946625

0.7377780850568456	0.3788173105063848	0.3093543072027245
0.2629452839503870	0.5795866914858152	0.8462365016456204
0.7380904320075103	0.4225146855868473	0.1530073371291678
0.6571710155194097	0.1907325690758910	0.5654967341462012
0.3500218635876493	0.8117307088943093	0.4339387770473166
0.7549320816931129	0.0172312160752810	0.6307744027302604
0.2523452529732566	0.9851326092936930	0.3684474637305044
0.7182154648330936	0.9530718360685100	0.7853867252645728
0.2865847935790100	0.0485222381980108	0.2136996653899246
0.5724488898078945	0.0577038719804861	0.8751750558643892
0.4294604051382649	0.9429393765316973	0.1239233926175913
0.4202677782849804	0.2151411576805629	0.8888481941951198
0.5798552810845052	0.7850055368097983	0.1103323091425708
0.3190723066423047	0.3870144409457410	0.8249499884086049
0.6813997692784497	0.6133024059024450	0.1743906194630682
0.3639378279907248	0.4547046912257571	0.6697510919446259
0.6392020019802089	0.5464658630306047	0.3297848508306700
0.5128285470927381	0.3507912191964877	0.5799212515884022
0.4928819531597028	0.6511751200831668	0.4196232361348393
0.9920641973551696	0.0938726056480945	0.5096048751615427
0.0211778766112261	0.9063788980655119	0.4910217113408351
0.3061051821782428	0.1273010177678415	0.5443188587440488
0.7076957114878653	0.8731601238393623	0.4556424797868743
0.5396741079509155	0.2056631660324015	0.4313398940461752
0.4723446507051037	0.7962458001409587	0.5682249071091690
0.4625565015411510	0.2486546573485668	0.2829453559810418
0.5471690099312312	0.7546588695742926	0.7169779558752225
0.2398655237164391	0.2499950877456456	0.1766641175548145
0.7683171470193457	0.7537342464120869	0.8237411605309362
0.9318812738277060	0.2103871523692860	0.1406492858052815
0.0756600679309045	0.7933302209517095	0.8604801423892425
0.6964808387166173	0.1304669759362866	0.2534337882220683
0.3129136907918237	0.8717966982578176	0.7481257112355024
0.7697172049525136	0.0921009873531702	0.4023218308078356
0.2422294015698299	0.9086122093948177	0.5989050003813716
0.4940949920006901	0.2389187420846639	0.0318877204911914
0.5066056291053940	0.7643470960724628	0.9669452870026944

2Ninaph HSLs

1.0000000000000000					
7.2635505097251825	-0.0185591948444922	0.0801032440006658			
-0.0070536494860078	13.4875463487865694	0.0323535482348631			
2.4376497463097175	4.2548539987749594	15.6606145033734343			
Fe	N	C	H	Ni	
2	12	76	48	2	

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000555929	0.5000000000143601	0.0000000000000000
0.9742672148758302	0.9075581504846042	0.1157684378994617
0.0257327850584801	0.0924418495270842	0.8842315621323209
0.1753138668575005	0.0857957552938657	0.0258564745279912
0.8246861332298678	0.9142042148976088	0.9741435515033317
0.8101430456170533	0.3758458847699941	0.0269554355804686
0.1898569542973974	0.6241541152389516	0.9730445755758055
0.2211122616981172	0.3999979628094081	0.9983510535077471

