Supporting Information

New insights into the key bifunctional role of sulfur

in Fe-N-C single-atom catalyst for ORR/OER

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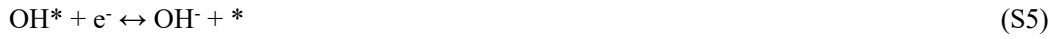*Technology and Equipment, Hefei University of Technology, Hefei 230009, China*

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Details of computational methods

ORR and OER processes are reversible. Previous research showed that ORR and OER process on SAC systems mainly followed the four-electron mechanism under alkaline conditions according to the electrochemical framework developed by Nørskov.[1] The overall reaction could be expressed as $O_2 + 2H_2O + 4e^- \leftrightarrow 4OH^-$. The whole reaction process was described as the following five elementary reactions (1)-(5):

$$* + O_2 \leftrightarrow O_2* \tag{S1}$$

$$O_2* + H_2O + e^- \leftrightarrow OOH* + OH^- \tag{S2}$$

$$OOH* + e^- \leftrightarrow O* + OH^- \tag{S3}$$

$$O* + H_2O + e^- \leftrightarrow OH* + OH^- \tag{S4}$$

$$OH* + e^- \leftrightarrow OH^- + * \tag{S5}$$

The first step (S1) is a pure chemical adsorption/desorption reaction involving no electron transfer. * represents clean catalyst surface, O_2*, $OOH*$, $O*$ and $OH*$ represent intermediates adsorbed on different catalyst surfaces (FeN$_4$C, FeN$_3$SC, Pt(111), RuO$_2$(110)), respectively. The corresponding reaction energies are expressed as:

$$\Delta E_{O_2^*} = E_{O_2*} - E^* - (2E_{H_2O} - 2E_{H_2})$$

$$\Delta E_{OOH^*} = E_{OOH*} - E^* - (2E_{H_2O} - \frac{3}{2}E_{H_2})$$

$$\Delta E_{O^*} = E_{O*} - E^* - (E_{H_2O} - E_{H_2})$$

$$\Delta E_{OH^*} = E_{OH*} - E^* - (E_{H_2O} - \frac{1}{2}E_{H_2})$$

where E_{H_2O} and E_{H_2} are the DFT electron energies of H$_2$O and H$_2$ molecules in the gas phase, respectively. E^*, E_{O_2*}, E_{OOH*}, E_{O*}, E_{OH*} are the energies of clean catalyst surface and adsorbed system O$_2$*, OOH*, O*, OH* respectively. The Gibbs free energy change of ORR/OER was calculated according to $\Delta G = \Delta E + \Delta ZPE - T\Delta S + \Delta pH$, where ΔZPE and ΔS represent the zero point energy and entropy change from the initial state to the end state of the reaction process, respectively, T is 298.15 K. VASPKIT, a postprocessing tool in the VASP code, was adopted to deal with electronic structures.[2] The free energy of liquid H_2O (l) molecules was calculated at the gas phase of T=298.15 K with a pressure of P=0.035 bar. The free energy of O$_2$ was calculated according to

the reaction $O_2 + 2H_2 = 2H_2O$ (the free energy change is 4.92 eV). Δ_{pH} is the free energy correction at any pH value, $\Delta G_{pH} = - kTln[H^+] = - kTln10 \times pH$. The theoretical overpotential (η) under standard conditions is calculated according to the following equation under alkaline conditions: $\eta^{ORR} = \{\Delta G1, - [\Delta G2, \Delta G3, \Delta G4, \Delta G5]^{max}/e + 0.460\ V\}^{max}$, $\eta^{OER} = \{\Delta G1, [\Delta G2, \Delta G3, \Delta G4, \Delta G5]^{max}/e - 0.460\ V\}^{max}$.

[1] Nørskov, J.; Rossmeisl, J.; Logadottir, A.; Lindqvist, L., Origin of the overpotential for oxygen reduction at a fuel-cell cathode. *J. Phys. Chem. B* **2004**, *108*, 17886-17892.

[2] Wang, V.; Xu, N.; Liu, J. C.; Tang, G.; Geng, W., 2019, arXiv: 1908.08269.

Bond length information and adsorption energy data

Table S1 Structural bond length information (unit: Å) and adsorption energy data (unit: eV) of ORR/OER intermediates on FeN_4C and FeN_3SC.

	d_{M-O} (FeN$_4$C)	d_{O-O} (FeN$_4$C)	d_{M-O} (FeN$_3$SC)	d_{O-O} (FeN$_3$SC)	E_{ad} (FeN$_4$C)	E_{ad} (FeN$_3$SC)
O_2	1.778	1.296	1.824/1.989	1.355	-2.123	-2.279
OOH	1.725	1.572	1.848	1.478	-1.596	-1.807
O	1.657	-	1.669	-	-4.249	-4.144
OH	1.826	-	1.876	-	-3.465	-3.577

Table S2 Structural bond length information (unit: Å) and adsorption energy data (unit: eV) of ORR/OER intermediates on Pt(111) and RuO_2(110).

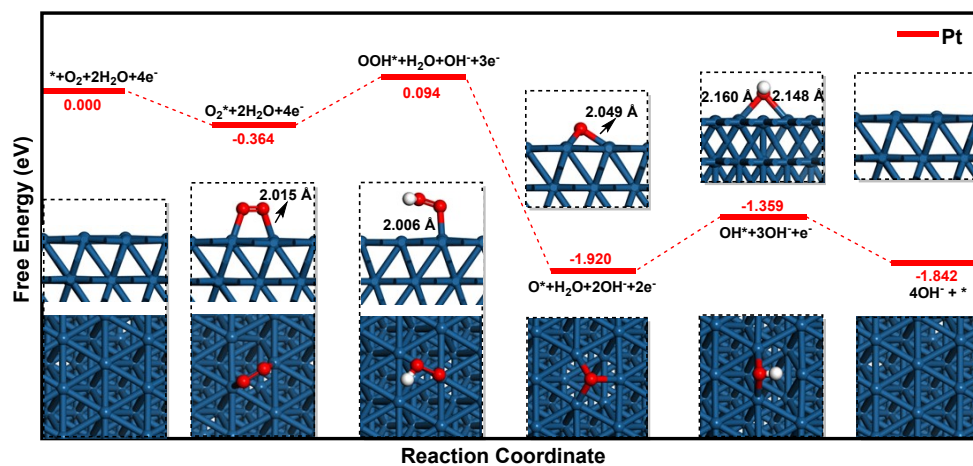|	d_{M-O} (Pt)	d_{O-O} (Pt)	d_{M-O} (RuO$_2$)	d_{O-O} (RuO$_2$)	E_{ad} (Pt)	E_{ad} (RuO$_2$)
O_2	2.015, 2.015	1.371	1.901	1.275	-1.613	-1.515
OOH	2.006	1.435	1.911	1.420	-1.046	-1.566
O	2.049,2.049,2.049	-	1.698	-	-4.119	-3.845
OH	2.160,2.148	-	1.902	-	-2.792	-3.347

Mechanism of ORR on Pt(111)

Figure S1 Energy profile of ORR catalyzed by Pt and optimized structures for related species (pH=13).

Mechanism of OER on FeN₄C, FeN₃SC and RuO₂

For FeN₄C, the reactant OH⁻ arrives near Fe-N₄ site. Due to the adsorption of OH⁻ by the positively charged Fe atom, Fe-O bond is formed. The first electron is released to obtain **OH@FeN₄C** intermediate. The energy decreases from -1.842 V to -2.051 eV, indicating that OH⁻ tends to adsorb on FeN₄C surface. Then, **OH@FeN₄C** releases the second electron and is oxidized to **O@FeN₄C** with further reduced energy of -0.020 eV. In the third electron-release step, the O-OH bond is formed to give **OOH@FeN₄C** intermediate. The instability of OOH on FeN₄C surface increases the free energy by 1.605 eV. It makes the step **O@FeN₄C→OOH@FeN₄C** difficult to proceed with. This step is the RDS of FeN₄C surface. Subsequently, **OOH@FeN₄C** undergoes the final electron-release step to give intermediate **O₂@FeN₄C** with declined energy of -0.414 eV. The final product O₂ is obtained by desorbing from FeN₄C surface with elevated energy of 0.880 eV. In summary, OH⁻ is oxidized to the final product O₂ through four electron-release steps and one desorption step on FeN₄C surface. The first (OH⁻→**OH@FeN₄C**), the second (**OH@FeN₄C→O@FeN₄C**) and the fourth (**OOH@FeN₄C→O₂@FeN₄C**) steps are exergonic, whereas the third (**O@FeN₄C→OOH@FeN₄C**) and last desorption (**O₂@FeN₄C→O₂**) steps are endergonic. The third step **O@FeN₄C→OOH@FeN₄C** has the highest energy demand of 1.605 eV.

For FeN₃SC surface, the OER process is similar to that of FeN₄C. OH⁻ first reaches near the active site Fe-N₃|S. **OH@FeN₃SC** is obtained after releasing the first electron with the reduced free energy of -0.329 eV. In the second electron-transfer process, **OH@FeN₃SC** reacts with OH⁻ to generate the intermediate **O@FeN₃SC** and a H₂O molecule. The shedding of H proton causes the bond length of Fe-O to be shortened to 1.669 Å in **O@FeN₃SC** (1.876 Å in **OH@FeN₃SC**) with the enhanced Fe-O interaction. The free energy increased by 0.199 eV after the step. Then the obtained **O@FeN₃SC** reacts with OH⁻ and releases the third electron to form **OOH@FeN₃SC**. The bonding of O-OH causes the Fe-O bond length to be stretched to 1.848 Å with increased free energy of 1.276 eV. The step is the RDS of OER on FeN₃SC surface, the same as FeN₄C. The much lower barrier makes facile RDS compared with FeN₄C. Subsequently, **OOH@FeN₃SC** releases the fourth electron to form **O₂@FeN₃SC** and the second H₂O molecule. The break of the OO-H bond induces the shortened O-O bond length of 1.355 Å in **O₂@FeN₃SC** (1.478 Å in **OOH@FeN₃SC**) with the

declined free energy of -0.325 eV. Finally, the adsorbed O_2 is dissociated from the FeN_3SC surface via a pure chemical desorption step. The free energy increased by 1.021 eV. In summary, OH^- undergoes four electron-release steps and one chemical desorption step on FeN_3SC surface to be oxidized to the final product O_2. The first ($OH^-\rightarrow OH@FeN_3SC$) and the fourth ($OOH@FeN_3SC\rightarrow O_2@FeN_3SC$) steps are exergonic, whereas the second ($OH@FeN_3SC\rightarrow O@FeN_3SC$), the third ($O@FeN_3SC\rightarrow OOH@FeN_3SC$) and the last desorption ($O_2@FeN_3SC\rightarrow O_2$) steps are endergonic. The third step $O@FeN_3SC\rightarrow OOH@FeN_3SC$ has the highest energy demand of 1.276 eV.
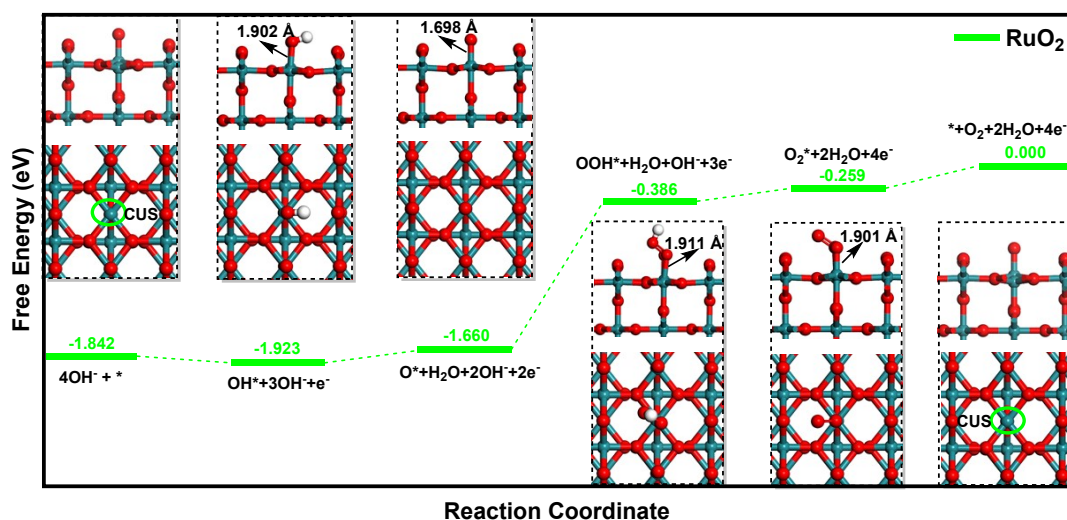
Figure S2 Energy profile of OER catalyzed by RuO_2 and optimized structures for related species (pH=13).

The OER mechanism on RuO_2(110) surface is investigated at U=0 V, pH=13, as shown in Figure S2. The coordination unsaturated site (CUS) Top Ru was considered as the active site on the RuO_2(110) surface.[1-2] First, OH^- is adsorbed on Top Ru and gives the first electron to obtain **OH@RuO₂** with Ru-O bond length of 1.902 Å. The adsorption energy of **OH@RuO₂** is -3.347 eV. The Gibbs free energy decreases from -1.842 eV to -1.923 eV. Then, **OH@RuO₂** releases the second electron to obtain **O@RuO₂** (The adsorption energy is -3.845 eV) with increased energy of 0.263 eV. The Ru-O bond length is shortened to 1.698 Å. Then, **O@RuO₂** releases the third electron and is oxidized to **OOH@RuO₂** (The adsorption energy is -1.566 eV), with increased free energy

of 1.275 eV. The bonding of O-OH re-stretches the Ru-O bond to 1.911 Å. This step is the RDS on RuO$_2$(110) surface, the same as FeN$_4$C and FeN$_3$SC surfaces. The energy trend of the first three electron-release steps is consistent with that of FeN$_3$SC surface. Subsequently, the fourth electron-transfer step gives **O$_2$@RuO$_2$**, the OO-H bond breaks and the Ru-O bond length is 1.901 Å with slight change (1.911 Å in **OOH@RuO$_2$**) due to the similar adsorption energy of -1.515 eV as **OOH@RuO$_2$** (-1.566 eV). The free energy increases by 0.126 eV. Compared with FeN$_4$C and FeN$_3$SC (-2.123 eV and -2.279 eV), the desorption of O$_2$ on RuO$_2$(110) surface becomes easier due to the instability of **O$_2$@RuO$_2$** (-1.515 eV). The free energy increases by 0.259 eV after O$_2$ desorption.

In summary, OH$^-$ undergoes four electron-transfer steps and one O$_2$-desorption step to evolve oxygen on RuO$_2$(110) surface. For the five steps, only the first step (OH$^-$→**OH@RuO$_2$**) is exergonic, while the following four steps (**OH@RuO$_2$**→**O@RuO$_2$**, **O@RuO$_2$**→**OOH@RuO$_2$**, **OOH@RuO$_2$**→**O$_2$@RuO$_2$**, **O$_2$@RuO**→O$_2$) are endergonic. The third step (**O@RuO$_2$**→**OOH@RuO$_2$**) has the highest energy demand of 1.275 eV.

[1] Rossmeisl, J.; Qu, Z.-W.; Zhu, H.; Kroes, G.-J.; Nørskov, J.K., Electrolysis of water on oxide surfaces. *J. Electroanal. Chem.* **2007**, *607*, 83-89.

[2] Briquet, L. G. V.; Sarwar, M.; Mugo, J.; Jones, G.; Federico, C.-V., *ChemCatChem* **2017**, *9*, 1261-1268.

Spin density and band structures of FeN$_4$C and FeN$_3$SC
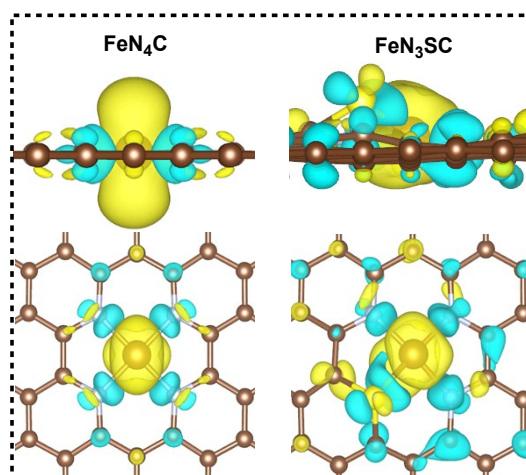
Figure S3 Spin density distributions of FeN$_4$C and FeN$_3$SC slabs. Yellow and turquoise iso-surfaces correspond to spin-up and spin-down density, respectively. The iso-surface levels are 0.002 eÅ^{-3}.

For both Fe-N$_4$ and Fe-N$_3$|S, the spin mainly locates on Fe and the coordination N atoms. The high spin of the active site stabilizes an unpaired electron in antibonding π^* orbitals of the O atom far away from the H atom in the OOH intermediate through exchange interactions.[1, 2]

[1]   Sun, Y.; Sun, S.; Yang, H.; Xi, S.; Gracia, J.; Xu, Z. J., Spin-related electron transfer and orbital interactions in oxygen electrocatalysis, *Adv. Mater.* **2020**, *32*, 2003297.

[2]   Li, Z.; Wang, Z.; Xi, S.; Zhao, X.; Sun, T.; Li, J.; Yu, W.; Xu, H.; Herng, T. S.; Hai, X.; Lyu, P.; Zhao, M.; Pennycook, S. J.; Ding, J.; Xiao, H.; Lu, J., Tuning the spin density of cobalt single-atom catalysts for efficient oxygen evolution, *ACS Nano* **2021**, *15*, 7105-7113.
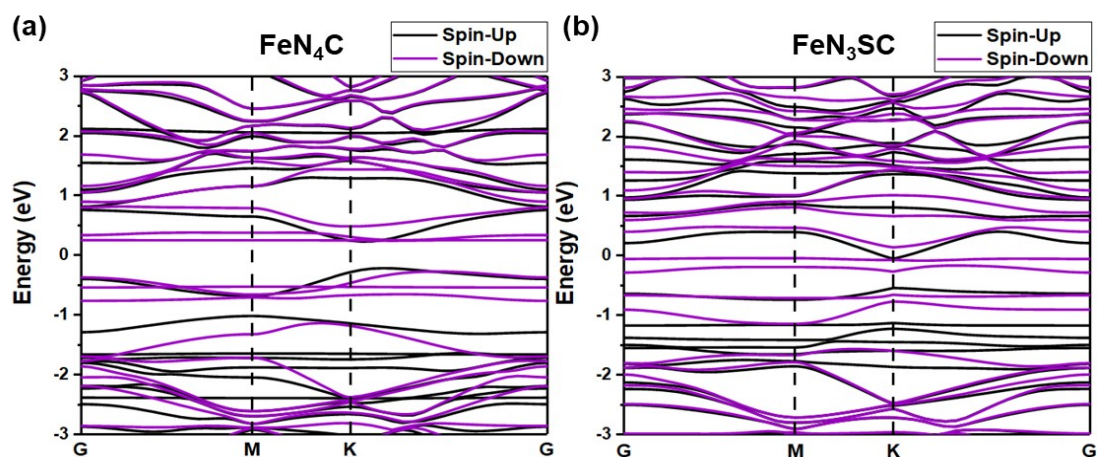
Figure S4 Band structures of (a) FeN_4C and (b) FeN_3SC slabs. The Fermi level is set at 0 eV.