0.7788877679975457	0.6000020074170891	0.0016489420742403
0.0027797859487393	0.5217550940645168	0.8639987601539616
0.9972202140385704	0.4782449059303460	0.1360012547528697
0.7980225774968730	0.0773350712989824	0.0329346436169331
0.2019774224833384	0.9226649436153025	0.9670653861649328
0.9505533002853284	0.9465769039573644	0.1844901252778683
0.0494466996407397	0.0534230848706159	0.8155099045675627
0.9452721193724187	0.8860442808225457	0.2671916368641192
0.0547278807050873	0.1139556968381470	0.7328083333540150
0.9666434162177850	0.7793200700713854	0.2813773632384269
0.0333565838755590	0.2206799299600206	0.7186226367297905
0.9862056182213763	0.7391707140688268	0.2096226750719197
0.0137943818381743	0.2608293157800290	0.7903773100212561
0.9890462337327719	0.8047453357549372	0.1288575952669504
0.0109537662406538	0.1952546940771143	0.8711424047012670
0.9720140451918269	0.7170101920156497	0.3644712545050766
0.0279859548626860	0.2829897781235786	0.6355287455267060
0.9799618601583973	0.6699185317826206	0.4386337525658632
0.0200381398491416	0.3300814682303113	0.5613662175886986
0.2983533205384390	0.1377962433319198	0.0330562178490439
0.7016466496369418	0.8622037417491910	0.9669437858697165
0.6828045563892289	0.3197242342248785	0.0308146160490921
0.3171954436017188	0.6802757657627581	0.9691853634500518
0.3269643202685373	0.3344137724213567	0.0130629766554051
0.6730356796061798	0.6655862276352664	0.9869370010002498
0.6700808770662192	0.1292754953290682	0.0401028030632844
0.3299191228872971	0.8707245344832728	0.9598971969685053
0.8487722226168373	0.5016166107965319	0.8334320203368151
0.1512277773704724	0.4983833891983522	0.1665679945700020
0.8419879112544564	0.5216538830822444	0.7466576136070699
0.1580120887855685	0.4783461169676215	0.2533424161748030
0.0010905444722837	0.5662731431249100	0.6867078142404921
0.9989094554819289	0.4337268569064960	0.3132921857277253
0.1615088321709379	0.5867491829920581	0.7191444033270997
0.8384911678690798	0.4132508170578006	0.2808556264547661
0.1558323999847460	0.5635882103605638	0.8069939576483875
0.8441676000555987	0.4364117896876465	0.1930060274447953
0.9971598788606215	0.5939039861773452	0.5981140454535918
0.0028401211796876	0.4060960138007133	0.4018859843282883
0.9898276343034311	0.6261494010545334	0.5214730143170812
0.0101723656308792	0.3738505989571479	0.4785269857147014
0.0443797747387720	0.1536845222821839	0.3770445024165099
0.9556202253089552	0.8463154627748111	0.6229554678016314
0.0764488656020177	0.1279932553317309	0.4631261335343240
0.9235511344522109	0.8720067148793049	0.5368738664974657
0.2474560162628805	0.1506966014896278	0.4821925223996644
0.7525439837706500	0.8493034134061901	0.5178074775685459
0.3924987263546527	0.2018800213376437	0.4161274121603569
0.6075012735202563	0.7981199638293219	0.5838725878078677
0.3654715846689669	0.2282019350174025	0.3319610164545495
0.6345284152845423	0.7717980947949385	0.6680389835772331
0.1924587586532240	0.2043247488958642	0.3100271394664915
0.8075412413803065	0.7956752659999609	0.6899728605017188
0.1614280966815969	0.2299799972848291	0.2239762269149352
0.8385719033125412	0.7700199878624474	0.7760237731168544
0.9920385225069879	0.2066159717716332	0.2040280130400873
0.0079614773483030	0.7933840133038217	0.7959719869917024
0.8465013001396571	0.1551943665965752	0.2698769887206822