For FeN_4C in Figure S4a, the valence band (VBM) of the spin-up channel is located at -0.215 eV and the conduction band (CBM) is located at 0.231 eV, so the band gap of the spin-up channel is 0.446 eV. The valence band and conduction band of the spin-down channel are located at -0.271 eV and 0.245 eV, respectively, so the band gap of the spin-down channel is 0.516 eV. Accordingly, the total band gap of FeN_4C is 0.447 eV. For FeN_3SC in Figure S4b, the VBM and the CBM of the spin-up channel are located at 0.000 eV and 0.028 eV, with a band gap of 0.028 eV. The VBM and CBM of the spin-down channel are located at -0.041 eV and 0.140 eV, with a band gap of 0.181 eV. That is, the total band gap of FeN_3SC is 0.028 eV. S-doping reduces the FeN_4C band gap and enhances the electrical conductivity, which is conducive to the electron transport in the catalytic reaction process.

DOS and d-band center of OOH@FeN$_4$C and OOH@FeN$_3$SC
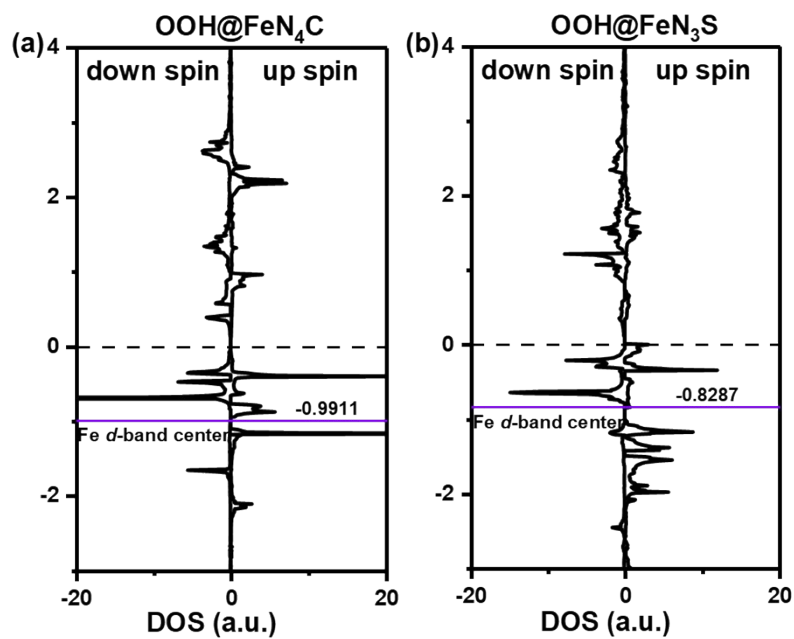
Figure S5 Density of states of (a) **OOH@FeN$_4$C** and (b) **OOH@FeN$_3$SC** slabs. The Fermi level is set at 0 eV.

ORR and OER on FeN$_2$S$_2$C, FeNS$_3$C and FeS$_4$C
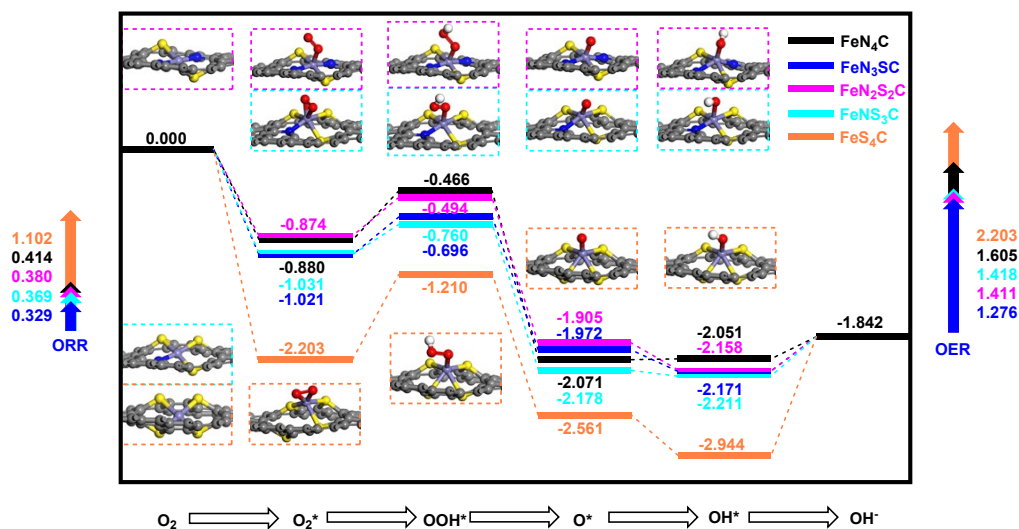
Figure S6 Energy profile of ORR catalyzed by FeN$_4$C, FeN$_3$SC, FeN$_2$S$_2$C, FeNS$_3$C and FeS$_4$C. The side views of related species for FeN$_2$S$_2$C, FeNS$_3$C and FeS$_4$C are displayed in pink, turquoise and orange boxes, respectively (pH=13).

O$_2$ adsorption at the doped S atom
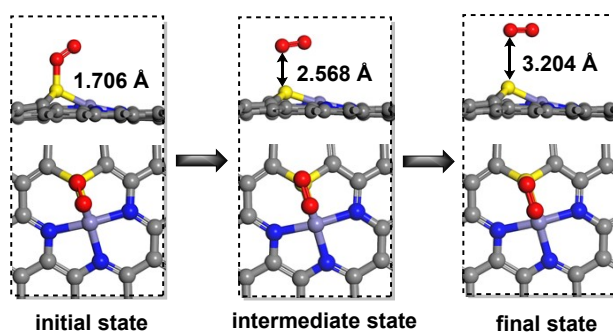
Figure S7 The structure optimization of O$_2$ adsorption at the protruding S

We investigated the O$_2$ species adsorption at the protruding S atom of the catalyst. Figure S7 shows the optimization process of the O$_2$@FeN$_3$SC structure, in which O$_2$ gradually moves away from S atoms. In the final configuration, the distance between O$_2$ and S atoms is 3.204 Å, and the corresponding energy is 1.419 eV higher than that adsorbed on Fe center. Therefore, O$_2$ cannot be stably adsorbed on S, which is not conducive to the subsequent reaction steps.

Electronic energies and Gibbs free energies of related compounds

	Electronic energies (eV)	Gibbs Free Energy (eV)
H_2O	-14.2168 (g)	-14.2186 (l)
$H_2(g)$	-6.7584 (g)	-6.8049 (g)
$O_2(g)$	-9.9970 (g)	-9.9074 (g)
FeN_4C	-446.1891	-446.1891
$OH@FeN_4C$	-456.7496	-457.2149
$O@FeN_4C$	-452.3310	-453.8326
$OOH@FeN_4C$	-461.0423	-463.0429
$O_2@FeN_4C$	-457.0446	-460.0550
FeN_3SC	-439.9843	-439.9843
$OH@FeN_3SC$	-450.6565	-451.1302
$O@FeN_3SC$	-446.0208	-447.5283
$OOH@FeN_3SC$	-455.0488	-457.0687
$O_2@FeN_3SC$	-450.9949	-453.9908
Pt(111)	-371.4430	-371.4430
OH@Pt(111)	-381.3307	-381.7761
O@Pt(111)	-377.4546	-378.9351
OOH@Pt(111)	-385.7463	-387.7370
O_2@Pt(111)	-381.7877	-384.7930
RuO_2(110)	-723.9835	-723.9835

OH@RuO$_2$(110)	-734.4255	-734.8806
O@RuO$_2$(110)	-729.7211	-731.2151
OOH@RuO$_2$(110)	-738.8070	-740.7570
O$_2$@RuO$_2$(110)	-734.2308	-737.2282
FeN$_2$S$_2$C	-434.2138	-434.2138
OH@FeN$_2$S$_2$C	-444.8318	-444.5769
O@ FeN$_2$S$_2$C	-440.1881	-440.1518
OOH@ FeN$_2$S$_2$C	-449.1094	-448.7868
O$_2$@FeN$_2$S$_2$C	-445.0665	-444.9947
FeNS$_3$C	-428.4830	-428.4830
OH@FeNS$_3$C	-439.1849	-438.8986
O@FeNS$_3$C	-434.7254	-434.6937
OOH@FeNS$_3$C	-443.6048	-443.3221
O$_2$@FeNS$_3$C	-439.4817	-439.4210
FeS$_4$C	-422.7368	-422.7368
OH@FeS$_4$C	-434.1204	-433.8861
O@FeS$_4$C	-429.3380	-429.3309
OOH@FeS$_4$C	-438.3172	-438.0263
O$_2$@FeS$_4$C	-434.7432	-434.6673

Fractional Coordinates of related compounds (Angstroms)

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     0.0000000000000000     10.0000000000000000      0.0000000000000000
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H₂

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   2
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O₂

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   O
   2
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FeN₄C

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44	4	1

Direct

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0.5832916817744150	0.3961053778022440	0.2481579738408794
0.4965440907481974	0.6512084424745662	0.2479607402991958
0.7108472518227207	0.6512252561994244	0.2481331140871033
0.5398906983319283	0.5236362986946563	0.2491457971290700

OH@FeN$_4$C
   1.00000000000000
      12.3236999512000001   0.0000000000000000   0.0000000000000000
      -6.1625538564999998   10.6730391195000003   0.0000000000000000
       0.0000000000000000   0.0000000000000000   15.0000000000000000
   C   N   Fe   O   H
   44   4   1   1   1
Direct

0.9726692284529156	0.9904439235198488	0.2452451207150230
0.1076515896607743	0.0606999561169100	0.2454053055762521
0.1764891699856140	0.9965794500484987	0.2456151248421151
0.3107265857484635	0.0667693754608196	0.2469484800738192
0.3747874358831818	0.9966003474829687	0.2461396405078294
0.5077761340350992	0.0606047534249386	0.2463400996027938
0.5725069982568368	0.9903354012611829	0.2464040167063220
0.7054894124773476	0.0544819255734841	0.2460763813360951
0.7695685003703508	0.9843474858432036	0.2467900700509806
0.9037808759417907	0.0545094958006795	0.2452844934263210
0.9708963727894946	0.1888953193858140	0.2437153029579868
0.1042729989352301	0.2578836491842432	0.2435578637416019
0.1745787211500549	0.1952721842338929	0.2452250919287402
0.3094622686659574	0.2685012873835054	0.2478025195673212
0.3788798649634215	0.2030174694040803	0.2488751022484420
0.5139436954354737	0.2684936890833858	0.2487288773540418
0.5754908688224606	0.1951333356112589	0.2463586022823454
0.7083723880423825	0.2578018696385510	0.2448395900844727
0.7727677894909913	0.1888662635818153	0.2445464611719198
0.9056212975121272	0.2564854223959609	0.2432345063128199
0.9725484676639634	0.3904077923881736	0.2420780563789377
0.1047458636545488	0.4588642850498537	0.2418696051035788
0.1696777744626959	0.3914041474336418	0.2428669777371853
0.3011835614917897	0.4585395339082424	0.2452258392801704
0.7119610074914179	0.4583849751007613	0.2456797986742448
0.7763673786989876	0.3913185476142144	0.2436871782270322

0.9087765121586662   0.4588204439941656   0.2421856119944176
0.9754523638664324   0.5922324216425067   0.2419877791102787
0.1076393344537520   0.6606839247183227   0.2422229084588831
0.1714194261053496   0.5922813370241485   0.2422704480086252
0.3038087741027178   0.6597942718744213   0.2440367695492332
0.3681683723587032   0.5926374683956593   0.2461829455286766
0.7789908885332395   0.5925812612613914   0.2448824270171073
0.9105107284225145   0.6597110784924075   0.2428769994143974
0.9760068073794484   0.7932448384278772   0.2435821140714604
0.1093413560399875   0.8622061348105131   0.2439531967462236
0.1746094252847659   0.7946050423652936   0.2434064316484708
0.3074826774234888   0.8622199802411917   0.2447369308188580
0.3718849402084791   0.7932711889901893   0.2451747120480081
0.5048045766540701   0.8558070268877594   0.2466911282942756
0.5664515387369753   0.7825653974170524   0.2492674231181111
0.7014586165862766   0.8481154462188997   0.2489403626125168
0.7708647518944276   0.7825656833217750   0.2474767192948472
0.9057869203514023   0.8558782801351754   0.2450306608373120
0.3699060704102042   0.3988356487777967   0.2484952496660879
0.5836762478439591   0.3985313805986871   0.2498257802052089
0.4966322627795228   0.6522487249755118   0.2507557379881485
0.7105292546449615   0.6524396699627389   0.2477090985248529
0.5401414720913722   0.5253905527052821   0.2676925628005566
0.5466382563827075   0.5250795557522602   0.3891451085457331
0.4827127862031897   0.5412522320790505   0.4141107888092993

O@FeN$_4$C
   1.00000000000000
     12.3236999512000001   0.0000000000000000   0.0000000000000000
     -6.1625538564999998   10.6730391195000003   0.0000000000000000
      0.0000000000000000   0.0000000000000000   15.0000000000000000
   C   N   Fe   O
   44   4   1   1
Direct
   0.9721795449286283   0.9886089168619817   0.2458107670633435
   0.1071247938903351   0.0587112184802383   0.2457386153024236
   0.1759405503806877   0.9944998464488382   0.2462785531381035
   0.3101063860219150   0.0645699591422281   0.2471324485443349
   0.3742092657796710   0.9944995643555361   0.2460900735247335
   0.5072350931322996   0.0587146770958753   0.2458303154488383
   0.5720757848453784   0.9886136843698805   0.2457146410728121
   0.7051047309630217   0.0528239053660634   0.2462461699276150
   0.7691986412413770   0.9827559849398720   0.2470773826810770

0.9033721938685629	0.0528238795689023	0.2460603572508557
0.9704967580709343	0.1871604253038514	0.2450999844761184
0.1038888928921459	0.2560334949280892	0.2444821388185383
0.1738009762586850	0.1930704784778330	0.2453747249646486
0.3088529778342333	0.2663208794057245	0.2472562710494455
0.3781436456398908	0.2006741121912471	0.2482872482868254
0.5131144809708812	0.2663195500841168	0.2477715624066990
0.5749242535629803	0.1930746577891504	0.2460580665602606
0.7078141603008035	0.2560559458078197	0.2454380707124166
0.7723405517702109	0.1871738876033386	0.2455563867183700
0.9052258099994115	0.2547736843379323	0.2449835270521780
0.9721802930981643	0.3886988517283178	0.2441720033402956
0.1043897319968816	0.4570069855361490	0.2433456086769674
0.1693952101319507	0.3895541204015954	0.2434287197061821
0.3010107932099861	0.4564626703177255	0.2442529720466395
0.7111174345535552	0.4564735094532413	0.2457026532151787
0.7758283084202533	0.3895827569002199	0.2448249332547717
0.9082800033724739	0.4570090029979439	0.2443242054379151
0.9749305524682688	0.5903139015168889	0.2443059123479337
0.1071438648120308	0.6586246304553320	0.2441452755856236
0.1710426040538517	0.5903173678293300	0.2433288975798536
0.3035044402158627	0.6577723504144102	0.2434049468915770
0.3682123222859748	0.5908666052853617	0.2442455259878160
0.7783034451705168	0.5908517845603191	0.2456854239555297
0.9099079008792248	0.6577417277902348	0.2447921464713941
0.9754183337651522	0.7912683962767678	0.2454068600457630
0.1088280573906162	0.8601491539671927	0.2455527695523937
0.1741118724627009	0.7925493975968169	0.2449704661753611
0.3069987311718820	0.8601635008569397	0.2450967239762436
0.3715154650385700	0.7912924387780494	0.2444569110187750
0.5043933224618282	0.8542562879215920	0.2453381811720807
0.5661970215396157	0.7810086647783199	0.2472143310042751
0.7011354029424284	0.8466537965688072	0.2482226613828894
0.7704514273848130	0.7810023504058735	0.2477199795782954
0.9055091966920705	0.8542474844428772	0.2460174636531577
0.3686733460206101	0.3958345134281784	0.2473449708722091
0.5828117975017131	0.3958122040475413	0.2481540757812285
0.4965090726713155	0.6514938610148100	0.2473390726524261
0.7106515153207357	0.6515049952298100	0.2481307698567648
0.5395039721118778	0.5236580374445290	0.2706581369159340
0.5389456145030087	0.5235807464963183	0.3811100698648688

OOH@FeN$_4$C

1.00000000000000

   12.3236999512000001   0.0000000000000000   0.0000000000000000

   -6.1625538564999998   10.6730391195000003   0.0000000000000000

   0.0000000000000000   0.0000000000000000   15.0000000000000000

C   N   Fe   O   H

44   4   1   2   1

Direct

0.9732721547580105 0.9901279424591533 0.2433587442685605
0.1082154852148487 0.0601732005507329 0.2434514892546387
0.1769477630176789 0.9959324451357153 0.2438344968238425
0.3112205108327654 0.0661115370300014 0.2446942821795867
0.3753387581963576 0.9959675796261501 0.2438799899555438
0.5083530682393330 0.0602119185820148 0.2434399270194913
0.5732395282969420 0.9901765863893461 0.2434659870137006
0.7062677776017702 0.0543834523732220 0.2439603668965648
0.7703400832311893 0.9842818186551415 0.2446171709038657
0.9045140268033169 0.0543784122645605 0.2438620962475704
0.9716176552881519 0.1887116399119835 0.2437308628655508
0.1050430546402780 0.2575267084387338 0.2437058743600924
0.1749667742277801 0.1945779739775655 0.2437810461892542
0.3099442412207651 0.2677100692427761 0.2452504756040608
0.3791784807357269 0.2020008313465458 0.2458859127834549
0.5142407694529081 0.2677638315377327 0.2455285028350263
0.5760364189347393 0.1945873354675290 0.2437202969730422
0.7088939469426446 0.2574901739543551 0.2435793542721750
0.7735178230122138 0.1886815904806908 0.2437257472076816
0.9063813808515570 0.2563459059949130 0.2438617299943057
0.9733093832882136 0.3902450159679675 0.2437366603911550
0.1055216868080960 0.4585400122386632 0.2436695792989205
0.1705720720966465 0.3910817352912628 0.2437928469966827
0.3021968684106610 0.4578123345870914 0.2442009149473409
0.7118912328398759 0.4576513405543571 0.2441103956887863
0.7768662709904065 0.3909959003367075 0.2433894558036199
0.9093615199139983 0.4584989710299915 0.2433243717643531
0.9760027092028526 0.5918184813487238 0.2430761421220427
0.1082229568661603 0.6601702216228599 0.2432603552656894
0.1721438165064119 0.5918672485062101 0.2433084234473071
0.3046524782367079 0.6592682503371531 0.2432131541144402
0.3694476698229369 0.5925239395026236 0.2442475874336537
0.7792957554255463 0.5923725912447811 0.2436209699733851
0.9108583719526673 0.6591713650535287 0.2428333626091322
0.9764625430645854 0.7927701301139860 0.2430204150426624
0.1098684720942930 0.8616287630032208 0.2433230103027207
0.1751747454835752 0.7940645550437543 0.2433751750592775