0.1534986997348469 0.8448056482795323 0.7301230113110933
0.8720520605041671 0.1293810771858475 0.3543705565744375
0.1279479395094540 0.8706189376902671 0.6456294434573451
0.5461950488100200 0.2150880331032141 0.6735451881925911
0.4538049512374229 0.7849119520255812 0.3264547820255430
0.5968055388970868 0.1406756519752932 0.6278267157246304
0.4031944611698606 0.8593243628823402 0.3721732544935037
0.6260895924640124 0.0406869184897474 0.6704697918133107
0.3739104074684008 0.9593131001934694 0.3295301783412512
0.6074241023591966 0.0111309878667356 0.7608963110261655
0.3925758976014038 0.9888689841945251 0.2391037038806587
0.5623566732282441 0.0821079153404156 0.8071383956623635
0.4376433268910844 0.9178920995738764 0.1928616341195024
0.5308788593309259 0.1851898853438101 0.7650304053379031
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0.4832125382830412 0.2598038832762199 0.8107663057237033
0.5167874915289374 0.7401961465545881 0.1892337241217348
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0.5519658971678396 0.6412185874089928 0.2311187989395407
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0.5105554982656670 0.3178128921912986 0.6320406505073919
0.4894445017554432 0.6821870779861214 0.3679593792744811
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0.0609743583954057 0.9709108493544250 0.8289342445914087
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0.9992457848733309 0.3425758267535528 0.7828698067210809
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0.9958020425749368 0.2238982584498430 0.9276132494711220
0.7281538348512626 0.4678782259011456 0.8811538958681595
0.2718461650694550 0.5321218038759099 0.1188460892250163
0.7159318955273264 0.5027324719911306 0.7251323566388592
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0.2867420012223079 0.6224444320992362 0.6757830996212917
0.7132579988710290 0.3775555679321627 0.3242169003469257
0.2756928203478068 0.5803638403495199 0.8341560825544292
0.7243071796597391 0.4196361596634048 0.1658438876001398
0.9637023156896873 0.0902019001288252 0.5139147869734302
0.0362976843137872 0.9097981222351166 0.4860852129947872
0.2714332411493814 0.1310422825115793 0.5481685076240552
0.7285667588240443 0.8689577473204722 0.4518314923441693
0.5260276897938070 0.2206413209502003 0.4319202685877244
0.4739723101607041 0.7793586790093840 0.5680797313804860
0.4765471345450862 0.2675808184777893 0.2807344067863511
0.5234528654425432 0.7324191815154535 0.7192655634317831
0.2738682451350556 0.2692195308484031 0.1736088638070044
0.7261317549042587 0.7307804989824049 0.8263911660384267
0.9701865595446648 0.2275156766541144 0.1377518371597830
0.0298134404621706 0.7724843531397525 0.8622481330583369
0.7145448660039335 0.1347795134525782 0.2535205722933398
0.2854551339344411 0.8652204642081003 0.7464793979247943
0.7610499120611678 0.0884294514829733 0.4048854002338942
0.2389500878440884 0.9115705261440823 0.5951145997343303
0.6134559878157262 0.1640236038690119 0.5582323296640226
0.3865440121576995 0.8359764259630467 0.4417676703041877
0.6641872176948524 0.9842442457480800 0.6347258195362286

0.3358127821776193	0.0157557696306867	0.3652741804955610
0.6323663536719764	0.9324806777785852	0.7938700010865176
0.3676336463724041	0.0675192998484704	0.2061299988816998
0.5500681346384582	0.0598211961290218	0.8765444738754624
0.4499318653258939	0.9401787964145498	0.1234555261563344
0.4713378628266227	0.2366600829425920	0.8802232070201867
0.5286621669795721	0.7633399319532259	0.1197767929480307
0.4065780665446752	0.4138509582175871	0.8056589254457833
0.5934219035447654	0.5861490120102602	0.1943410597109505
0.4307459430033020	0.4660005479988527	0.6458291187516068
0.5692540570042368	0.5339994520140792	0.3541708514029622
0.5210511751047022	0.3401593939802225	0.5625501964146835
0.4789488248687235	0.6598406358518218	0.4374498035535268
0.4909533154330390	0.2294212444125847	0.0338602338597056
0.5090467143665123	0.7705787704943958	0.9661397475464923

2Ninaph LSLS

1.0000000000000000		
7.1387826389432805	-0.0133916622167724	0.0121175560757374
-0.0290740227622939	13.3456145945846316	0.0168769565839647
-1.8321513423066271	-4.6386426849151912	15.6110445576935266

Fe	N	C	H	Ni	
2	12	76	48	2	

Direct

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0.0000000000070912	0.4999999999636842	0.0000000000000000
0.9791386278211860	0.9062229263209503	0.8828268078082502
0.0208613722494491	0.0937770587759701	0.1171731921534516
0.8204129516659506	0.9125915424300786	0.0255991664158373
0.1795870484282531	0.0874084650600011	0.9744008336096925
0.0063882370847992	0.5236026549668580	0.1247392506664511
0.9936117629995493	0.4763973747991912	0.8752607492952507
0.8027397650192682	0.5963272127958419	0.0049716777441944
0.1972602349305959	0.4036727872130825	0.9950283222813354
0.8170543454349755	0.3908660591620361	0.9818164070274662
0.1829456546569332	0.6091339408468741	0.0181835929980636
0.2006391091500035	0.9191737214614051	0.0292940559443977
0.7993608907923146	0.0808263083046370	0.9707059440173040
0.9549469115549485	0.9462569358372406	0.8154279850341624
0.0450530884006355	0.0537430827656493	0.1845720149913674
0.9489296836063801	0.8850625848133689	0.7315147520168779
0.0510703163199011	0.1149373928023820	0.2684852479448239
0.9704297981870695	0.7764375629309441	0.7144929520374674
0.0295702017627946	0.2235624370779661	0.2855070479880695
0.9918846547269098	0.7352452525155968	0.7849883837020357
0.0081153453482870	0.2647547474710237	0.2150116162596660
0.9948763676048884	0.8015852245531931	0.8671290944361800
0.0051236324778614	0.1984147456763026	0.1328709055893569
0.9748327983355125	0.7138521519355550	0.6296886682002167
0.0251672017488715	0.2861478779031188	0.3703113317614850
0.9840529184124733	0.6674911535905679	0.5541604921651100
0.0159470816794283	0.3325088464183494	0.4458395078604269
0.6980404742275468	0.8571113752460136	0.0317443018070946
0.3019595258552101	0.1428885949834822	0.9682556982184423
0.6894021377391439	0.3319068821206130	0.9747616587748382

0.3105978622107273	0.6680931178883043	0.0252383412506916
0.6833899487584674	0.6576169445521245	0.0144964054443832
0.3166100511746990	0.3423830554345031	0.9855035945173185
0.3253323702791562	0.8636617163825520	0.0357479510366261
0.6746676296661320	0.1363382687366581	0.9642520489889108
0.8484486957418795	0.5095709362816763	0.1597449556564641
0.1515513041988328	0.4904290339478194	0.8402550443690657
0.8451460312313728	0.5286788686422810	0.2470787853229552
0.1548539687276502	0.4713211611460508	0.7529212147025746
0.0097912020059070	0.5670471485940212	0.3035185567621284
0.9902087979272522	0.4329528513926064	0.6964814431995663
0.1728402618632927	0.5819182743464708	0.2664729615971311
0.8271597380865714	0.4180817256624394	0.7335270384283987
0.1658275668937819	0.5588638105831905	0.1782504604830777
0.8341724330393703	0.4411361894034371	0.8217495394786170
0.0072920297498555	0.5937977732174460	0.3928419169733672
0.9927079703329014	0.4062021970120426	0.6071580830521697
0.9966358981551977	0.6246114170052692	0.4701975056688923
0.0033641019458770	0.3753886128556800	0.5298024943566375
0.9567652746464361	0.8469256369473541	0.3758782260717979
0.0432347254408896	0.1530743481718631	0.6241217739537319
0.9192599879089443	0.8712954474853234	0.4625494535027173
0.0807400120409270	0.1287045525236010	0.5374505465228196
0.7450542594124698	0.8473641281779081	0.4827655651942493
0.2549457406840219	0.1526358867207236	0.5172344348312947
0.6018078503438105	0.7964054989506621	0.4171626338738079
0.3981921496014778	0.2035944861685479	0.5828373661517219
0.6336408039169754	0.7722146624577135	0.3324359095547678
0.3663591961627901	0.2277853524186213	0.6675640904069269
0.8101291385646618	0.7971978578053864	0.3094318016443580
0.1898708615272469	0.2028021422035309	0.6905681983811647
0.8460628818692726	0.7728958697100410	0.2227587531256887
0.1539371182013483	0.2271041153868794	0.7772412468360130
0.0193707118827362	0.7962713690393244	0.2017335148736947
0.9806292880762726	0.2037286607490145	0.7982664851518422
0.1635124791601257	0.8470734744745556	0.2670595225082621
0.8364875209196541	0.1529265404017934	0.7329404774534467
0.1329246499442647	0.8718366199990157	0.3520926435319041
0.8670753499889088	0.1281633799876261	0.6479073564297977
0.4466185200858632	0.7810716136031104	0.6729529167341539
0.5533814800060455	0.2189283864058069	0.3270470832913688
0.3948820666351125	0.8549597669610733	0.6277113667027479
0.6051179333101828	0.1450402181581296	0.3722886333227819
0.3738309074610839	0.9585187903928301	0.6708819003254263
0.6261690924743775	0.0414812170749670	0.3291180996362755
0.4016762963802236	0.9922933151977702	0.7614949110623570
0.5983237035494966	0.0077066736034226	0.2385050888993447
0.4473977071646189	0.9219714185709904	0.8074808229035000
0.5526022927898282	0.0780285963276270	0.1925191771220369
0.4709931616343042	0.8152885674972836	0.7647532186568924
0.5290068384500373	0.1847114622687656	0.2352467813048094
0.5181647440284891	0.7411091815726891	0.8101633456332777
0.4818352560725643	0.2588908482156285	0.1898366543922521
0.5443121336470682	0.6383507917740374	0.7673392887890316
0.4556878662769179	0.3616491783605440	0.2326607111726702
0.5234473421397183	0.6048268163716557	0.6766002081352411
0.4765526578193047	0.3951732134166761	0.3233997918902958
0.4739939718119714	0.6746418996291936	0.6305388673042742