0.3080669789851220   0.8616748527068603   0.2434639078601021
0.3726426750970905   0.7928500214935990   0.2433444884846177
0.5055097577432247   0.8557927852931112   0.2436201708417949
0.5673157013720738   0.7826202411993661   0.2455162286118283
0.7022880947081843   0.8482281421449834   0.2457886744575584
0.7715098330388417   0.7825471338705149   0.2449915073471165
0.9065290464935822   0.8557082007330848   0.2433420177429954
0.3697903607660549   0.3971526293577261   0.2453169971319485
0.5837159634953721   0.3970844985434757   0.2464499530592869
0.4978408133782447   0.6531217169734025   0.2469600588874629
0.7114272573158151   0.6528915758348556   0.2455958374523134
0.5404968787415343   0.5249572141896274   0.2671444369262711
0.5385875593864627   0.5262641291384809   0.3821186351109513
0.4836195961309792   0.3954191986532356   0.4295149001956124
0.4987418708447883   0.4270767336659433   0.4908650199809386

O$_2$@FeN$_4$C
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   12.3236999512000001   0.0000000000000000   0.0000000000000000
   -6.1625538564999998   10.6730391195000003   0.0000000000000000
    0.0000000000000000   0.0000000000000000   15.0000000000000000
   C   N   Fe   O
   44   4   1   2
Direct
   0.9728630373319987   0.9886556196868134   0.2434992920168004
   0.1078668801681243   0.0589195707259461   0.2434681326890894
   0.1766823623864195   0.9947305632999379   0.2439950099106054
   0.3108707642780971   0.0648390645303644   0.2450847287923164
   0.3750029604015169   0.9947700344846109   0.2438991642795661
   0.5080139043546603   0.0589500549731937   0.2437366943374579
   0.5727619115781495   0.9886797579513159   0.2434173768635215
   0.7057587235358126   0.0528690680315947   0.2438938549491209
   0.7698323665430912   0.9827579578534114   0.2447472877316199
   0.9040267167317094   0.0528306455020125   0.2436707634604268
   0.9711421862517023   0.1872334396794233   0.2429031968898372
   0.1045482684885326   0.2562055679915562   0.2425744327024791
   0.1746356843964119   0.1934129700386941   0.2433678128568697
   0.3096179967180533   0.2667146680333072   0.2458054662733307
   0.3789622779021347   0.2010495976012541   0.2471208423014981
   0.5138688495843667   0.2666722789302878   0.2474389441436433
   0.5756562160794778   0.1934678786400740   0.2446431555762004
   0.7085157125077137   0.2561473115170634   0.2441108142681490
   0.7729544886626165   0.1872292733683813   0.2435911833860378

0.9058651511200343	0.2548507437074182	0.2431946405352375
0.9728108636584407	0.3887975214572688	0.2430331759324980
0.1049722958886225	0.4571277072357290	0.2424409139406351
0.1699087351823719	0.3896481946191334	0.2423382096533237
0.3014292702218078	0.4567252955337230	0.2434514931450729
0.7121990124161337	0.4568186567235180	0.2466113823430071
0.7765035344015505	0.3896695381526016	0.2443858279488258
0.9089904138093325	0.4571608780158480	0.2435941127479423
0.9756491040190884	0.5904498317049345	0.2435788397098161
0.1078349653413440	0.6587967759289037	0.2429905517584819
0.1716567626730882	0.5904645190494636	0.2423952029333994
0.3040728993946501	0.6579325536183147	0.2421416347715166
0.3685017658170645	0.5908442552556773	0.2432323886051040
0.7792162592449507	0.5908222311997904	0.2465249649669393
0.9106760505196213	0.6579511545498240	0.2442744038258490
0.9761854153524678	0.7914649518358353	0.2438917420793614
0.1095366570765317	0.8603691109118874	0.2435245846295439
0.1748300526176743	0.7927476636285549	0.2431549337817689
0.3077211883569547	0.8603593432149464	0.2428908687018773
0.3721623584181021	0.7913903164580023	0.2423582951769299
0.5050430844586901	0.8541812321219290	0.2430633944139834
0.5667330185483489	0.7808887601331848	0.2453024355600520
0.7017293761342762	0.8465539003824410	0.2466557030687730
0.7710390381878223	0.7809557476025291	0.2470716522394015
0.9060167460091206	0.8541505152891955	0.2443003818102210
0.3697629275909672	0.3966391589816522	0.2462994374536008
0.5835301362804005	0.3967817331018039	0.2500012924668802
0.4969494573267086	0.6509526948124728	0.2457628011538175
0.7106323728036088	0.6508916371161118	0.2498206362483700
0.5393140634037578	0.5239186222855069	0.2671793673961602
0.5319971283587467	0.5246625230581571	0.3855695238834894
0.4389092014671252	0.5243477534744156	0.4260470386895331

FeN$_3$SC
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     -6.1625538564999998   10.6730391195000003   0.0000000000000000
      0.0000000000000000   0.0000000000000000   15.0000000000000000
   C   S   N   Fe
   44   1   3   1
Direct
  0.9718521527164433   0.9879682735759491   0.2448361393982988
  0.1060058718281080   0.0565188845924530   0.2477339012578072

0.1753255179739472	0.9928931615491442	0.2414921435023915
0.3095443925882530	0.0611588031394378	0.2428733940563931
0.3747117892273147	0.9931969523237829	0.2375006214438552
0.5076008552365932	0.0584961566268149	0.2395818526898633
0.5728869434362043	0.9891675975426240	0.2415927612238609
0.7057364440252155	0.0533808487216245	0.2429034736598080
0.7701450197277487	0.9835950705838328	0.2459185442977387
0.9040983083330659	0.0532241046301112	0.2473731704231845
0.9719633250674249	0.1880201244355152	0.2497835710517488
0.1041393721089506	0.2560320250415220	0.2612466422327218
0.1720665646699646	0.1891098313715764	0.2623630689829314
0.3036802091252219	0.2509897611839641	0.2729803422545496
0.3772629725275844	0.1954682461351238	0.2548993626123519
0.5134913587787577	0.2655675261551122	0.2479727827055379
0.5751592846928846	0.1931841908922161	0.2402900943767622
0.7082177757084775	0.2560169346110924	0.2363203077420413
0.7730682601214312	0.1874430768163684	0.2388685871463910
0.9061327314247403	0.2550534399681735	0.2407660450200925
0.9724753895900691	0.3885274413987385	0.2348254895789158
0.1045224744467079	0.4569352296970016	0.2401780068749412
0.1686028258659703	0.3909155276347788	0.2593693961326769
0.2969837871021488	0.4650882081068320	0.2756813959684581
0.7107470599926904	0.4562933256522246	0.2366599134024021
0.7756987157192575	0.3894701485935217	0.2325807966891959
0.9082927346912245	0.4567185795755984	0.2294131608104191
0.9749779517966815	0.5899016869696049	0.2274970177507442
0.1072943095951336	0.6583190584732479	0.2292190347112816
0.1717397505062346	0.5906148670687588	0.2360178428866289
0.3036891211655552	0.6596793847705772	0.2428967212285459
0.3681560913506934	0.5946004968043422	0.2602810337979361
0.7786896972499997	0.5908225454599271	0.2355640636628563
0.9097723876911298	0.6573082252994971	0.2298184467730603
0.9753416785051031	0.7908975133499206	0.2337628083044541
0.1082169559704073	0.8590805213300393	0.2338643083539417
0.1741451031533172	0.7919116548369826	0.2308346211154534
0.3071440762483162	0.8595965020065575	0.2339915264624907
0.3722457416021089	0.7920760311095628	0.2389909569532951
0.5052236723115401	0.8552304171065777	0.2444428197555958
0.5671917948226135	0.7829898172736306	0.2521889244910744
0.7022119861683567	0.8477131580489714	0.2484477601963954
0.7715992259440994	0.7821552950301589	0.2446587688765360
0.9056512824026988	0.8541404225452940	0.2401309188939771
0.3734479106755685	0.3968013543095996	0.3289757567380907
0.5824290993501084	0.3964934142499080	0.2472433534250270

0.4977094568920379   0.6544461169920067   0.2627841049655861
0.7122691980192902   0.6526354380742156   0.2451564080785800
0.5461319438526004   0.5303334483354635   0.2702378180431109

OH@FeN$_3$SC
  1.00000000000000
   12.3236999512000001   0.0000000000000000   0.0000000000000000
   -6.1625538564999998   10.6730391195000003   0.0000000000000000
    0.0000000000000000   0.0000000000000000   15.0000000000000000
  C   S   N   Fe   O   H
  44   1   3   1   1   1
Direct
0.9704716692563802   0.9899831261746654   0.2427531913057148
0.1045848756461667   0.0586494803360439   0.2449681104549886
0.1740297849582624   0.9949334217592373   0.2395918922375150
0.3081534376371598   0.0632581263214337   0.2421929194163020
0.3732645785049697   0.9951574495154177   0.2375413437679189
0.5061812878512330   0.0604093096299363   0.2405378094792333
0.5713937036314137   0.9910637201394825   0.2422641595154393
0.7041709797436577   0.0552651429508190   0.2432235628142807
0.7682977048856208   0.9851796849999079   0.2461446924530346
0.9023421035970741   0.0548696565219571   0.2456981471929098
0.9700208366392906   0.1896707749760280   0.2464928129355299
0.1022523613198678   0.2578355554074634   0.2564647698391106
0.1704137098705635   0.1914290670867826   0.2584850120716949
0.3021263118416719   0.2535083003576343   0.2707254673915069
0.3757026856759776   0.1976860430064295   0.2545584323470292
0.5121839155876343   0.2676662417588374   0.2494048373496609
0.5736943955093077   0.1950889933644114   0.2415702225102073
0.7065351786685712   0.2581204425997177   0.2363759377692320
0.7713460250660440   0.1892454421734304   0.2381855972670819
0.9041972096921881   0.2568634381960398   0.2379458401411062
0.9704844315592447   0.3903380679360313   0.2304508294597108
0.1027524693134027   0.4587609763374043   0.2348298101846128
0.1666920054289958   0.3927956076028573   0.2542271136949955
0.2946529444397063   0.4661238027979324   0.2716854700078554
0.7084305475194491   0.4582313106109056   0.2373150205014894
0.7738212781944664   0.3914997476052079   0.2313705725515307
0.9062866520441459   0.4585615247648296   0.2257606487156762
0.9734569753646214   0.5920840075634787   0.2232745214594319
0.1059235391264405   0.6602800939307067   0.2247685089276102
0.1704648577599592   0.5924717661962468   0.2310301053021115
0.3026127989633500   0.6612102468773235   0.2392882742315233

0.3671210409466655   0.5959856615021297   0.2576654735405097
0.7771380645738432   0.5933915958082900   0.2356088937130972
0.9083895039493248   0.6595196781823559   0.2270756939404035
0.9739259809782160   0.7928553372986832   0.2315402189255543
0.1070942037754978   0.8611802602106577   0.2316185114963082
0.1729418586481202   0.7940560017492689   0.2280539965110037
0.3059120510110988   0.8616469158207151   0.2326108868519403
0.3710168058148214   0.7939054978550786   0.2374532777253832
0.5037144875150296   0.8569051223456285   0.2443388799080117
0.5655022743195968   0.7841925601010052   0.2533034058171668
0.7006563222034086   0.8495179567682718   0.2502166619841743
0.7705735780331486   0.7842678211517811   0.2459092325122423
0.9043853957652860   0.8560794904649274   0.2387445104190989
0.3680440453300651   0.3977519331411863   0.3277272736855189
0.5811440620206352   0.3982958817793255   0.2492979812835258
0.4961066371148856   0.6560348600945376   0.2645021730478518
0.7124042621894989   0.6553671312842511   0.2487466886058938
0.5543413150610600   0.5371655152342256   0.2935717792873237
0.6213216536880000   0.5659239067805063   0.4091148955515334
0.5569558077649672   0.5309771499285617   0.4552540078973893

O@FeN$_3$SC
  1.00000000000000
   12.3236999512000001   0.0000000000000000   0.0000000000000000
   -6.1625538564999998   10.6730391195000003   0.0000000000000000
    0.0000000000000000   0.0000000000000000   15.0000000000000000
  C   S   N   Fe   O
  44   1   3   1   1
Direct
  0.9710213382845212   0.9875659411362807   0.2422459814028358
  0.1052332121742827   0.0561603722814258   0.2447093758982576
  0.1744874406698989   0.9923737455558798   0.2392844662965710
  0.3086506082592644   0.0606248958591282   0.2420994017685338
  0.3739071706481833   0.9925095792021138   0.2381051815159492
  0.5067209475878997   0.0578507072131983   0.2413303308381327
  0.5720395293756418   0.9885286934522381   0.2432383834908383
  0.7048492744766809   0.0529656844168415   0.2440934284810597
  0.7692060847933189   0.9831297288713348   0.2461892398417197
  0.9030908396463807   0.0526647398396044   0.2458601107324928
  0.9708054307393935   0.1874193439537073   0.2479497433617140
  0.1029595395451329   0.2554671951887983   0.2584027532229559
  0.1711377225727804   0.1888031305030287   0.2589528875537537
  0.3025666272031490   0.2505889434515320   0.2711843990536425

0.3761149392238475	0.1947628162706145	0.2550718183400920
0.5126660183437961	0.2649773146587863	0.2508255833870047
0.5742095863782598	0.1926654773741266	0.2427406090288972
0.7072007814203858	0.2557874955044462	0.2379802962535664
0.7719864167049688	0.1870194671529595	0.2397344783947005
0.9048945849431942	0.2545971574504391	0.2401039951498513
0.9711398116837548	0.3880563202726944	0.2337026749308758
0.1034321267270084	0.4564392117677661	0.2385599571582276
0.1673906073271286	0.3903232884883448	0.2573101146086196
0.2956705866889187	0.4635886843030557	0.2748240304753961
0.7088154865059119	0.4558315915121568	0.2374129863564542
0.7743415247125739	0.3891301659100057	0.2329370727809819
0.9069313306304818	0.4562280756163341	0.2284080292644834
0.9741253491881751	0.5895454016490282	0.2257503251080512
0.1066143133705080	0.6578021922005622	0.2279657565335705
0.1711979413834046	0.5900356045657200	0.2347645137272098
0.3034089579596171	0.6585908352571007	0.2423539280186889
0.3678983648067958	0.5932553042453070	0.2604772239325254
0.7773676607259483	0.5908160522576048	0.2335798309306062
0.9089156309039491	0.6569419950164297	0.2272471477745149
0.9744854699174970	0.7904086375441863	0.2310030076057822
0.1075813979463147	0.8585397706332859	0.2318895728883791
0.1735049816105654	0.7913920970778749	0.2299057745714871
0.3065663643514348	0.8589336377094434	0.2341592351489162
0.3716838333858129	0.7912791707859413	0.2395942281598123
0.5044024685758026	0.8545006177720608	0.2457798692485191
0.5664400498287010	0.7819737715709627	0.2542662590668490
0.7013575699282715	0.8473195314124582	0.2494894713515647
0.7709443501296226	0.7820653388085430	0.2433162738515929
0.9051280458060829	0.8539951204850424	0.2372738186589332
0.3669643007861218	0.3929444746866226	0.3310373661394589
0.5814383742844119	0.3958273036304493	0.2504096268112406
0.4974519557895399	0.6538547871110022	0.2657578513796869
0.7126951970482547	0.6535828851200465	0.2434733792816844
0.5554368476485665	0.5356091109768287	0.2937259323225684
0.6050416143578490	0.5569274072766432	0.3992023869007267

OOH@FeN$_3$SC

   1.00000000000000

    12.3236999512000001   0.0000000000000000   0.0000000000000000

    -6.1625538564999998   10.6730391195000003   0.0000000000000000

    0.0000000000000000   0.0000000000000000   15.0000000000000000

   C   S   N   Fe   O   H

		44	1	3	1	2	1

Direct

0.9791385600175859	0.9861101918074811	0.2401345837836950
0.1133459810017470	0.0548802812064047	0.2425116975195922
0.1827809065424635	0.9911678033903359	0.2371545919601690
0.3168950509701894	0.0594387043492244	0.2398272257479953
0.3820724948420864	0.9913780937739882	0.2359816151646715
0.5150281349802199	0.0566414683121957	0.2389554470939560
0.5801919650797991	0.9872652999089019	0.2413016733045286
0.7129654980502413	0.0514444108734417	0.2421070353092444
0.7771156316878751	0.9813850515796660	0.2445830427973645
0.9111974517493544	0.0511275803035827	0.2438820054091353
0.9788659015940930	0.1859494216465718	0.2457344019659708
0.1111002380845795	0.2540296738362079	0.2561187199407810
0.1791901289120753	0.1875047844158062	0.2567334370786855
0.3110739886355610	0.2497625710756396	0.2686517734547611
0.3845448435612656	0.1939802803205140	0.2519783702637933
0.5210657055123277	0.2640301056700303	0.2468112934088890
0.5825607240567261	0.1913538744204856	0.2393409118611494
0.7153998711043108	0.2543009975477165	0.2344562258299508
0.7802004109073145	0.1854555459614246	0.2370903141791602
0.9129825943200666	0.2531017293931754	0.2375295074281629
0.9793321326746702	0.3866780776290797	0.2308642725865894
0.1114917205676436	0.4550799638639182	0.2365728535236789
0.1755428317401576	0.3890884097362075	0.2554284587300565
0.3035271012086503	0.4622136574670210	0.2730006434680251
0.7173060858390601	0.4544978612500952	0.2329826842423807
0.7826393831380497	0.3876464535166615	0.2285677106908215
0.9151805979576193	0.4548018757245716	0.2245816377690736
0.9823093536098026	0.5883323126664390	0.2217986979979899
0.1146720860166115	0.6564825951740288	0.2251419592274835
0.1791538883100069	0.5887565827255989	0.2329981386580429
0.3113135738936821	0.6574476516132798	0.2415193272529412
0.3759891737214488	0.5922931181642850	0.2596233395361219
0.7857281791671958	0.5895877254919849	0.2304234659099601
0.9171491856871886	0.6557885556651335	0.2233875949080038
0.9825958790459720	0.7890908190271090	0.2282784924209274
0.1158172607067961	0.8574048103901623	0.2294400542773174
0.1816536300176714	0.7902687325255243	0.2275335919144771
0.3146274669570619	0.8578076536514744	0.2324099858580861
0.3796649512013923	0.7901058745937178	0.2383923357771144
0.5124598021929962	0.8531584688576782	0.2443968416564735
0.5742809405360785	0.7804531129286246	0.2532132475204904
0.7093588095543188	0.8456277763690175	0.2485010469103535