0.5260060282799373	0.3253581003797166	0.3694611327212556
0.9432606136211490	0.0301801833513053	0.8308154998654587
0.0567393864776307	0.9698198390284887	0.1691845001600711
0.9323372868750255	0.9218676274878561	0.6800572408894539
0.0676627132070280	0.0781323947970094	0.3199427590722408
0.0075826742891181	0.6520778108624441	0.7755037515871024
0.9924173257936388	0.3479221593670587	0.2244962484384416
0.0108869975079955	0.7720938151189713	0.9226549913780460
0.9891130026077448	0.2279061700002458	0.0773450086474980
0.7229970943630448	0.4819975062554036	0.1152210197460448
0.2770029055868264	0.5180024937535137	0.8847789802794708
0.7161346730050013	0.5143578328914060	0.2718236547617181
0.2838653270960450	0.4856421968969258	0.7281763452638117
0.3029193009284299	0.6128256607956786	0.3066904295285298
0.6970806991634788	0.3871743392132316	0.6933095704969929
0.2885909774170230	0.5702869514616964	0.1479669731512629
0.7114090225419858	0.4297130783266283	0.8520330268742669
0.0306514498722308	0.9088709350825610	0.5128843672475440
0.9693485500517767	0.0911290351246592	0.4871156327141506
0.7172060132862796	0.8656953915167165	0.5492006437464028
0.2827939866681675	0.1343046233819010	0.4507993562791270
0.4659660591737875	0.7760666259676654	0.4336648557019842
0.5340339409226900	0.2239333889309520	0.5663351443235527
0.5237190281810555	0.7337223607340206	0.2814787070278939
0.4762809718941341	0.2662776392526069	0.7185212929338078
0.7344956066360240	0.7347055666088309	0.1727407738759936
0.2655043933138401	0.2652944334000793	0.8272592261495362
0.0451230618375931	0.7763182157703596	0.1349831430048525
0.9548769381001563	0.2236817991059823	0.8650168569568635
0.2979325151783172	0.8684236122902078	0.2498541124333045
0.7020674847646760	0.1315763653478328	0.7501458875922253
0.2428329646683807	0.9123805729434764	0.4022149619025583
0.7571670354068161	0.0876194270431512	0.5977850380591363
0.3702325619123101	0.8282548637100504	0.5581345681127559
0.6297674381750227	0.1717451214091597	0.4418654319127739
0.3347659678338033	0.0144621125856617	0.6354387423470342
0.6652340321188532	0.9855378965023434	0.3645612576784956
0.3822341760047365	0.0736561370104170	0.7950990919488845
0.6177658239542936	0.9263438927779006	0.2049009080766524
0.4660040809526507	0.9474595067730149	0.8771100254324082
0.5339959191346750	0.0525404783461880	0.1228899745931358
0.5363201222578340	0.7673925311894862	0.8798712752153222
0.4636798776828641	0.2326074389673778	0.1201287248102147
0.5846190675529499	0.5834362290420572	0.8036523026486435
0.4153809325222468	0.4165637709445704	0.1963476973130582
0.5465215721270766	0.5237591175741514	0.6428830532056651
0.4534784278227946	0.4762408824347588	0.3571169468198647
0.4560559810479674	0.6489914267360106	0.5607217509109077
0.5439440188851847	0.3510085732506170	0.4392782490507869
0.5059025084853914	0.7624618221905095	0.0309853625713785
0.4940974916110932	0.2375381927081008	0.9690146374541584