0.7789731306305603	0.7801164007989859	0.2424810495270963
0.9129431692638490	0.8521894920914614	0.2354295623109286
0.3772039711096477	0.3927977463532646	0.3272676953106018
0.5901304150092034	0.3948309509498846	0.2460765440912400
0.5052001136344955	0.6524685111881282	0.2656826198752047
0.7206567814035040	0.6511263007228667	0.2440404263299963
0.5631862754553859	0.5320767314833631	0.2903748544327458
0.6125988816940693	0.5479639350267449	0.4082006452904409
0.7454111377096234	0.5887721956581173	0.4275740238684193
0.7590366417357083	0.6446186159027557	0.4780624186252326

O$_2$@FeN$_3$SC

1.00000000000000

12.3236999512000001	0.0000000000000000	0.0000000000000000
-6.1625538564999998	10.6730391195000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

C	S	N	Fe	O
44	1	3	1	2

Direct

0.9692929959718459	0.9871116193613805	0.2440843523532000
0.1035085488259656	0.0557786692775323	0.2461300870528256
0.1730244145526349	0.9921500905862547	0.2406388284560009
0.3070713235435621	0.0605213164928053	0.2432440948446508
0.3722377285075199	0.9922821569419435	0.2389227103844161
0.5051330025600759	0.0576731887276882	0.2423611237357382
0.5701958168179930	0.9878815583910032	0.2439252817760973
0.7028984041672921	0.0522152118617342	0.2449288089774344
0.7670182487868785	0.9820864961984803	0.2478242641995033
0.9011283387720854	0.0518932184944044	0.2476626407799322
0.9686927727397414	0.1867087712510523	0.2487662778842479
0.1009436013037992	0.2548018721894844	0.2588118133248966
0.1690258515934176	0.1882996405352934	0.2602931778370236
0.3007510896409884	0.2505640460120511	0.2731254208342639
0.3743183677004832	0.1950937295677989	0.2558869666148560
0.5105481882013384	0.2653744568028558	0.2505510857543948
0.5723977701532892	0.1926720016862553	0.2432921234350810
0.7051456757623715	0.2552678383855120	0.2378454979160037
0.7699353135956150	0.1863023025427881	0.2399009206977870
0.9027726405871859	0.2538464801510079	0.2399277388860238
0.9692326071519558	0.3874196748174621	0.2324673336961873
0.1017051999819462	0.4556893548800112	0.2366696007645512
0.1659270072093600	0.3898493563555830	0.2559601545586518
0.2944777877247698	0.4626803716738683	0.2724879639851901

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0.7069025012872687    0.4557342245565745    0.2383322924988047
0.7722483291046149    0.3886884298553946    0.2325688098547506
0.9049191293897860    0.4556125180020297    0.2273333244774411
0.9724367129406856    0.5892792192291462    0.2246223755567825
0.1049939273889277    0.6572845179164460    0.2263685699763523
0.1696045130623396    0.5894014505595172    0.2325375927861273
0.3019620016430622    0.6576803607064340    0.2395172742136295
0.3670106295197778    0.5920777604039722    0.2561706547142212
0.7762179446460308    0.5909630562705178    0.2377883509771715
0.9076894703469968    0.6569856095739920    0.2282569660159544
0.9731347662859013    0.7901491930596513    0.2329248949063736
0.1063462500318134    0.8584083210351151    0.2328026091722347
0.1720249615769303    0.7911448947227367    0.2293653650815723
0.3050816782628729    0.8586041149159152    0.2337822831632775
0.3701124402850056    0.7905444098630637    0.2379262768924927
0.5026934431988174    0.8534282325259773    0.2448523219151500
0.5644113655212718    0.7800575402964045    0.2524316780121431
0.6996152319837091    0.8463804032261538    0.2515305454838763
0.7698175695690852    0.7814006773054505    0.2487248992504378
0.9035616308959343    0.8533053310666082    0.2402592621457559
0.3636139954931611    0.3928256598491607    0.3328703832780018
0.5791341590775135    0.3968708775105092    0.2494958924757017
0.4957177875148411    0.6513419680061705    0.2599918630164448
0.7123636150575444    0.6528145226530040    0.2537605269261037
0.5544535158709135    0.5316140503258091    0.3017286373870899
0.6196669859971153    0.5155634780067017    0.4068073778563938
0.5835033381959693    0.6005565853732804    0.4248308152167331
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Pt(111)
   1.00000000000000
     11.1501998900999997   0.0000000000000000   0.0000000000000000
     -5.5750999450999998   9.6563563621000004   0.0000000000000000
      0.0000000000000000   0.0000000000000000   21.8281002045000001
   Pt
   64
Selective dynamics
Direct
   0.0000000000000000   0.0000000000000000   0.1832499960000007   F   F   F
   0.3333300199999982   0.1666700039999967   0.2875199960000003   F   F   F
   0.1666649706331170   0.3333350703668828   0.3919795207144938   T   T   T
   0.0000015077671374 -0.0000015077671374   0.4978901235604116   T   T   T
   0.0000000060000005   0.2500000120000010   0.1832499960000007   F   F   F
   0.3333300319999992   0.4166700270000021   0.2875199960000003   F   F   F

0.1666649656331131	0.0833350403668803	0.3919795207144938	T	T	T
0.0000015137671379	0.2499985042328636	0.4978901235604116	T	T	T
0.2500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.0833300099999974	0.4166700270000021	0.2875199960000003	F	F	F
0.4166649656331131	0.0833350403668803	0.3919795207144938	T	T	T
0.2500015137671380	0.2499985042328636	0.4978901235604116	T	T	T
0.2500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.0833299980000035	0.1666700039999967	0.2875199960000003	F	F	F
0.4166649596331197	0.3333350703668828	0.3919795207144938	T	T	T
0.2500015077671375	-0.0000015077671374	0.4978901235604116	T	T	T
0.5000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.8333299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.6666650236331180	0.3333350703668828	0.3919795207144938	T	T	T
0.5000015077671376	-0.0000015077671374	0.4978901235604116	T	T	T
0.5000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.8333299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.6666650086331132	0.0833350403668803	0.3919795207144938	T	T	T
0.5000015137671381	0.2499985042328636	0.4978901235604116	T	T	T
0.7500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.5833299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.9166650086331132	0.0833350403668803	0.3919795207144938	T	T	T
0.7500015137671381	0.2499985042328636	0.4978901235604116	T	T	T
0.7500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.5833299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.9166650236331180	0.3333350703668828	0.3919795207144938	T	T	T
0.7500015077671376	-0.0000015077671374	0.4978901235604116	T	T	T
0.0000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.3333300159999979	0.6666700390000031	0.2875199960000003	F	F	F
0.1666649556331193	0.8333350193668820	0.3919795207144938	T	T	T
0.0000015197671384	0.4999985152328609	0.4978901235604116	T	T	T
0.0000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.3333300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.1666649856331147	0.5833350573668852	0.3919795207144938	T	T	T
0.0000015247671353	0.7499985272328618	0.4978901235604116	T	T	T
0.2500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.0833300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.4166649746331174	0.5833350573668852	0.3919795207144938	T	T	T
0.2500015247671353	0.7499985272328618	0.4978901235604116	T	T	T
0.2500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.0833299949999997	0.6666700390000031	0.2875199960000003	F	F	F
0.4166649556331194	0.8333350193668820	0.3919795207144938	T	T	T
0.2500015197671385	0.4999985152328609	0.4978901235604116	T	T	T
0.5000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.8333299729999979	0.6666700390000031	0.2875199960000003	F	F	F

0.6666649986331195	0.8333350193668820	0.3919795207144938	T	T	T
0.5000015197671386	0.4999985152328609	0.4978901235604116	T	T	T
0.5000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.8333300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.6666650176331175	0.5833350573668852	0.3919795207144938	T	T	T
0.5000015247671354	0.7499985272328618	0.4978901235604116	T	T	T
0.7500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.5833300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.9166650176331175	0.5833350573668852	0.3919795207144938	T	T	T
0.7500015247671354	0.7499985272328618	0.4978901235604116	T	T	T
0.7500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.5833299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.9166649986331195	0.8333350193668820	0.3919795207144938	T	T	T
0.7500015197671386	0.4999985152328609	0.4978901235604116	T	T	T

OOH@Pt(111)
   1.00000000000000
     11.1501998900999997   0.0000000000000000   0.0000000000000000
     -5.5750999450999998   9.6563563621000004   0.0000000000000000
      0.0000000000000000   0.0000000000000000   21.8281002045000001
   Pt   O   H
     64   1   1
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.3333300199999982	0.1666700039999967	0.2875199960000003	F	F	F
0.1616944465078768	0.3304416390475797	0.3916366158034038	T	T	T
-0.0097600908286562	-0.0041963685988275	0.4981670058746161	T	T	T
0.0000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.3333300319999992	0.4166700270000021	0.2875199960000003	F	F	F
0.1644384523600124	0.0826337917086113	0.3918754423224987	T	T	T
-0.0132018795721636	0.2436691891060634	0.4986148158685291	T	T	T
0.2500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.0833300099999974	0.4166700270000021	0.2875199960000003	F	F	F
0.4127797515987129	0.0817774718072451	0.3920778554862295	T	T	T
0.2347619909449383	0.2410010701306992	0.4990546316999880	T	T	T
0.2500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.0833299980000035	0.1666700039999967	0.2875199960000003	F	F	F
0.4144140290476266	0.3364249204363345	0.3957478210619573	T	T	T
0.2392724786831085	-0.0047485667335506	0.4988921371085572	T	T	T
0.5000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.8333299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.6618742298236693	0.3311058342846754	0.3921308348130473	T	T	T

0.4887340538582380	-0.0030877844032123	0.4989514044371478	T	T	T
0.5000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.8333299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.6618355822468392	0.0813613109104643	0.3921059789653674	T	T	T
0.4887887939478027	0.2430748017196184	0.4991342788028324	T	T	T
0.7500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.5833299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.9126563540543166	0.0813404198877892	0.3919048747463120	T	T	T
0.7386090894825265	0.2448268780149437	0.4987101226667939	T	T	T
0.7500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.5833299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.9118014570888755	0.3312378171076474	0.3921037334070582	T	T	T
0.7393668559137693	-0.0044372001308817	0.4977408130970409	T	T	T
0.0000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.3333300159999979	0.6666700390000031	0.2875199960000003	F	F	F
0.1644398163879637	0.8324771635539975	0.3918501820841003	T	T	T
-0.0132094278433974	0.4940725991409268	0.4985991467209258	T	T	T
0.0000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.3333300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.1617252560627111	0.5817636724675770	0.3916238938939324	T	T	T
-0.0096992280618252	0.7455942068592901	0.4981444140114931	T	T	T
0.2500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.0833300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.4125434853663613	0.5815078757910600	0.3923537389005235	T	T	T
0.2346430165773480	0.7448271327431247	0.4989308133571751	T	T	T
0.2500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.0833299949999997	0.6666700390000031	0.2875199960000003	F	F	F
0.4143672645817028	0.8286064459330067	0.3955678028287969	T	T	T
0.2308031029570971	0.4908126808691980	0.4960095451974991	T	T	T
0.5000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.8333299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.6625770759108255	0.8315606423943133	0.3922893351092203	T	T	T
0.4829511408326824	0.4889223836121858	0.5017675757979252	T	T	T
0.5000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.8333300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.6625878769197461	0.5815582071290490	0.3923316801052855	T	T	T
0.4824750848000292	0.7454048942751739	0.5014110810678847	T	T	T
0.7500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.5833300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.9127012540759900	0.5819915330526031	0.3919395592837938	T	T	T
0.7478438641255593	0.7493758550789512	0.4949011247009047	T	T	T
0.7500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.5833299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.9145977410538836	0.8326400292504598	0.3906329562982817	T	T	T

0.7393676156555569	0.4947973478446850	0.4978255573270229	T	T	T
0.4932840760789507	0.6236586443464759	0.5751628894528132	T	T	T
0.5893237416134293	0.6729791425323903	0.5902984804054070	T	T	T

O@Pt(111)

1.00000000000000

11.1501998900999997	0.0000000000000000	0.0000000000000000
-5.5750999450999998	9.6563563621000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.8281002045000001

Pt   O

64   1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.3333300199999982	0.1666700039999967	0.2875199960000003	F	F	F
0.1682334923489040	0.3364822572090512	0.3940016741117275	T	T	T
0.0000275589108451	0.0000746434674971	0.4990488589030985	T	T	T
0.0000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.3333300319999992	0.4166700270000021	0.2875199960000003	F	F	F
0.1663137936187318	0.0831978562152402	0.3919198241056049	T	T	T
-0.0025587397890888	0.2471305635825599	0.4987720729170522	T	T	T
0.2500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.0833300099999974	0.4166700270000021	0.2875199960000003	F	F	F
0.4163478626379075	0.0832944207398028	0.3918729187675949	T	T	T
0.2496702860889053	0.2471273899995053	0.4987720893676701	T	T	T
0.2500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.0833299980000035	0.1666700039999967	0.2875199960000003	F	F	F
0.4163539242251743	0.3331330925364144	0.3918807357448681	T	T	T
0.2496717460970793	0.0026543572634520	0.4987664084491580	T	T	T
0.5000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.8333299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.6666673674201832	0.3333444909664530	0.3922034719078846	T	T	T
0.5021239506282869	0.0042684566068976	0.4973377342101169	T	T	T
0.5000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.8333299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.6669286681470530	0.0832920956490810	0.3918738811566330	T	T	T
0.5003215199396142	0.2502211650317425	0.4985038887663041	T	T	T
0.7500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.5833299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.9168666877018907	0.0831976530170417	0.3919195561231985	T	T	T
0.7498795075514310	0.2502217402356948	0.4985038231483220	T	T	T
0.7500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.5833299549999964	0.1666700039999967	0.2875199960000003	F	F	F

0.9167643534146721	0.3331329843748095	0.3918805057143924	T	T	T
0.7529615075768523	0.0026517349302738	0.4987668589316755	T	T	T
0.0000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.3333300159999979	0.6666700390000031	0.2875199960000003	F	F	F
0.1682233658149328	0.8318224190054964	0.3939981212868577	T	T	T
-0.0041677649163141	0.4979804625226803	0.4973355065156984	T	T	T
0.0000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.3333300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.1669198811426327	0.5834964942193038	0.3926464714514434	T	T	T
-0.0025735991055668	0.7504273441395440	0.4987665066174147	T	T	T
0.2500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.0833300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.4165594079475348	0.5834966275676617	0.3926460709843994	T	T	T
0.2447078065911815	0.7553945080859386	0.5007182621109062	T	T	T
0.2500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.0833299949999997	0.6666700390000031	0.2875199960000003	F	F	F
0.4165606870389363	0.8331385243626882	0.3926491375820045	T	T	T
0.2447025751601975	0.4894250043371277	0.5007155675567833	T	T	T
0.5000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.8333299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.6635813938512991	0.8318210889650289	0.3939989559253855	T	T	T
0.5021281310124267	0.4979799255657221	0.4973351759749159	T	T	T
0.5000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.8333300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.6669284453368535	0.5836907714379297	0.3918746396686652	T	T	T
0.5106679451304911	0.7553950064996642	0.5007176721937507	T	T	T
0.7500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.5833300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.9167450460281479	0.5836915580713279	0.3918734332994245	T	T	T
0.7529831011858001	0.7504278131284803	0.4987670039280475	T	T	T
0.7500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.5833299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.9168622736066969	0.8337422863708165	0.3919212613964176	T	T	T
0.7498818484183897	0.4997832555610355	0.4985039335281984	T	T	T
0.3333517738187423	0.6667172553713970	0.5522644980585737	T	T	T

OOH@Pt(111)
  1.00000000000000
    11.1501998900999997   0.0000000000000000   0.0000000000000000
    -5.5750999450999998   9.6563563621000004   0.0000000000000000
     0.0000000000000000   0.0000000000000000   21.8281002045000001
   Pt   O   H
    64   2   1

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.3333300199999982	0.1666700039999967	0.2875199960000003	F	F	F
0.1671244113661301	0.3339495447782728	0.3939939367128840	T	T	T
-0.0010616685614077	-0.0024859987027982	0.4981419613460783	T	T	T
0.0000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.3333300319999992	0.4166700270000021	0.2875199960000003	F	F	F
0.1660901135252438	0.0822997363079572	0.3915459153031907	T	T	T
-0.0025128748519076	0.2463141819395041	0.4976876482298110	T	T	T
0.2500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.0833300099999974	0.4166700270000021	0.2875199960000003	F	F	F
0.4161401413502873	0.0825265203844430	0.3919810593890322	T	T	T
0.2484712435977835	0.2447163278526182	0.4972077255625558	T	T	T
0.2500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.0833299980000035	0.1666700039999967	0.2875199960000003	F	F	F
0.4167821254530824	0.3329213206191419	0.3920775642209474	T	T	T
0.2494429935087779	-0.0020321148864671	0.4981093270805421	T	T	T
0.5000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.8333299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.6666994509752834	0.3329245656734936	0.3920804147702340	T	T	T
0.4997921842228071	-0.0009354640354642	0.4980506927002082	T	T	T
0.5000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.8333299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.6666352952099723	0.0826181042526578	0.3921008924537729	T	T	T
0.4997682329345500	0.2480823139001991	0.4980328646431662	T	T	T
0.7500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.5833299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.9168150678577313	0.0824882304284360	0.3917999813933892	T	T	T
0.7494686795709379	0.2486757249894650	0.4982432975659449	T	T	T
0.7500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.5833299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.9164870328705196	0.3326568227803983	0.3920675702312931	T	T	T
0.7496288206999846	-0.0011669402733437	0.4982834152612388	T	T	T
0.0000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.3333300159999979	0.6666700390000031	0.2875199960000003	F	F	F
0.1660987522032571	0.8318806057658897	0.3918185541840362	T	T	T
-0.0016893642981973	0.4986133959902074	0.4981052337202304	T	T	T
0.0000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.3333300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.1677517104426674	0.5815151932907344	0.3945282139890987	T	T	T
-0.0008954473045396	0.7484073889973200	0.4983156151043124	T	T	T
0.2500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.0833300469999969	0.9166700999999975	0.2875199960000003	F	F	F

0.4154297789810494	0.5821689736823088	0.3931759589465896	T	T	T
0.2494832015568280	0.7501553803518068	0.4979191781617691	T	T	T
0.2500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.0833299949999997	0.6666700390000031	0.2875199960000003	F	F	F
0.4164146871989992	0.8327896879800786	0.3918375600807349	T	T	T
0.2496683502805263	0.4976792761750046	0.5045230827885360	T	T	T
0.5000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.8333299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.6669813565738767	0.8326589731424214	0.3916884608892411	T	T	T
0.5002931536111216	0.4986541078997462	0.4981907606869843	T	T	T
0.5000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.8333300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.6661362992837637	0.5827839137027042	0.3921209638214943	T	T	T
0.5019931686081999	0.7517554601946517	0.4971494396593057	T	T	T
0.7500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.5833300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.9168775839474953	0.5826121314164803	0.3919027580403918	T	T	T
0.7500233971972626	0.7489933582899658	0.4983759520116787	T	T	T
0.7500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.5833299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.9165137719164350	0.8321659988109874	0.3921371846621533	T	T	T
0.7494042821960362	0.4982630030380640	0.4983474885332833	T	T	T
0.2629993677491165	0.4923084037135669	0.5960428412412734	T	T	T
0.3939390695850514	0.5098492669630478	0.6152706114612212	T	T	T
0.4528332545107008	0.6117986354228038	0.6166141543161431	T	T	T

O_2@Pt(111)
   1.00000000000000
     11.1501998900999997   0.0000000000000000   0.0000000000000000
     -5.5750999450999998   9.6563563621000004   0.0000000000000000
      0.0000000000000000   0.0000000000000000   21.8281002045000001
   Pt   O
     64   2
Selective dynamics
Direct

0.0000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.3333300199999982	0.1666700039999967	0.2875199960000003	F	F	F
0.1675733777492605	0.3326443676089819	0.3935628135242598	T	T	T
-0.0016728688819271	-0.0014311348007402	0.4992021837461779	T	T	T
0.0000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.3333300319999992	0.4166700270000021	0.2875199960000003	F	F	F
0.1684737573153095	0.0864809559617665	0.3952295952729381	T	T	T
-0.0022305331460076	0.2498746026627915	0.4978477753286896	T	T	T

0.2500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.0833300099999974	0.4166700270000021	0.2875199960000003	F	F	F
0.4162047941675828	0.0817574358271497	0.3912183777789318	T	T	T
0.2504297142293395	0.2509579425140437	0.5024138119772089	T	T	T
0.2500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.0833299980000035	0.1666700039999967	0.2875199960000003	F	F	F
0.4172494387306724	0.3326378183334321	0.3921013742047624	T	T	T
0.2502214725828292	-0.0017156301820249	0.4981151965627483	T	T	T
0.5000000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.8333299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.6681754742947010	0.3337196642480157	0.3912421427211466	T	T	T
0.5008319287325111	-0.0011592356111933	0.4980494583260709	T	T	T
0.5000000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.8333299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.6671581486734136	0.0828620912801477	0.3920024362225287	T	T	T
0.5042514953914466	0.2458049591327843	0.4952137328914223	T	T	T
0.7500000060000005	0.2500000120000010	0.1832499960000007	F	F	F
0.5833299669999974	0.4166700270000021	0.2875199960000003	F	F	F
0.9169279119784354	0.0829802284875138	0.3921573213005966	T	T	T
0.7513754700115119	0.2492740122036602	0.4980965650417131	T	T	T
0.7500000000000000	0.0000000000000000	0.1832499960000007	F	F	F
0.5833299549999964	0.1666700039999967	0.2875199960000003	F	F	F
0.9175615770076759	0.3341530845913508	0.3916787753958775	T	T	T
0.7505142400864016	-0.0004710634499457	0.4987587151982237	T	T	T
0.0000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.3333300159999979	0.6666700390000031	0.2875199960000003	F	F	F
0.1653882527286811	0.8337299939059468	0.3918245659112455	T	T	T
-0.0016034075754434	0.5008314539380680	0.4982779643464159	T	T	T
0.0000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.3333300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.1659102777319934	0.5840438911261380	0.3908358690014990	T	T	T
-0.0005050009801322	0.7506225275150775	0.4988098883414419	T	T	T
0.2500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.0833300469999969	0.9166700999999975	0.2875199960000003	F	F	F
0.4173854590517063	0.5824392044088293	0.3935833177239091	T	T	T
0.2492096353550196	0.7516414038108362	0.4982365247536861	T	T	T
0.2500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.0833299949999997	0.6666700390000031	0.2875199960000003	F	F	F
0.4158465947236457	0.8324419530739046	0.3916668692113164	T	T	T
0.2453126059568608	0.5049363690271539	0.4958976842135653	T	T	T
0.5000000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.8333299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.6669998031534423	0.8330471885920445	0.3921604387664219	T	T	T
0.4995727595949973	0.4996245219357950	0.5024354868890055	T	T	T

0.5000000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.8333300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.6634338693025392	0.5814340934336234	0.3952965489548056	T	T	T
0.5001895327081072	0.7523660101618108	0.4978295666362264	T	T	T
0.7500000169999979	0.7500000349999993	0.1832499960000007	F	F	F
0.5833300039999969	0.9166700999999975	0.2875199960000003	F	F	F
0.9161667816584060	0.5845293240404991	0.3918679272731588	T	T	T
0.7515111707426215	0.7517383377965881	0.4992390364728307	T	T	T
0.7500000120000010	0.5000000229999984	0.1832499960000007	F	F	F
0.5833299729999979	0.6666700390000031	0.2875199960000003	F	F	F
0.9163640660129428	0.8335642561598702	0.3920339393539432	T	T	T
0.7518623504740632	0.4998271944727272	0.4981973339150361	T	T	T
0.4361174498814732	0.4370031018462388	0.5889666312859047	T	T	T
0.3153017705499083	0.3119382627865999	0.5889360638282370	T	T	T

RuO$_2$(110)

   1.00000000000000

    6.2244000435000002   0.0000000000000000   0.0000000000000000

    0.0000000000000000   12.6898002625000004   0.0000000000000000

    0.0000000000000000   0.0000000000000000   28.3910999297999993

O   **Ru**

  68   **32**

Selective dynamics

Direct

0.4515300210000035	0.2257600020000012	0.1056699989999998	F	F	F
0.4515300210000035	0.4757600209999993	0.2174100060000015	F	F	F
0.4515300210000035	0.2257600020000012	0.3291500039999988	F	F	F
0.4515300210000035	0.4757624720757741	0.4394139862592512	T	T	T
0.4515300210000035	0.2257608099211764	0.5553006718644905	T	T	T
0.2015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.2015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.2007094591219178	0.1288010415544830	0.3982173059408936	T	T	T
0.2053842734361825	0.3804117920359218	0.5113100092264762	T	T	T
0.4515300210000035	0.4757600209999993	0.1303700050000032	F	F	F
0.4515300210000035	0.2257600020000012	0.2421100030000005	F	F	F
0.4515300210000035	0.4757597913140785	0.3543714691220153	T	T	T
0.4515300210000035	0.2257621300000819	0.4668192617857423	T	T	T
0.2015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.2007080826075016	0.3227225797255421	0.3982155256854639	T	T	T
0.2053855078460810	0.0711085235657759	0.5113105336955470	T	T	T
0.9515299830000004	0.4757600209999993	0.2174100060000015	F	F	F
0.9515299830000004	0.2257600020000012	0.3291500039999988	F	F	F

0.9515299830000004	0.4757632449560734	0.4442851832534890	T	T	T
0.9515299830000004	0.2257598042049105	0.5491747399129489	T	T	T
0.7015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.7015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.7023505448780790	0.1288010415544830	0.3982173059408936	T	T	T
0.6976757305638142	0.3804117920359218	0.5113100092264762	T	T	T
0.9515299830000004	0.4757600209999993	0.1303700050000032	F	F	F
0.9515299830000004	0.2257600020000012	0.2421100030000005	F	F	F
0.9515299830000004	0.4757595573780621	0.3541268332510050	T	T	T
0.9515299830000004	0.2257620341004444	0.4669918382546058	T	T	T
0.9515299830000004	0.4757595370677710	0.5782916437163689	T	T	T
0.7015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.7023519213924954	0.3227225797255421	0.3982155256854639	T	T	T
0.6976744961539159	0.0711085235657759	0.5113105336955470	T	T	T
0.4515300210000035	0.7257599830000032	0.1056699989999998	F	F	F
0.4515300210000035	0.9757599830000032	0.2174100060000015	F	F	F
0.4515300210000035	0.7257599830000032	0.3291500039999988	F	F	F
0.4515300210000035	0.9757624340757779	0.4394139862592512	T	T	T
0.4515300210000035	0.7257607909211783	0.5553006718644905	T	T	T
0.2015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.2015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.2007094591219178	0.6288010695544850	0.3982173059408936	T	T	T
0.2053842734361825	0.8804118290359212	0.5113100092264762	T	T	T
0.4515300210000035	0.9757599830000032	0.1303700050000032	F	F	F
0.4515300210000035	0.7257599830000032	0.2421100030000005	F	F	F
0.4515300210000035	0.9757597533140824	0.3543714691220153	T	T	T
0.4515300210000035	0.7257621110000839	0.4668192617857423	T	T	T
0.2015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.2007080826075016	0.8227225797255420	0.3982155256854639	T	T	T
0.2053855078460810	0.5711085375657766	0.5113105336955470	T	T	T
0.9515299830000004	0.9757599830000032	0.2174100060000015	F	F	F
0.9515299830000004	0.7257599830000032	0.3291500039999988	F	F	F
0.9515299830000004	0.9757632069560771	0.4442851832534890	T	T	T
0.9515299830000004	0.7257597852049126	0.5491747399129489	T	T	T
0.7015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.7015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.7023505448780790	0.6288010695544850	0.3982173059408936	T	T	T
0.6976757305638142	0.8804118290359212	0.5113100092264762	T	T	T
0.9515299830000004	0.9757599830000032	0.1303700050000032	F	F	F
0.9515299830000004	0.7257599830000032	0.2421100030000005	F	F	F
0.9515299830000004	0.9757595193780656	0.3541268332510050	T	T	T
0.9515299830000004	0.7257620151004465	0.4669918382546058	T	T	T

0.9515299830000004	0.9757594990677748	0.5782916437163689	T	T	T
0.7015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.7023519213924954	0.8227225797255420	0.3982155256854639	T	T	T
0.6976744961539159	0.5711085375657766	0.5113105336955470	T	T	T
0.2015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.2015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.1967076299651749	0.4757621499384360	0.3980497395078793	T	T	T
0.2064551721889062	0.2257610285191779	0.5134889219013860	T	T	T
0.4515300210000035	0.2257600020000012	0.1738899970000034	F	F	F
0.4515300210000035	0.4757600209999993	0.2856299780000029	F	F	F
0.4515300210000035	0.2257610100022569	0.3982752880717050	T	T	T
0.4515300210000035	0.4757593288256493	0.5050401513987834	T	T	T
0.7015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.7015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.7063523740348220	0.4757621499384360	0.3980497395078793	T	T	T
0.6966048318110908	0.2257610285191779	0.5134889219013860	T	T	T
0.9515299830000004	0.2257600020000012	0.1738899970000034	F	F	F
0.9515299830000004	0.4757600209999993	0.2856299780000029	F	F	F
0.9515299830000004	0.2257609031864704	0.3987644959387591	T	T	T
0.9515299830000004	0.4757597431132219	0.5181404160715474	T	T	T
0.2015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.2015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.1967076299651749	0.9757621119384401	0.3980497395078793	T	T	T
0.2064551721889062	0.7257610095191795	0.5134889219013860	T	T	T
0.4515300210000035	0.7257599830000032	0.1738899970000034	F	F	F
0.4515300210000035	0.9757599830000032	0.2856299780000029	F	F	F
0.4515300210000035	0.7257609910022590	0.3982752880717050	T	T	T
0.4515300210000035	0.9757592908256534	0.5050401513987834	T	T	T
0.7015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.7015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.7063523740348220	0.9757621119384401	0.3980497395078793	T	T	T
0.6966048318110908	0.7257610095191795	0.5134889219013860	T	T	T
0.9515299830000004	0.7257599830000032	0.1738899970000034	F	F	F
0.9515299830000004	0.9757599830000032	0.2856299780000029	F	F	F
0.9515299830000004	0.7257608841864723	0.3987644959387591	T	T	T
0.9515299830000004	0.9757597051132260	0.5181404160715474	T	T	T

OH@RuO$_2$(110)

1.00000000000000

   6.2244000435000002   0.0000000000000000   0.0000000000000000

   0.0000000000000000   12.6898002625000004   0.0000000000000000

   0.0000000000000000   0.0000000000000000   28.3910999297999993

O	Ru	H						
69	32	1						

Selective dynamics

Direct

0.4515300210000035	0.2257600020000012	0.1056699989999998	F	F	F
0.4515300210000035	0.4757600209999993	0.2174100060000015	F	F	F
0.4515300210000035	0.2257600020000012	0.3291500039999988	F	F	F
0.4515053994605225	0.4782274377954074	0.4414854004199247	T	T	T
0.4517403924073283	0.2340607676466429	0.5551604450486890	T	T	T
0.2015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.2015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.2003651023273726	0.1288691724212949	0.3980196830263582	T	T	T
0.2023968404682749	0.3796126235471893	0.5081471318792694	T	T	T
0.4515300210000035	0.4757600209999993	0.1303700050000032	F	F	F
0.4515300210000035	0.2257600020000012	0.2421100030000005	F	F	F
0.4515317731338160	0.4757102309580192	0.3547672209324957	T	T	T
0.4515990879711639	0.2237208065380436	0.4662255111409881	T	T	T
0.2015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.2010975695827417	0.3230043325467122	0.3982746181235156	T	T	T
0.2066758519146771	0.0711042725971364	0.5125974713457307	T	T	T
0.9515299830000004	0.4757600209999993	0.2174100060000015	F	F	F
0.9515299830000004	0.2257600020000012	0.3291500039999988	F	F	F
0.9515200365974590	0.4772450641204337	0.4436867234522920	T	T	T
0.9516628145229583	0.2261494848141997	0.5484868496321207	T	T	T
0.7015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.7015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.7028173816460976	0.1289169134936216	0.3980302340689755	T	T	T
0.7010130671655702	0.3795484557131688	0.5080788630928393	T	T	T
0.9515299830000004	0.4757600209999993	0.1303700050000032	F	F	F
0.9515299830000004	0.2257600020000012	0.2421100030000005	F	F	F
0.9515076619216818	0.4760981862461775	0.3546143299149050	T	T	T
0.9517401595098303	0.2244938060628327	0.4667333805296526	T	T	T
0.9508452497372050	0.4709601327687903	0.5766505777515010	T	T	T
0.7015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.7020753846739078	0.3229557099004970	0.3982705731832034	T	T	T
0.6966274392044187	0.0711291251350832	0.5125690614409877	T	T	T
0.4515300210000035	0.7257599830000032	0.1056699989999998	F	F	F
0.4515300210000035	0.9757599830000032	0.2174100060000015	F	F	F
0.4515300210000035	0.7257599830000032	0.3291500039999988	F	F	F
0.4515876388754324	0.9759303115819140	0.4398214448950713	T	T	T
0.4516894939049689	0.7259588075369980	0.5542001876656976	T	T	T
0.2015300019999984	0.6284000260000013	0.1738899970000034	F	F	F

0.2015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.2012820325165978	0.6290731603718225	0.3979827833672688	T	T	T
0.2042571785656410	0.8808380562642009	0.5119889735475911	T	T	T
0.4515300210000035	0.9757599830000032	0.1303700050000032	F	F	F
0.4515300210000035	0.7257599830000032	0.2421100030000005	F	F	F
0.4515860798965031	0.9757022945189940	0.3545328160995427	T	T	T
0.4515496986249942	0.7266462482925438	0.4665194296723619	T	T	T
0.2015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.2003061289229839	0.8230478906077365	0.3982622308444151	T	T	T
0.2040349191815430	0.5715243223035062	0.5109405781618208	T	T	T
0.9515299830000004	0.9757599830000032	0.2174100060000015	F	F	F
0.9515299830000004	0.7257599830000032	0.3291500039999988	F	F	F
0.9515934378452731	0.9764561690510781	0.4446235131881631	T	T	T
0.9515917104724618	0.7267177443496248	0.5489886615113713	T	T	T
0.7015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.7015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.7018068095144753	0.6291284557509985	0.3979900555016836	T	T	T
0.6990132391986799	0.8808251380403774	0.5119638377619369	T	T	T
0.9515299830000004	0.9757599830000032	0.1303700050000032	F	F	F
0.9515299830000004	0.7257599830000032	0.2421100030000005	F	F	F
0.9515629971473742	0.9758399479989092	0.3543136047708499	T	T	T
0.9517573836020283	0.7255039854139710	0.4666608501377711	T	T	T
0.9514861479848840	0.9773281888014715	0.5793529108491013	T	T	T
0.7015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.7027997112079164	0.8230023755065218	0.3982790696899194	T	T	T
0.6993695154114375	0.5715596674480602	0.5107874121090396	T	T	T
0.4522572107834441	0.4653771025315770	0.5779713329364877	T	T	T
0.2015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.2015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.1999281955277855	0.4759273915621293	0.3986651821061558	T	T	T
0.2066992496833210	0.2256095942667645	0.5126238027193030	T	T	T
0.4515300210000035	0.2257600020000012	0.1738899970000034	F	F	F
0.4515300210000035	0.4757600209999993	0.2856299780000029	F	F	F
0.4515477188272718	0.2257338838031828	0.3979926207603490	T	T	T
0.4517912492091263	0.4756084423244049	0.5111428987414491	T	T	T
0.7015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.7015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.7030975983986423	0.4759326506832566	0.3986663487744990	T	T	T
0.6967200663740477	0.2256126093690023	0.5125970462804199	T	T	T
0.9515299830000004	0.2257600020000012	0.1738899970000034	F	F	F
0.9515299830000004	0.4757600209999993	0.2856299780000029	F	F	F
0.9516240139471642	0.2259888802146870	0.3983645921138350	T	T	T

0.9517349139132402	0.4750197243561424	0.5168131828432495	T	T	T
0.2015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.2015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.1966179537689736	0.9760164987842828	0.3984045928268246	T	T	T
0.2059120642561954	0.7252634423218632	0.5130554535872781	T	T	T
0.4515300210000035	0.7257599830000032	0.1738899970000034	F	F	F
0.4515300210000035	0.9757599830000032	0.2856299780000029	F	F	F
0.4515110688108052	0.7261799712917482	0.3981791294382349	T	T	T
0.4516279227548306	0.9756123540010615	0.5054936934905340	T	T	T
0.7015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.7015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.7065578975306461	0.9760169538073092	0.3984078517745003	T	T	T
0.6974036450363900	0.7252691343303019	0.5130019749791782	T	T	T
0.9515299830000004	0.7257599830000032	0.1738899970000034	F	F	F
0.9515299830000004	0.9757599830000032	0.2856299780000029	F	F	F
0.9515799219709246	0.7258350658029954	0.3984575266147006	T	T	T
0.9516166416798061	0.9756987871148268	0.5192077974516061	T	T	T
0.4538078087735352	0.3909669960104047	0.5880533599589222	T	T	T

O@RuO$_2$(110)

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    6.2244000435000002   0.0000000000000000   0.0000000000000000
    0.0000000000000000   12.6898002625000004   0.0000000000000000
    0.0000000000000000   0.0000000000000000 28.3910999297999993
  O   Ru
  69   32
Selective dynamics
Direct