2Pdnaph

1.0000000000000000		
7.5270137830788810	-0.0371087142834050	-0.0524226009812228
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-1.5359932700484467	-3.3435572756055754	15.5412546651600660
Pd	Fe	N C H

	2	2	12	76	48
Direct					
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0.0073495715454897				0.7626031637451618	0.5357680925104944
0.4999999999425242				0.9999999999787406	0.5000000000127187
0.4999999999891500				0.5000000000171170	0.5000000000127187
0.5258680800078039				0.1052219133269645	0.6190624184469868
0.4741319199505725				0.8947780792245013	0.3809375815148712
0.6660441490026727				0.0906668644932296	0.4500498557091603
0.3339558509850349				0.9093331429172906	0.5499501144991896
0.3282215891869598				0.3783740776024160	0.4825918221513703
0.6717784109551772				0.6216259522298699	0.5174081778740600
0.7221476211978413				0.4082772263527588	0.4997927194023575
0.2778523788111968				0.5917228034795272	0.5002072806230657
0.5015860444007529				0.5182342803669115	0.6365788202771725
0.4984139555775471				0.4817657196673295	0.3634211797482578
0.2756455562007787				0.0727877686451706	0.4566684992722472
0.7243544437575267				0.9272122238365128	0.5433315006896109
0.5587447851899938				0.0703255429237188	0.6917162090974500
0.4412552149136246				0.9296744495737741	0.3082837909279803
0.5600591467461840				0.1287073587488692	0.7729326841446778
0.4399408532167044				0.8712926263514547	0.2270673158807597
0.5252597512401493				0.2288913337648069	0.7801731875658859
0.4747402487259293				0.7711086662536175	0.2198268123959721
0.4944685272058322				0.2651668705177244	0.7039522481829010
0.5055315026170177				0.7348331593145616	0.2960477518425293
0.4958866111620353				0.2013545436387147	0.6253553922596069
0.5041133888347957				0.7986454861777545	0.3746446077022441
0.5198942634229908				0.2893416111079077	0.8619283047125990
0.4801057365737620				0.7106584186387863	0.1380716952492591