0.4515300210000035	0.2257600020000012	0.1056699989999998	F	F	F
0.4515300210000035	0.4757600209999993	0.2174100060000015	F	F	F
0.4515300210000035	0.2257600020000012	0.3291500039999988	F	F	F
0.4516641475529514	0.4757785331468226	0.4429915726378953	T	T	T
0.4516594683975099	0.2281963542989857	0.5543822925355691	T	T	T
0.2015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.2015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.2002470150630714	0.1287168026885649	0.3980307558455455	T	T	T
0.2035115395350563	0.3798116445657952	0.5091319468644941	T	T	T
0.4515300210000035	0.4757600209999993	0.1303700050000032	F	F	F
0.4515300210000035	0.2257600020000012	0.2421100030000005	F	F	F
0.4516165133978299	0.4758034913259199	0.3548133850901184	T	T	T
0.4515731173899795	0.2231042284289257	0.4663196672149307	T	T	T
0.2015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.0731299959999987	0.2856299780000029	F	F	F

0.2022368461949576	0.3228125698741390	0.3982184413516279	T	T	T
0.2050138328434138	0.0706883123088853	0.5120363353393426	T	T	T
0.9515299830000004	0.4757600209999993	0.2174100060000015	F	F	F
0.9515299830000004	0.2257600020000012	0.3291500039999988	F	F	F
0.9516714721802674	0.4756696579541424	0.4433076277928661	T	T	T
0.9515997738833977	0.2249299879594532	0.5486944377554139	T	T	T
0.7015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.7015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.7029783165852248	0.1287384626454744	0.3980428911168254	T	T	T
0.6996590372019478	0.3797675272136986	0.5090000124837334	T	T	T
0.9515299830000004	0.4757600209999993	0.1303700050000032	F	F	F
0.9515299830000004	0.2257600020000012	0.2421100030000005	F	F	F
0.9515725638149565	0.4757502224707202	0.3546441215761479	T	T	T
0.9517179192606754	0.2259782955506385	0.4666433471419686	T	T	T
0.9508779977635043	0.4756011297365838	0.5752785747331578	T	T	T
0.7015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.7009787912431176	0.3227781280366298	0.3982328579095067	T	T	T
0.6982134093719298	0.0707053725711484	0.5120047844028830	T	T	T
0.4515300210000035	0.7257599830000032	0.1056699989999998	F	F	F
0.4515300210000035	0.9757599830000032	0.2174100060000015	F	F	F
0.4515300210000035	0.7257599830000032	0.3291500039999988	F	F	F
0.4515762387932843	0.9757890679406269	0.4396227445569579	T	T	T
0.4516653010736454	0.7232437046850786	0.5543418647568994	T	T	T
0.2015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.2015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.2021907003941889	0.6287410467205343	0.3982320294873622	T	T	T
0.2050527872080653	0.8808677096072720	0.5120410583846026	T	T	T
0.4515300210000035	0.9757599830000032	0.1303700050000032	F	F	F
0.4515300210000035	0.7257599830000032	0.2421100030000005	F	F	F
0.4515851539377566	0.9757853892187861	0.3544289913265865	T	T	T
0.4515748164739638	0.7284793934923932	0.4663142133648210	T	T	T
0.2015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.2002775329245638	0.8228483098193821	0.3980105089796447	T	T	T
0.2028440730969662	0.5717890956010889	0.5089429941091994	T	T	T
0.9515299830000004	0.9757599830000032	0.2174100060000015	F	F	F
0.9515299830000004	0.7257599830000032	0.3291500039999988	F	F	F
0.9515959923554768	0.9757822028290571	0.4444433358452833	T	T	T
0.9516025567583950	0.7266417228373067	0.5486869094749188	T	T	T
0.7015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.7015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.7010324911028849	0.6287750819934385	0.3982463003254998	T	T	T
0.6981766154605630	0.8808519255765455	0.5120084775195858	T	T	T

0.9515299830000004	0.9757599830000032	0.1303700050000032	F	F	F
0.9515299830000004	0.7257599830000032	0.2421100030000005	F	F	F
0.9515600310912660	0.9757769031827414	0.3542238298037196	T	T	T
0.9517225899767308	0.7257339044763569	0.4666148585047617	T	T	T
0.9514483886324108	0.9757516452140366	0.5789916045293542	T	T	T
0.7015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.7029480290629788	0.8228261458342709	0.3980223629902055	T	T	T
0.7003286276677013	0.5718347221443518	0.5088097950665393	T	T	T
0.4526169008696466	0.4771604501647193	0.5761827979415576	T	T	T
0.2015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.2015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.2014799930088265	0.4757745475088629	0.3988242746887883	T	T	T
0.2066047090393911	0.2252458467375761	0.5127568365513716	T	T	T
0.4515300210000035	0.2257600020000012	0.1738899970000034	F	F	F
0.4515300210000035	0.4757600209999993	0.2856299780000029	F	F	F
0.4515814395505031	0.2254544500393156	0.3980353221228111	T	T	T
0.4515521189839632	0.4757718054825205	0.5163767075374329	T	T	T
0.7015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.7015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.7017833053094521	0.4757746816541413	0.3988230475602734	T	T	T
0.6966892907630137	0.2252686936580072	0.5127219331011007	T	T	T
0.9515299830000004	0.2257600020000012	0.1738899970000034	F	F	F
0.9515299830000004	0.4757600209999993	0.2856299780000029	F	F	F
0.9516258259219387	0.2260493946989819	0.3984170496351464	T	T	T
0.9514899777332740	0.4758793412740635	0.5152738632364811	T	T	T
0.2015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.2015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.1965399794019974	0.9757817981790640	0.3982571678018199	T	T	T
0.2065693498193052	0.7263023205788940	0.5127355705931319	T	T	T
0.4515300210000035	0.7257599830000032	0.1738899970000034	F	F	F
0.4515300210000035	0.9757599830000032	0.2856299780000029	F	F	F
0.4515829559811110	0.7260904069442304	0.3980356591455061	T	T	T
0.4516172049460437	0.9757678031027447	0.5053418657222980	T	T	T
0.7015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.7015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.7066262176628085	0.9757813525835995	0.3982588838892754	T	T	T
0.6967330875797136	0.7262813963671111	0.5127005865011107	T	T	T
0.9515299830000004	0.7257599830000032	0.1738899970000034	F	F	F
0.9515299830000004	0.9757599830000032	0.2856299780000029	F	F	F
0.9516277282568589	0.7255328009639274	0.3983914425745526	T	T	T
0.9515956182626266	0.9757757715523584	0.5188101226573532	T	T	T

OOH@RuO₂(110)

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6.2244000435000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	12.6898002625000004	0.0000000000000000
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O	Ru	H
70	32	1

Selective dynamics

Direct

0.4515300210000035	0.2257600020000012	0.1056699989999998	F	F	F
0.4515300210000035	0.4757600209999993	0.2174100060000015	F	F	F
0.4515300210000035	0.2257600020000012	0.3291500039999988	F	F	F
0.4526883375822225	0.4750060095647191	0.4417457103984975	T	T	T
0.4504175023188746	0.2241244588213442	0.5546193797651017	T	T	T
0.2015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.2015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.2000939716751823	0.1281244820785564	0.3979607212765182	T	T	T
0.1988750905558019	0.3760746751253919	0.5091093481917575	T	T	T
0.4515300210000035	0.4757600209999993	0.1303700050000032	F	F	F
0.4515300210000035	0.2257600020000012	0.2421100030000005	F	F	F
0.4516006148754476	0.4749538822934841	0.3547676218635968	T	T	T
0.4510458765915065	0.2222992351968896	0.4665048064708529	T	T	T
0.2015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.2006939711829611	0.3216893948182018	0.3984499761378065	T	T	T
0.2045307027826661	0.0685953225835160	0.5118752405888731	T	T	T
0.9515299830000004	0.4757600209999993	0.2174100060000015	F	F	F
0.9515299830000004	0.2257600020000012	0.3291500039999988	F	F	F
0.9523925947230503	0.4756068133659359	0.4436765601202562	T	T	T
0.9500650956614357	0.2224315345141069	0.5490408360351715	T	T	T
0.7015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.7015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.7021365666326993	0.1276479758747965	0.3978990690036923	T	T	T
0.7008482459824190	0.3779146355194526	0.5089182181632109	T	T	T
0.9515299830000004	0.4757600209999993	0.1303700050000032	F	F	F
0.9515299830000004	0.2257600020000012	0.2421100030000005	F	F	F
0.9519694868598648	0.4750003111120993	0.3546775461474151	T	T	T
0.9498821072635055	0.2224845369774607	0.4667379658321320	T	T	T
0.9673964916566256	0.4711699588579950	0.5768638367564954	T	T	T
0.7015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.7014636415404397	0.3221922686590063	0.3984921572629749	T	T	T
0.6964672482403915	0.0685766713906739	0.5118248496618624	T	T	T
0.4515300210000035	0.7257599830000032	0.1056699989999998	F	F	F

0.4515300210000035	0.9757599830000032	0.2174100060000015	F	F	F
0.4515300210000035	0.7257599830000032	0.3291500039999988	F	F	F
0.4511521155837008	0.9746632874836352	0.4395235807078387	T	T	T
0.4504255645242454	0.7264127003950309	0.5543184549471910	T	T	T
0.2015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.2015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.2014327510036871	0.6281334940346017	0.3980858441470224	T	T	T
0.2037089128995358	0.8788213696003915	0.5114135611318521	T	T	T
0.4515300210000035	0.9757599830000032	0.1303700050000032	F	F	F
0.4515300210000035	0.7257599830000032	0.2421100030000005	F	F	F
0.4512911476205342	0.9749018992499114	0.3544169710316030	T	T	T
0.4515847496791522	0.7248400641941490	0.4665357477088186	T	T	T
0.2015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.2001863512437935	0.8216349419462093	0.3984175131120584	T	T	T
0.2031394893726396	0.5699502834587075	0.5094682866385880	T	T	T
0.9515299830000004	0.9757599830000032	0.2174100060000015	F	F	F
0.9515299830000004	0.7257599830000032	0.3291500039999988	F	F	F
0.9511807975402219	0.9748279611754302	0.4442959536056832	T	T	T
0.9516865136492634	0.7249391650568080	0.5490015514853012	T	T	T
0.7015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.7015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.7016741358266814	0.6277147840430709	0.3979227201733785	T	T	T
0.6978387476953577	0.8786605655915277	0.5112375649227531	T	T	T
0.9515299830000004	0.9757599830000032	0.1303700050000032	F	F	F
0.9515299830000004	0.7257599830000032	0.2421100030000005	F	F	F
0.9514617692761904	0.9749706686248941	0.3542301276977438	T	T	T
0.9495928050219826	0.7237110299273175	0.4666971827178474	T	T	T
0.9501803390361433	0.9737750931193024	0.5787197384991181	T	T	T
0.7015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.7025713136444245	0.8220533040590722	0.3982632830085130	T	T	T
0.6980704115903039	0.5693389016371234	0.5127603074937671	T	T	T
0.5266562247309547	0.5348053056914489	0.6066507645965270	T	T	T
0.4280715994510431	0.4569004275401039	0.5779936200321670	T	T	T
0.2015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.2015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.2002314767218346	0.4750014723315181	0.3987198651837259	T	T	T
0.2047404371380190	0.2238470962323452	0.5129937023895891	T	T	T
0.4515300210000035	0.2257600020000012	0.1738899970000034	F	F	F
0.4515300210000035	0.4757600209999993	0.2856299780000029	F	F	F
0.4514223850743931	0.2247218415672723	0.3981769463268900	T	T	T
0.4476738997847569	0.4734920573526472	0.5112400380633072	T	T	T
0.7015300019999984	0.4757600209999993	0.1738899970000034	F	F	F

0.7015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.7036153166474066	0.4750197321504719	0.3986994956857328	T	T	T
0.6954829943406906	0.2233359011152578	0.5129735551787261	T	T	T
0.9515299830000004	0.2257600020000012	0.1738899970000034	F	F	F
0.9515299830000004	0.4757600209999993	0.2856299780000029	F	F	F
0.9507784107565072	0.2248512604722981	0.3984770143670260	T	T	T
0.9495241949056208	0.4728172825495189	0.5169688210318931	T	T	T
0.2015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.2015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.1964396347272659	0.9749084384521801	0.3982148398618632	T	T	T
0.2049839691882202	0.7236884603339965	0.5125461047418430	T	T	T
0.4515300210000035	0.7257599830000032	0.1738899970000034	F	F	F
0.4515300210000035	0.9757599830000032	0.2856299780000029	F	F	F
0.4518190184483558	0.7251144709826751	0.3981705137331027	T	T	T
0.4506012443146425	0.9736421502255351	0.5051340534599621	T	T	T
0.7015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.7015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.7061681000137757	0.9748648893391211	0.3982259444414893	T	T	T
0.6963665114009497	0.7232456842454654	0.5134063960416364	T	T	T
0.9515299830000004	0.7257599830000032	0.1738899970000034	F	F	F
0.9515299830000004	0.9757599830000032	0.2856299780000029	F	F	F
0.9511470861554465	0.7247769326505775	0.3985107839287239	T	T	T
0.9506445735093456	0.9735445227572109	0.5185228564921357	T	T	T
0.5005350452369639	0.5046432693991115	0.6381275123680089	T	T	T

O$_2$@RuO$_2$(110)
   1.00000000000000
      6.2244000435000002   0.0000000000000000   0.0000000000000000
      0.0000000000000000   12.6898002625000004   0.0000000000000000
      0.0000000000000000   0.0000000000000000   28.3910999297999993
   O   Ru
   70   32
Selective dynamics
Direct

0.4515300210000035	0.2257600020000012	0.1056699989999998	F	F	F
0.4515300210000035	0.4757600209999993	0.2174100060000015	F	F	F
0.4515300210000035	0.2257600020000012	0.3291500039999988	F	F	F
0.4517520195028372	0.4761953488114727	0.4411724833718474	T	T	T
0.4516764969018204	0.2252620035595589	0.5532763716097210	T	T	T
0.2015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.2015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.2010469192789107	0.1282627529942890	0.3978466823525760	T	T	T
0.2008910745958382	0.3801641990457387	0.5096161889019974	T	T	T

0.4515300210000035	0.4757600209999993	0.1303700050000032	F	F	F
0.4515300210000035	0.2257600020000012	0.2421100030000005	F	F	F
0.4515666198311994	0.4753648631329956	0.3548886229379911	T	T	T
0.4516093247022412	0.2242389401586392	0.4664484132068821	T	T	T
0.2015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.2011276145576455	0.3222443630034798	0.3980065014439504	T	T	T
0.2048383344038708	0.0705840226441091	0.5117125351016881	T	T	T
0.9515299830000004	0.4757600209999993	0.2174100060000015	F	F	F
0.9515299830000004	0.2257600020000012	0.3291500039999988	F	F	F
0.9516199873958364	0.4754653331278019	0.4435061789966940	T	T	T
0.9516038079507095	0.2247227801520237	0.5488363638221726	T	T	T
0.7015300019999984	0.1283999979999990	0.1738899970000034	F	F	F
0.7015300019999984	0.3783999890000018	0.2856299780000029	F	F	F
0.7020869565694543	0.1282701201482453	0.3978463433541478	T	T	T
0.7019924101797923	0.3801410218196864	0.5097612924760001	T	T	T
0.9515299830000004	0.4757600209999993	0.1303700050000032	F	F	F
0.9515299830000004	0.2257600020000012	0.2421100030000005	F	F	F
0.9515853184686033	0.4759563690528020	0.3544892839215749	T	T	T
0.9516334090136038	0.2238877861158201	0.4662290350362619	T	T	T
0.9522868369263170	0.4767325966323276	0.5772296283386580	T	T	T
0.7015300019999984	0.3231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.0731299959999987	0.2856299780000029	F	F	F
0.7020104288277458	0.3222345313544585	0.3979989793699136	T	T	T
0.6983324404325744	0.0705957286161776	0.5116647102287079	T	T	T
0.4515300210000035	0.7257599830000032	0.1056699989999998	F	F	F
0.4515300210000035	0.9757599830000032	0.2174100060000015	F	F	F
0.4515300210000035	0.7257599830000032	0.3291500039999988	F	F	F
0.4515511035152850	0.9754559712959892	0.4395141156458342	T	T	T
0.4515919644695010	0.7245477246531401	0.5544601398563231	T	T	T
0.2015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.2015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.2012172185433988	0.6282723138537126	0.3982727665623559	T	T	T
0.2055404415966021	0.8808587444231657	0.5115606374069572	T	T	T
0.4515300210000035	0.9757599830000032	0.1303700050000032	F	F	F
0.4515300210000035	0.7257599830000032	0.2421100030000005	F	F	F
0.4515583338111727	0.9752390036881491	0.3543838234079679	T	T	T
0.4515674440297900	0.7265599260673369	0.4665806530098264	T	T	T
0.2015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.2015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.2005747661327764	0.8222987014177409	0.3981160673067470	T	T	T
0.2001510584279942	0.5722242998100744	0.5101507534512331	T	T	T
0.9515299830000004	0.9757599830000032	0.2174100060000015	F	F	F
0.9515299830000004	0.7257599830000032	0.3291500039999988	F	F	F

0.9515684231041915	0.9755501177910957	0.4441936660935075	T	T	T
0.9515432923238860	0.7273095278897362	0.5490158076202608	T	T	T
0.7015300019999984	0.6284000260000013	0.1738899970000034	F	F	F
0.7015300019999984	0.8784000260000013	0.2856299780000029	F	F	F
0.7018946423522958	0.6282864192801547	0.3982676342102029	T	T	T
0.6975660151986494	0.8808360018260394	0.5115309229621057	T	T	T
0.9515299830000004	0.9757599830000032	0.1303700050000032	F	F	F
0.9515299830000004	0.7257599830000032	0.2421100030000005	F	F	F
0.9515540690469477	0.9753808829685473	0.3542056803578515	T	T	T
0.9515791185161532	0.7264691729530107	0.4666952174416902	T	T	T
0.9513716455009528	0.9748511322431986	0.5786976979441786	T	T	T
0.7015300019999984	0.8231300099999999	0.1738899970000034	F	F	F
0.7015300019999984	0.5731300099999999	0.2856299780000029	F	F	F
0.7025241150497680	0.8222900851651774	0.3981182105703158	T	T	T
0.7030277248064568	0.5721984401463137	0.5100743427429396	T	T	T
0.4522969715172074	0.4692085827807416	0.5782738668481385	T	T	T
0.4572073456073086	0.3860062417290280	0.6034514033983557	T	T	T
0.2015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.2015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.1992540450413055	0.4750472059756242	0.3987402915563859	T	T	T
0.2044360056835536	0.2262755539699063	0.5126849819028244	T	T	T
0.4515300210000035	0.2257600020000012	0.1738899970000034	F	F	F
0.4515300210000035	0.4757600209999993	0.2856299780000029	F	F	F
0.4515557267998174	0.2250164557817482	0.3980592009189091	T	T	T
0.4513898754004018	0.4759719494787329	0.5113992657520815	T	T	T
0.7015300019999984	0.4757600209999993	0.1738899970000034	F	F	F
0.7015300019999984	0.2257600020000012	0.2856299780000029	F	F	F
0.7038864915220884	0.4750587493284500	0.3987316735133466	T	T	T
0.6987419026404486	0.2262608469414894	0.5126778951681084	T	T	T
0.9515299830000004	0.2257600020000012	0.1738899970000034	F	F	F
0.9515299830000004	0.4757600209999993	0.2856299780000029	F	F	F
0.9515778402164240	0.2251539044579003	0.3982431528652900	T	T	T
0.9515122867543878	0.4766197713594075	0.5173120167837304	T	T	T
0.2015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.2015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.1967045088427794	0.9752320056921638	0.3981939027459095	T	T	T
0.2058504212468120	0.7260980642641440	0.5130588512372839	T	T	T
0.4515300210000035	0.7257599830000032	0.1738899970000034	F	F	F
0.4515300210000035	0.9757599830000032	0.2856299780000029	F	F	F
0.4515393018741001	0.7254454265357796	0.3981906460900612	T	T	T
0.4515359378839129	0.9758678637062295	0.5051963150410647	T	T	T
0.7015300019999984	0.9757599830000032	0.1738899970000034	F	F	F
0.7015300019999984	0.7257599830000032	0.2856299780000029	F	F	F
0.7064212259104361	0.9752321329904131	0.3981949948286833	T	T	T

0.6972728053418237	0.7260974935171240	0.5130469241784466	T	T	T
0.9515299830000004	0.7257599830000032	0.1738899970000034	F	F	F
0.9515299830000004	0.9757599830000032	0.2856299780000029	F	F	F
0.9515616248107597	0.7252984437512109	0.3984299131535253	T	T	T
0.9515569964950331	0.9760152038300909	0.5185432597647749	T	T	T

FeN$_2$S$_2$C

    1.00000000000000
     12.4588003158999996   0.0000000000000000   0.0000000000000000
     -6.2367124682000004   10.5828929508999998   0.0000000000000000
      0.0058500891000000   -0.0107090795000000   14.9636953188999993
   C   S   N   Fe
     44   2   2   1
Direct
0.9742885749825311	0.9896371818643809	0.2439158552678081
0.1080059432711509	0.0575488217819937	0.2474985319488557
0.1763904534248326	0.9932938136660102	0.2385412114954296
0.3103567322081360	0.0607308946651645	0.2411891835604052
0.3756863493818370	0.9932496517810724	0.2389512580116984
0.5083336190997489	0.0575002627821893	0.2442572429126251
0.5739283009633367	0.9897592752063389	0.2476370230753820
0.7065908998434928	0.0540184792270642	0.2526003273681213
0.7719418454057270	0.9865701926089681	0.2500616600477523
0.9059023739862582	0.0539481970449065	0.2527450226549714
0.9739930447836882	0.1885903982725600	0.2618581035189550
0.1061777701244480	0.2561993721717692	0.2713359806375710
0.1749819545888510	0.1905109978167349	0.2650507015653819
0.3068500481324329	0.2523327222136372	0.2712405356052067
0.3788026719408781	0.1957458717060884	0.2514276379309290
0.5147102724402883	0.2633553488091796	0.2432266972128371
0.5766082176899251	0.1919609241756235	0.2439917669796994
0.7097439252245155	0.2548157585638887	0.2459087043187966
0.7748588861425870	0.1878212412661400	0.2528941080635267
0.9074344141343218	0.2550587848830549	0.2568262920240988
0.9740762645696358	0.3889401489025653	0.2512426117621813
0.1054757884585907	0.4572187973165477	0.2567757994277038
0.1703318978411132	0.3916827623642367	0.2732003652353798
0.2996226934905325	0.4656659995386705	0.2843350168410737
0.7125079089319482	0.4519043801436609	0.2249615202813162
0.7782358573311446	0.3873088211867622	0.2378424441605099
0.9100164076025424	0.4560003376849922	0.2396090265595112
0.9770024051439059	0.5899577873349340	0.2323809317898251
0.1084018966170554	0.6582845564695227	0.2380944881731399
0.1724177326360853	0.5911739600223703	0.2496264047626273

0.3041642153099622   0.6598951170737672   0.2521591954495832
0.3698111032489359   0.5953065621662665   0.2654501184777220
0.7826997648977319   0.5816395808920769   0.2062606954057125
0.9121032478036109   0.6556175216991225   0.2169280984059937
0.9761820107010174   0.7911025889371817   0.2194223146540008
0.1083844004564805   0.8587177078213276   0.2290267012004714
0.1749908505334428   0.7922316096419526   0.2335229509605929
0.3075623857556773   0.8594231255892434   0.2381173254991346
0.3726934284322049   0.7924300554446370   0.2449276874781322
0.5057583329235043   0.8553172507218643   0.2474494608687854
0.5676418113777510   0.7838829280058207   0.2478574787043761
0.7034836059089222   0.8515727569387413   0.2397533963892270
0.7754612577617719   0.7950342754370741   0.2198938610647201
0.9073269001256216   0.8567098985606422   0.2261781197697872
0.3837956234720171   0.3991637040378602   0.3272231743466615
0.6984990472762517   0.6483094116064936   0.1636600516471286
0.5841891374003102   0.3929707933977067   0.2325708802113617
0.4981347971390802   0.6542247309108340   0.2580556667548772
0.5410630570841561   0.5235158866463422   0.2452266325184129

OH@FeN$_2$S$_2$C
   1.00000000000000
    12.4588003158999996   0.0000000000000000   0.0000000000000000
    -6.2367124682000004   10.5828929508999998   0.0000000000000000
     0.0058500891000000   -0.0107090795000000   14.9636953188999993
   C   S   N   Fe   O   H
   44   2   2   1   1   1
Direct
   0.9677119388127680   0.9862750773718969   0.2408061266982506
   0.1016242115206737   0.0540882516881634   0.2443579768041053
   0.1697633654952454   0.9897469520312930   0.2355190141823149
   0.3037483353617464   0.0575189539139970   0.2393164966145146
   0.3692973966002120   0.9898342746842358   0.2359283422558712
   0.5017596060013868   0.0541871994826939   0.2411258161859006
   0.5679329641555410   0.9868239742557035   0.2443372956070364
   0.7004477518940863   0.0512189915314498   0.2496321728016287
   0.7661523717726560   0.9838404562734827   0.2480589769586660
   0.8998871890681036   0.0509735101977781   0.2496912778781082
   0.9683723578254765   0.1859293626341092   0.2575952351331370
   0.1002027941252771   0.2532748899639927   0.2674639474956466
   0.1682615122568490   0.1865223326675301   0.2626905304712708
   0.2996888295022902   0.2480069278898387   0.2726907548581256
   0.3721576201845235   0.1922776405421997   0.2526182401166720

0.5091914090087603   0.2604416291372976   0.2446491599872230
0.5704034737114995   0.1883383143339183   0.2421177012378312
0.7035628539779011   0.2514968931852405   0.2425921403227757
0.7690012200379786   0.1848042355381505   0.2489250792473293
0.9016505300627258   0.2521420067684496   0.2518265382921419
0.9685196373169244   0.3857450403630792   0.2449634794536638
0.1001371824014625   0.4540297443381932   0.2501709939211020
0.1650950970722935   0.3890031149697127   0.2685133199046424
0.2939051910437196   0.4623635929858891   0.2840921897834757
0.7049854613940579   0.4472024097975249   0.2231040674417431
0.7720991741615159   0.3836676699055300   0.2336433098855143
0.9039994979485082   0.4524415561439483   0.2337016085148001
0.9702760098583723   0.5862082372565928   0.2263599596125119
0.1019910007252203   0.6546069119698824   0.2317308413958907
0.1667973326313892   0.5878080561126234   0.2429409323483079
0.2985532046259825   0.6562352263595753   0.2478562548114561
0.3650934990833089   0.5927627666490949   0.2662451669167208
0.7743201613918852   0.5773556830396227   0.2027391107445319
0.9042047718750362   0.6514976011209705   0.2122260606277430
0.9690488000783525   0.7873481429363974   0.2154422698447821
0.1012190363935774   0.8548574593465453   0.2248007709947547
0.1683691734806195   0.7885647838413050   0.2284568555686557
0.3008449850173639   0.8558796147380733   0.2338416399382810
0.3663278067948312   0.7889712387134685   0.2413348851049893
0.4992327422922511   0.8527662535452163   0.2450756682445111
0.5609481034214546   0.7812833656319225   0.2499015172665138
0.6976904217155050   0.8490557496119950   0.2396439487830639
0.7687744446999837   0.7922780206736748   0.2182884595919258
0.9007140289726455   0.8536169681934181   0.2232824641577258
0.3675107299875308   0.3898930864790297   0.3346664552704335
0.6865081127090396   0.6431376197737839   0.1681444620592798
0.5783014266966812   0.3886928430760925   0.2361711972055096
0.4931946708226886   0.6545939121918458   0.2666643261859242
0.5658497605861559   0.5379027360980204   0.2977407051849011
0.6694129753171152   0.5881994394142871   0.3955178266890103
0.6423384951087967   0.6062601146312712   0.4517065733990749

O@FeN$_2$S$_2$C

   1.00000000000000

   12.4588003158999996   0.0000000000000000   0.0000000000000000
   -6.2367124682000004   10.5828929508999998   0.0000000000000000
    0.0058500891000000   -0.0107090795000000   14.9636953188999993
   C   S   N   Fe   O

44   2   2   1   1
Direct

0.9724571160462848	0.9886124469593378	0.2410819971063723
0.1060926786234541	0.0565017991889146	0.2455188722535002
0.1748211109270438	0.9923043790148597	0.2379001427578739
0.3086820961916792	0.0599699988871283	0.2429979332171597
0.3741056192283077	0.9923706119842860	0.2398878965546920
0.5066123307697334	0.0567936884020831	0.2447431709907444
0.5722944268719370	0.9888735967999308	0.2470852883288716
0.7048991705994849	0.0530725864348368	0.2509757224975439
0.7700152958822137	0.9855340484758747	0.2484539985854919
0.9039963324256559	0.0527295804585547	0.2495611283061644
0.9719207320015746	0.1873418039850073	0.2579908541485288
0.1037793927219810	0.2548344739676653	0.2682278452460601
0.1724369999434150	0.1891408855453534	0.2634913540302861
0.3038353880205441	0.2507047280896401	0.2743291479651271
0.3771487575711907	0.1948848228100966	0.2561930930862046
0.5130333424163159	0.2630546517861150	0.2494715112394835
0.5747730325950480	0.1913998212005029	0.2457713598181716
0.7079092717102310	0.2538102837692708	0.2453015419857141
0.7729803118669865	0.1867635692395634	0.2504857796679011
0.9055529189938689	0.2538770647668380	0.2527939673782562
0.9724796038341553	0.3876160169687315	0.2464231506752809
0.1038510730430301	0.4559476675421586	0.2524606831020653
0.1681465783264015	0.3902934308892451	0.2703222304419660
0.2967271557962397	0.4634209717891563	0.2853762202747367
0.7109926244433799	0.4507996374599679	0.2262491924396563
0.7766814197297293	0.3860305563647891	0.2357244134170220
0.9085602122054959	0.4547501099988118	0.2350403585292871
0.9756491295801892	0.5886527687219610	0.2276886451488815
0.1070099322398967	0.6570893335578466	0.2341634749991966
0.1709372241522933	0.5899555234040293	0.2461821001926672
0.3025213322022985	0.6585210121349457	0.2513811255208163
0.3677748923347368	0.5939869995887845	0.2679562267354740
0.7809452661170119	0.5796707070985639	0.2052023952117974
0.9106574583487221	0.6544793292923858	0.2134518248692154
0.9745721092738265	0.7898659162386510	0.2170804193726620
0.1068699481729573	0.8577286101838627	0.2269928446290509
0.1734915440631352	0.7911806237129241	0.2312889817602323
0.3059529417903867	0.8584402115159077	0.2374460950042554
0.3710217957632206	0.7912865246230270	0.2448125242194605
0.5039138278465116	0.8544654921595992	0.2480696359567424
0.5657436146167069	0.7825750056803498	0.2515845543554188
0.7017208505100478	0.8505080645964006	0.2413354442562432

0.7738331507014446   0.7942255922521730   0.2208574292326097
0.9055984627309901   0.8554312618559219   0.2243087772733301
0.3724469861421417   0.3923213176845691   0.3358605519430836
0.6913266375298266   0.6437727417839527   0.1739392449924588
0.5840019990207341   0.3937438667859154   0.2418721418662072
0.4955914569636892   0.6543875482492858   0.2657144213613128
0.5490789442640588   0.5278391253261946   0.2739244197542530
0.6395661728497554   0.5867700977740375   0.3635880143004647

OOH@FeN$_2$S$_2$C
  1.00000000000000
   12.4588003158999996   0.0000000000000000   0.0000000000000000
   -6.2367124682000004   10.5828929508999998   0.0000000000000000
    0.0058500891000000   -0.0107090795000000   14.9636953188999993
  C   S   N   Fe   O   H
  44   2   2   1   2   1
Direct

0.9735472441410133   0.9859214773219460   0.2403431530406323
0.1072229553096981   0.0538306470538743   0.2442220073484722
0.1758167592351960   0.9895833569828141   0.2363537844195754
0.3096584041447818   0.0573873586545123   0.2412033109169289
0.3750694288743109   0.9897327260288178   0.2384330161335222
0.5076419198251222   0.0541632316446197   0.2432946242460165
0.5732958623536900   0.9861137031087576   0.2459568648491264
0.7059546784274570   0.0504171829832172   0.2494834563951876
0.7711104461737145   0.9828742187718427   0.2479374618842356
0.9051155135253974   0.0500593791146087   0.2487541201789237
0.9731388359775417   0.1847682710130097   0.2559766213464169
0.1050132501374726   0.2522178155284939   0.2661436661480742
0.1736000924989919   0.1864135504441842   0.2620234025282599
0.3051818037261974   0.2483018607713117   0.2724946850909869
0.3781549922619183   0.1923197552335835   0.2538085282348301
0.5140634744266601   0.2604359499564101   0.2464083653486398
0.5758625102654810   0.1888365197493128   0.2433579569727292
0.7089442338274534   0.2510758616854449   0.2418271863889713
0.7741202818008286   0.1840961307032727   0.2475634053344256
0.9067373565884632   0.2512321988043328   0.2498062064886591
0.9736779292283023   0.3849270670142844   0.2430418979562782
0.1051042711490276   0.4532992911138762   0.2496728122207555
0.1695240821933105   0.3877377533043407   0.2678412567628506
0.2980197207495601   0.4606903714423342   0.2830404801095616
0.7117345831301286   0.4479701461333830   0.2229579618792787
0.7775525173609661   0.3831609170724344   0.2317378299656823

0.9095931365335289   0.4519448813419526   0.2311579676290291
0.9767813866250646   0.5859044887528979   0.2242601291524992
0.1080761764207017   0.6543814800809412   0.2314820901194931
0.1720212291805632   0.5872797226342308   0.2438071357391502
0.3036010341408360   0.6559186361072070   0.2499659727968132
0.3687876970231720   0.5915376812815250   0.2667549179671469
0.7818125597597058   0.5773118593546877   0.2035712028744118
0.9116254708334487   0.6517894110918940   0.2107768012246603
0.9754461415222961   0.7872070802997956   0.2152700633956380
0.1078232947181684   0.8550057699378757   0.2251798379674715
0.1744374435431315   0.7884660227153468   0.2292184900087842
0.3068396619909309   0.8558019405944716   0.2359696391058305
0.3719727289748161   0.7887092485883057   0.2436184527455807
0.5048194415186433   0.8517400896044095   0.2471040880369411
0.5665023924482138   0.7796487917195565   0.2512250161322981
0.7028178086716258   0.8477961464156102   0.2416865063786908
0.7745688511377512   0.7911802489416909   0.2212911514921747
0.9065741659288101   0.8528060661166430   0.2235943448931707
0.3752453320384528   0.3907758161840379   0.3332781732356116
0.6910054902558055   0.6408674642164960   0.1740199347449673
0.5841542253880824   0.3909417741532228   0.2376051757329878
0.4969115029976631   0.6517029090204928   0.2655689990295679
0.5466522219356407   0.5219699984640902   0.2668950142366600
0.6534874398681210   0.5908839680628485   0.3591462381250051
0.6276950638339183   0.4991590102261023   0.4335455847724876
0.7059156453781846   0.5475335094586636   0.4667131652739024

O$_2$@FeN$_2$S$_2$C

1.00000000000000

   12.4588003158999996   0.0000000000000000   0.0000000000000000
   -6.2367124682000004   10.5828929508999998   0.0000000000000000
    0.0058500891000000   -0.0107090795000000   14.9636953188999993
   C   S   N   Fe   O
   44   2   2   1   2
Direct
 0.9755624361614892   0.9905526775398179   0.2408503353806112
 0.1092398018623096   0.0585058057617487   0.2448764122953631
 0.1777846507629131   0.9943116158069689   0.2364551085095102
 0.3116512479682575   0.0619941597941077   0.2407411916048904
 0.3769453671430014   0.9942772065078993   0.2372097259653108
 0.5095584574171208   0.0586001008401589   0.2418367701960147
 0.5751002802224849   0.9904258194016686   0.2443429328017596
 0.7077864535501465   0.0547325743269864   0.2489278739486640

S56

0.7730250450977468	0.9872232088884934	0.2477767856499838
0.9069772391233119	0.0545161810812985	0.2493902043704757
0.9749120648104632	0.1892320756013508	0.2570586020737458
0.1068072726109471	0.2567338515477784	0.2669962384401758
0.1755901346060960	0.1910899639843538	0.2627669898187776
0.3073635422432555	0.2530561357800125	0.2722358107988109
0.3801270976383049	0.1969863221097996	0.2532705758093710
0.5161329053522085	0.2651240968622274	0.2455392688816356
0.5778134893189087	0.1932355395570715	0.2424248248916807
0.7108506583997559	0.2555231306099418	0.2422721366718961
0.7759553547485908	0.1884401925852059	0.2480358292490855
0.9085057639934241	0.2557179996478532	0.2509533730268060
0.9752989343992593	0.3894668094170787	0.2442713275959232
0.1065673023575127	0.4578229223074275	0.2502830035715868
0.1708798367589769	0.3922398197132766	0.2681817589704522
0.2994148702775633	0.4654456738727584	0.2817651658122740
0.7138767093234432	0.4526163834601782	0.2245050939943010
0.7795536874067491	0.3877743808140337	0.2333556716349635
0.9114428900654057	0.4565722984250136	0.2328896896559677
0.9785667988304564	0.5905084062754099	0.2259219787459670
0.1098652154501209	0.6590487023552486	0.2320165895292161
0.1736959365709615	0.5917926332986442	0.2436960964981829
0.3053422371780687	0.6604399106390988	0.2482296216288371
0.3702698779599791	0.5956128420933913	0.2640241947162024
0.7838530937679126	0.5820890726458842	0.2054744628578412
0.9135625801275901	0.6564044940644278	0.2124796058830432
0.9774688143651155	0.7919071645452752	0.2159121886946966
0.1097580363233523	0.8597598757806507	0.2254846977888843
0.1763488921658239	0.7931446362254926	0.2291913519218625
0.3088362867307065	0.8604072083624940	0.2348312700767042
0.3738462977072236	0.7931624203318329	0.2416648190904167
0.5066571881158806	0.8559922197790378	0.2447629915237386
0.5683071964504113	0.7839112818301630	0.2481152011402539
0.7047785412254035	0.8521253310794804	0.2400982767412877
0.7768851356992481	0.7959541447440700	0.2201514284721520
0.9086773613357055	0.8575389062161475	0.2237224139259573
0.3785965254697704	0.3973466371092277	0.3306120126903503
0.6945986285726387	0.6460305362896995	0.1713777387308352
0.5865326421891910	0.3955122346227100	0.2384181760674956
0.4987523493139295	0.6552212486418344	0.2613810959154809
0.5494360804135919	0.5285564627656077	0.2642675007334752
0.6570381504441923	0.5934307968261645	0.3559687808182612
0.6396234069730488	0.5180067372335098	0.4225849371888151