2Pdnaph HSHS

1.0000000000000000					
7.5270137830788810				-0.0371087142834050	-0.0524226009812228
-0.0801671209892343				13.9527771939873233	0.1198741358483286
-1.5359932700484467				-3.3435572756055754	15.5412546651600660
Pd	Fe	N	C	H	
2	2	12	76	48	
Direct					
0.9926504284499913				0.2373968512021065	0.4642318776978627
0.0073495715454897				0.7626031637451618	0.5357680925104944
0.4999999999425242				0.9999999999787406	0.5000000000127187
0.4999999999891500				0.5000000000171170	0.5000000000127187
0.5258680800078039				0.1052219133269645	0.6190624184469868
0.4741319199505725				0.8947780792245013	0.3809375815148712
0.6660441490026727				0.0906668644932296	0.4500498557091603
0.3339558509850349				0.9093331429172906	0.5499501144991896
0.3282215891869598				0.3783740776024160	0.4825918221513703
0.6717784109551772				0.6216259522298699	0.5174081778740600
0.7221476211978413				0.4082772263527588	0.4997927194023575
0.2778523788111968				0.5917228034795272	0.5002072806230657
0.5015860444007529				0.5182342803669115	0.6365788202771725
0.4984139555775471				0.4817657196673295	0.3634211797482578
0.2756455562007787				0.0727877686451706	0.4566684992722472
0.7243544437575267				0.9272122238365128	0.5433315006896109
0.5587447851899938				0.0703255429237188	0.6917162090974500
0.4412552149136246				0.9296744495737741	0.3082837909279803

0.5600591467461840	0.1287073587488692	0.7729326841446778
0.4399408532167044	0.8712926263514547	0.2270673158807597
0.5252597512401493	0.2288913337648069	0.7801731875658859
0.4747402487259293	0.7711086662536175	0.2198268123959721
0.4944685272058322	0.2651668705177244	0.7039522481829010
0.5055315026170177	0.7348331593145616	0.2960477518425293
0.4958866111620353	0.2013545436387147	0.6253553922596069
0.5041133888347957	0.7986454861777545	0.3746446077022441
0.5198942634229908	0.2893416111079077	0.8619283047125990
0.4801057365737620	0.7106584186387863	0.1380716952492591
0.5138281197761714	0.3360787185351413	0.9353258359846706
0.4861718801591692	0.6639212516852311	0.0646741639771804
0.7879559083445642	0.1449749638118689	0.4538547835659443
0.2120440916508457	0.8550250510656099	0.5461451866424127
0.2005265066334232	0.3271644556479956	0.4752453616224273
0.7994734934349239	0.6728355145025944	0.5247546383394237
0.8253021879887612	0.3462502549476696	0.4850799429450774
0.1746978119913081	0.6537497450656744	0.5149200272632797
0.1644180946232865	0.1306278593299979	0.4537146853080074
0.8355819053549354	0.8693721406344608	0.5462853147174229
0.3529324216115057	0.5007965201531803	0.6726686728976290
0.6470675783545019	0.4992034797954688	0.3273313270642291
0.3462181392720964	0.5179873446760226	0.7608487450721597
0.6537818905077017	0.4820126552726123	0.2391512548896984
0.4993983736441052	0.5573425328038155	0.8159163674344256
0.5006016264672155	0.4426574671606431	0.1840836325909976
0.6548852294648313	0.5739575688023635	0.7777082258270624
0.3451147705012474	0.4260424312160538	0.2222917741347956
0.6500547722499590	0.5532926708279646	0.6889772145801984
0.3499452278613617	0.4467073291364798	0.3110227854452319
0.4963635168622531	0.5847560854259015	0.9054177347166430
0.5036364831038256	0.4152439145925229	0.0945822652452080
0.4931972437005783	0.6187575514551895	0.9823476339595771
0.5068027860792981	0.3812424485632349	0.0176523660022738
0.4569482499966213	0.1726087699688819	0.2507724636255588
0.5430517797972598	0.8273912300444621	0.7492275065827982
0.3076110857570455	0.1204370722502190	0.2065141359390239
0.6923889143114792	0.8795629575148283	0.7934858789631534
0.2959876705571816	0.0891686104300504	0.1160272971353891
0.7040123592272067	0.9108313821372320	0.8839727028900413
0.4329864712966227	0.1113665680688527	0.0709168432863123
0.5670135585491067	0.8886334244800693	0.9290831417987917
0.6022274099514817	0.1941317734039174	0.2064015644659065
0.3977725901476958	0.8058682266144999	0.7935984354959515
0.7598873528163352	0.2447400290710817	0.2504212236138983
0.2401126471790747	0.7552599858063971	0.7495787465944517
0.8984469229596144	0.2656362183872787	0.2058604267027988
0.1015530770492603	0.7343637518305570	0.7941395583823052
0.8854886241583344	0.2364592833154546	0.1152804406893821
0.1145113758413601	0.7635407018184921	0.8847195518976747
0.7350923338488968	0.1856542783310218	0.0706312542078678
0.2649076662410934	0.8143457366035136	0.9293687532559431
0.5897972536663616	0.1634284090972429	0.1146878515464849
0.4102027462996460	0.8365715908513920	0.8853121484153661
0.0467101608642935	0.2113766701770246	0.8306144396215345
0.9532898353718622	0.7886233149232993	0.1693855604039030
0.0993515854992353	0.1399394659575321	0.8795537959766619
0.9006484293583270	0.8600605191269750	0.1204462039851890

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0.5829318056808148 0.9926600684941036 0.6831659630988511
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0.5854686166582042 0.0969378058344716 0.8296158148399329
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0.7631670431573596 0.5281412625143744 0.3717932992556356
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0.2243417598581203 0.3955113498206089 0.1823300589919299
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0.2336145729886923 0.4336648861658858 0.3428265353348792
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0.5332854086898777 0.8031185954773576 0.6796372482239050
0.1975803639996911 0.1033041329684394 0.2408727762632381
0.8024196210581493 0.8966958521807697 0.7591271939451119
0.1771071572055334 0.0480857750009989 0.0822306189912680
0.8228928130264492 0.9519142547951205 0.9177693735957888
0.4232883895591470 0.0886269001875206 0.0012241611301249
0.5767116401634738 0.9113731147680042 0.9987758155629649
0.7696505187236440 0.2670666898987619 0.3201106431509615
0.2303494812238966 0.7329332803374271 0.6798893568744759
0.0191236727243265 0.3036134263371153 0.2408600728088501
0.9808763272844701 0.6963865438109309 0.7591399122762397
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0.1134158917006687 0.1608871646094130 0.9494579231718348
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0.1460631178504386 0.9448220498047206 0.7176330910128925
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0.0554235942385617 0.0664638251232859 0.6291646173557197
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0.0350192209463458 0.7657633892148112 0.3803534625309766

0.8980837818839547	0.4021452287172735	0.6903878471414160
0.1019162256501360	0.5978547415189155	0.3096121528840143
0.9259755808623211	0.4500202995992524	0.8511811736890635
0.0740244153462157	0.5499796705513376	0.1488188262727945
0.0213961082065310	0.3291669917340130	0.9395742729364898
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2Pdnaph HSLs

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2.2980556120933247	4.0966796920094097	15.5751583954199475			
Pd	Fe	N	C	H	
2	2	12	76	48	

Direct

0.4917690224796445	0.2292742908464476	0.0354613740777125
0.5082310073439515	0.7707257240387335	0.9645386259733257
0.0000000000000000	0.0000000000000000	0.0000000000000000
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0.9775125327675269	0.9079501450056213	0.1149126910348386
0.1696257197042002	0.0835516551343005	0.0286847883397812
0.8303742951035460	0.9164483671995285	0.9713152041820408
0.2206077754654387	0.4046061686163469	0.9989990030229023
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0.7792842108628477	0.0084712936638383	0.3299061595694752
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0.9755945130768637	0.7083375269749368	0.0801435320668631
0.0244054739530455	0.2916624730283743	0.9198564530698121
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0.8266900770491361	0.3356227827757934	0.1711353036768202
0.1733099229476309	0.6643771874629891	0.8288647037280086
0.6279506650785436	0.3945381327093003	0.0569863109680355
0.3720493349978113	0.6054618673279109	0.9430136629003911
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Pd	Fe	N	C	H	O	
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0.9917691270309916	0.1550081917688715	0.7823982195800880
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0.5214019337216058	0.7355637558719508	0.2224129020882231
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Pd	Fe	N	C	H	O	
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Direct

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0.3166586840616219	0.4095083647839175	0.4376387071767383
0.6833413457228730	0.5904916351994984	0.5623613226359936
0.3177298542130274	0.0962871825696823	0.4944102676554465

0.6822701159624387	0.9037127950864345	0.5055897621572782
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