FeNS₃C

1.00000000000000

12.3236999512000001	0.0000000000000000	0.0000000000000000
-6.1625538564999998	10.6730391195000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

C   S   N   Fe
44   3   1   1

Direct

0.9735771506187542	0.9902618909840085	0.2366791825289494
0.1068024701875908	0.0567597790402872	0.2413963893173178
0.1744854019901121	0.9915810127629855	0.2347777559596962
0.3083667187602850	0.0588810191598611	0.2376323853860352
0.3742250144361163	0.9918319283567615	0.2377152393185104
0.5072731515040362	0.0583328524024036	0.2383258883327735
0.5738326939617274	0.9921073743243440	0.2436351189556237
0.7072297490696747	0.0576073320033844	0.2429627968881669
0.7747197557850255	0.9927290438852080	0.2427635623806550
0.9075563208033101	0.0571464155172726	0.2423207873974615
0.9742904784118082	0.1902667933506568	0.2502606442230497
0.1049489173352636	0.2553151207516717	0.2646469398326660
0.1723585036453137	0.1880144787728358	0.2601757614222119
0.3038836787043019	0.2487916664417086	0.2698534514589354
0.3763561142392606	0.1933791511116246	0.2477701919170052
0.5122835670613300	0.2621077537681380	0.2378281753450458
0.5749967258908680	0.1918395234444476	0.2343305566044373
0.7085915891093212	0.2558228526057664	0.2329363948438587
0.7747367251835240	0.1901336687204660	0.2391226069708074
0.9076458688572604	0.2568809687488819	0.2438120279333623
0.9738918449590246	0.3898606602676176	0.2415592875541515
0.1050477211015772	0.4572397813381920	0.2556528704107089
0.1671409437725822	0.3887296913114940	0.2737995914453215
0.2931586998917519	0.4595663410203027	0.2987879912121106
0.7089807682894989	0.4514867848397384	0.2185869409389414
0.7764280495201630	0.3874956379498769	0.2259601074798443
0.9090239535517243	0.4565615614705675	0.2292518955201379
0.9752269073773272	0.5899221323560107	0.2258495313121321
0.1070141389888547	0.6578523972469047	0.2374076143610875
0.1714397467198529	0.5911042825263513	0.2544527090323405
0.3023641511904895	0.6598699713901037	0.2714834758860605
0.3580841908573281	0.5890907653347660	0.2973679768985524
0.7776318960974136	0.5815844168335789	0.2037538122658039
0.9085928615056961	0.6554180048194164	0.2122147945275847
0.9740036506182664	0.7903334948077223	0.2158848125329727
0.1066766150061934	0.8573711200953428	0.2264168554740511
0.1736235231929334	0.7910866441104426	0.2351991519147123

0.3069616906344110   0.8583261097801966   0.2441980725538071
0.3722580948925122   0.7929911187564171   0.2612443824768042
0.5073866966812278   0.8597462612259581   0.2582053403699236
0.5780023618297569   0.7993764478017412   0.2651403970473064
0.7075901918333750   0.8594450700829788   0.2443839449482877
0.7743763128297192   0.7968814627110139   0.2241898480833782
0.9061021345188542   0.8572238713126266   0.2230475706474824
0.3749811073976133   0.3844194661797072   0.3367343357411207
0.5165988735032054   0.6614321091813303   0.3302061191577522
0.6846501087586608   0.6467000216565454   0.1764573026766807
0.5800241048089019   0.3910422203129088   0.2306229057983663
0.5403384771162286   0.5162121681274270   0.2660344537159942

OH@FeNS$_3$C

1.00000000000000

  12.3236999512000001   0.0000000000000000   0.0000000000000000
  -6.1625538564999998   10.6730391195000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000   15.0000000000000000

C   S   N   Fe   O   H
44   3   1   1   1   1

Direct

0.9724929784047522   0.9909850058334547   0.2340999910914663
0.1059050763962291   0.0576934214396273   0.2378753606558341
0.1738481601122033   0.9927676463800795   0.2327722913976932
0.3077331163536853   0.0601237733825530   0.2378408599308200
0.3734516197858062   0.9930539613269271   0.2365170020396371
0.5064344291037496   0.0592743549092321   0.2368488132015382
0.5731545097278127   0.9926874248474056   0.2413982310981419
0.7064236688171565   0.0583403439084298   0.2397782618724764
0.7737694122451808   0.9933168197653901   0.2411939706417921
0.9065504823108529   0.0579308350550090   0.2382764531430535
0.9737517838426278   0.1914961135866363   0.2423275633057979
0.1045523382507506   0.2571294143438748   0.2558861697390163
0.1714698350756178   0.1892821605763689   0.2548050620083255
0.3021072318015958   0.2495450033133924   0.2691671309147815
0.3760116050297981   0.1943169320235667   0.2516035826078136
0.5127129531074978   0.2636348906276514   0.2451580439356340
0.5746052867584329   0.1926963821494220   0.2348798454077801
0.7079508520516300   0.2562158584560936   0.2302838758688523
0.7741022085637684   0.1906859745550348   0.2337271661299326
0.9071978244305329   0.2578951455702359   0.2355161437152484
0.9736889051117125   0.3907830027556325   0.2320820492368357
0.1048164604442966   0.4585585499095148   0.2456202547371559

S59

0.1668179358335023	0.3904871612103084	0.2638524694538459
0.2921042406671842	0.4615984999283826	0.2911989469230370
0.7094786363015669	0.4521434589275690	0.2231410873472374
0.7762839577377433	0.3879033743616603	0.2227768576709355
0.9087598127590611	0.4574882550124859	0.2220222847735904
0.9744380707941124	0.5908539979192593	0.2197033109635000
0.1064732174616765	0.6590953123185852	0.2302557506884944
0.1710809432013153	0.5923665708848350	0.2460561901093769
0.3011611117720941	0.6610097943482351	0.2657736415343777
0.3568285432640098	0.5906350945547506	0.2929503289678570
0.7754798535329684	0.5817452432423750	0.2073440754677591
0.9069681680749736	0.6562203349773204	0.2105476233918259
0.9726288427230246	0.7910537809694496	0.2147250241033400
0.1055251040039774	0.8584624390973699	0.2235186496596561
0.1727977874815282	0.7922367739162707	0.2303689780735339
0.3059851857324614	0.8594721318791040	0.2405466124212627
0.3711596215567886	0.7941321454460516	0.2576759856333847
0.5063952617238459	0.8605651684485716	0.2570486214227338
0.5768342793100193	0.8002390685755576	0.2682249710884421
0.7064258360989947	0.8603080338231028	0.2470901541788122
0.7728844485401966	0.7973511764707987	0.2275412978263224
0.9043586809035596	0.8574562604103085	0.2235082537216766
0.3675239584544543	0.3850873338992085	0.3346039190629895
0.5101373784892376	0.6653002433267993	0.3375238889308692
0.6783369153451356	0.6443254257668692	0.1877175286157455
0.5836191620144365	0.3925390522671799	0.2461821970269962
0.5574223858925886	0.5192476138062856	0.2988983520638702
0.6486316092905922	0.5452303576445401	0.4044449385318820
0.6950089793132522	0.5001938928512314	0.4067799536670352

O@FeNS$_3$C

    1.00000000000000
      12.3236999512000001   0.0000000000000000   0.0000000000000000
      -6.1625538564999998   10.6730391195000003   0.0000000000000000
       0.0000000000000000   0.0000000000000000   15.0000000000000000
   C   S   N   Fe   O
    44   3   1   1   1
Direct
   0.9726425330781150   0.9903492606831763   0.2335712928032544
   0.1059721707722216   0.0567965901003425   0.2376748121794827
   0.1735296580774823   0.9916166891180532   0.2328131894188531
   0.3074642264880270   0.0588490097589084   0.2376702557954074
   0.3732958947929620   0.9917876102117062   0.2362504259598386

0.5061299404036831	0.0580382239274025	0.2365830672314227
0.5729858938316486	0.9915875166347303	0.2412727242273724
0.7062739967493056	0.0576674588496929	0.2397881343195117
0.7738197237725597	0.9926618939533753	0.2409520675137354
0.9066763012631707	0.0573512730494221	0.2380796102041090
0.9738570735839278	0.1908964629988533	0.2432407032149249
0.1045950159601342	0.2563110802411752	0.2574806935730609
0.1715920442678804	0.1883438936349743	0.2554803835494836
0.3018652989265251	0.2481494779054364	0.2697350160337002
0.3756348084987014	0.1929270184136566	0.2512616015452413
0.5123974140164804	0.2624177595465085	0.2440087320131754
0.5741494180652632	0.1915757671546022	0.2344602560144627
0.7077849981282683	0.2557259586403102	0.2304664792746735
0.7739893362552001	0.1901695334598998	0.2343983043877394
0.9071529821106928	0.2572868449368865	0.2369318464796003
0.9734541568400921	0.3901030475925612	0.2343064596150268
0.1046175736703222	0.4576254966418633	0.2481548726239350
0.1670444074664319	0.3896312587119210	0.2662381314482664
0.2924377602730518	0.4607558742307709	0.2940839204226149
0.7079882121590317	0.4509710437529845	0.2209580239719904
0.7756606164850769	0.3873053127275709	0.2228961359604473
0.9081948703242838	0.4565606500015840	0.2234752573526808
0.9738196979628277	0.5897418144004982	0.2206847925420907
0.1059630450632077	0.6578634430647907	0.2316805959134302
0.1708912538267611	0.5913661077954742	0.2481900334711367
0.3012047051862977	0.6599996248876551	0.2675472058603514
0.3572973820692982	0.5899789382849776	0.2956725389797661
0.7747626926765396	0.5809045049139545	0.2050877852221707
0.9061928186916548	0.6549432267223465	0.2102481389272223
0.9723097847698821	0.7900015874858672	0.2147600616784334
0.1051173758149473	0.8571859628278036	0.2238988385956824
0.1724561594755418	0.7910040763898849	0.2311404859392383
0.3057111658937907	0.8581511716652058	0.2408728234917014
0.3710353426991995	0.7929213696495838	0.2582671796264552
0.5062658720303259	0.8593439316821092	0.2570887585206429
0.5770635746728219	0.7993752782545444	0.2689317204574734
0.7067511822294369	0.8596022036578327	0.2470369915228894
0.7731406350818822	0.7968347857330820	0.2262900752793361
0.9046768266986335	0.8570030892702217	0.2227731839407806
0.3663788988601400	0.3824070418740416	0.3371958925733496
0.5097172924009146	0.6672932609860881	0.3414769444847887
0.6782144548463402	0.6442096844076017	0.1894248156355031
0.5816241589787479	0.3912868751629173	0.2422139937548842
0.5641677005800937	0.5196790318092014	0.3158653185836902

0.6830122442301683   0.5718019851959411   0.3869994508649883

OOH@FeNS₃C

1.00000000000000
    12.3236999512000001   0.0000000000000000   0.0000000000000000
    -6.1625538564999998   10.6730391195000003   0.0000000000000000
     0.0000000000000000   0.0000000000000000   15.0000000000000000
  C   S   N   Fe   O   H
  44   3   1   1   2   1
Direct
0.9714011120269517   0.9892583142613706   0.2323912492823813
0.1048183067320464   0.0559016102955259   0.2361970740394395
0.1725820053993586   0.9908742555437164   0.2312697291066599
0.3064878069831795   0.0582357045306017   0.2358524554380975
0.3723084817470976   0.9912477461437976   0.2347830710047318
0.5052221410321170   0.0575744995928659   0.2346472964143351
0.5719685873499130   0.9909806354329821   0.2395539885172452
0.7052165321771870   0.0567290421554736   0.2378525010191882
0.7727052782849839   0.9917072221303352   0.2394362001119854
0.9054579144373650   0.0562310077872801   0.2365883344641489
0.9726708793900080   0.1897785357793213   0.2407090540000503
0.1034166103221605   0.2553461972424036   0.2543995090935443
0.1704983608783402   0.1875608908721887   0.2531220015352774
0.3011368526276154   0.2477652589445638   0.2668454181186664
0.3748031369756445   0.1925246629672680   0.2487930326867545
0.5116379602206782   0.2621048514545358   0.2415315422828694
0.5734080732264176   0.1909933591490000   0.2318629847560677
0.7067530169564440   0.2546048191964231   0.2272784889368397
0.7729347298681072   0.1890551078048027   0.2315666996416910
0.9060585644792705   0.2561910696696380   0.2336279124028749
0.9724750641470488   0.3890501250464923   0.2301920636184445
0.1035700036332583   0.4567363610460831   0.2441894543957563
0.1656475821823431   0.3886098840298393   0.2623265180255057
0.2911792444964477   0.4596197364480243   0.2893714291220337
0.7078835598660896   0.4500824902085483   0.2190301634956973
0.7749069093816661   0.3860656662565825   0.2191087341241697
0.9074177840993142   0.4555838468458877   0.2193943776479219
0.9731136469031199   0.5888774388545568   0.2176418913547241
0.1051036077729541   0.6571349963692660   0.2289206903687084
0.1697848454228160   0.5904826665686536   0.2447845734050894
0.2999243872671055   0.6591277928990977   0.2644631250542255
0.3557023256521282   0.5886262000974094   0.2910885961261511
0.7743309014043726   0.5800031819390138   0.2041171608326173

0.9056480661987097   0.6543045928764913   0.2083010908474416
0.9714051161595421   0.7892043730361916   0.2129945577416399
0.1041851604722932   0.8564813898557231   0.2222601207461111
0.1715201611069270   0.7903058991374999   0.2293548588471281
0.3047704465782481   0.8576399373599899   0.2394344119941429
0.3699836254834128   0.7923022145238156   0.2564358381639292
0.5052455339298040   0.8588466290141000   0.2554882659921224
0.5757621387079445   0.7985332009411688   0.2662892748677659
0.7053585096564862   0.8587107463737889   0.2452339313965387
0.7717716430042594   0.7957346763053406   0.2255983741148747
0.9032472435379855   0.8557950594356991   0.2216322312805141
0.3672444677539745   0.3833861810537579   0.3324170972706842
0.5093464036921341   0.6631013205637636   0.3351441641816439
0.6772703131400344   0.6429261001255192   0.1856499849808260
0.5820508884350599   0.3905977011783393   0.2411299841899270
0.5569561674026910   0.5184396707523093   0.2968795298896004
0.6498207466984933   0.5486045666754502   0.3990797859359215
0.7169343268249555   0.4769223989879814   0.4130590729163063
0.7694134658734880   0.5246992122395148   0.4635401212190010

O₂@FeNS₃C

  1.00000000000000

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   -6.1625538564999998   10.6730391195000003   0.0000000000000000
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   C   S   N   Fe   O
   44   3   1   1   2
Direct
   0.9718927623476940   0.9888798025562734   0.2335423386636788
   0.1057008251689908   0.0559016980338621   0.2363765513732378
   0.1733633862864128   0.9909659182737134   0.2320101026630487
   0.3074672904049165   0.0583538068754170   0.2370971293608963
   0.3731388599008981   0.9913018953525148   0.2361461446376868
   0.5059692938667617   0.0573805820109939   0.2363682717827448
   0.5729117616994662   0.9909018594598666   0.2413909814818157
   0.7061422546102235   0.0566430505606761   0.2394013958905953
   0.7735706837222420   0.9916101943219841   0.2415766311549234
   0.9063095164107101   0.0561241247695574   0.2374488779443676
   0.9737672180224772   0.1898821191308962   0.2399321942243847
   0.1047630972115728   0.2559152104161931   0.2521128633026965
   0.1721517941289184   0.1883500517888337   0.2514735560185609
   0.3028755132179239   0.2490599028743965   0.2646054139615854
   0.3760062418879304   0.1924451436198433   0.2499218255382353

0.5128931377719200	0.2618371266742343	0.2457868844205895
0.5743649580611241	0.1910247384219381	0.2344593597260089
0.7079013766491525	0.2545621673832389	0.2291739101908340
0.7738870598465187	0.1889873072918519	0.2322589298752067
0.9071282891590768	0.2562255033724215	0.2330875832389355
0.9733626748632339	0.3889827233645508	0.2290019406972475
0.1045976472020304	0.4569720755821130	0.2419080883401270
0.1670468635761067	0.3891495131401259	0.2589641423836526
0.2928220495735147	0.4605335642741457	0.2851590139714619
0.7093086287105320	0.4502447468306962	0.2247874227056882
0.7760014416480707	0.3860752471457382	0.2215317901176712
0.9083439316234452	0.4556992738742106	0.2195580816868195
0.9736666864316151	0.5889438027717744	0.2178231215114211
0.1058534396159029	0.6573414417276291	0.2282611459640775
0.1707707714679281	0.5907546693292522	0.2431289484099624
0.3007916306095355	0.6594245959214299	0.2631974827843197
0.3569437488049252	0.5888867274023818	0.2887955046362969
0.7742470549042479	0.5796430268479049	0.2089835045672788
0.9057091661927781	0.6541111254026244	0.2104899970109852
0.9716399595674184	0.7889472498058716	0.2152826497450819
0.1046415490609350	0.8564424681673701	0.2231512479853777
0.1722116476792557	0.7904136380312123	0.2293598011389465
0.3053969311876945	0.8576754497894341	0.2398173568572872
0.3706697077126259	0.7924600752149777	0.2567085241184766
0.5059274382264443	0.8587683859498693	0.2574324345519834
0.5765627180449158	0.7987423922928857	0.2700027557800818
0.7061905834416989	0.8587833807262911	0.2493658092014373
0.7713436164565209	0.7942258776101029	0.2310324141681452
0.9030903810773611	0.8548605318525658	0.2247291133687017
0.3699996075168078	0.3866643099488838	0.3281744469386842
0.5076127818780842	0.6622041046842926	0.3377110109353192
0.6729674647268329	0.6389838440617320	0.1966341265181085
0.5847005054903356	0.3908081306252478	0.2500811358156411
0.5635860541622321	0.5171644686863042	0.3161957189518739
0.7164735101393290	0.5846013241294290	0.3948349970666477
0.6012251450327047	0.5072006736202427	0.4317753796211836

FeS$_4$C

1.00000000000000

12.3236999512000001	0.0000000000000000	0.0000000000000000
-6.1625538564999998	10.6730391195000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

C	S	Fe
44	4	1

Direct

0.9738879000143682	0.9909480472762777	0.2426214774076872
0.1059649504637346	0.0557000190554158	0.2490937385134321
0.1722512572430025	0.9887209281558045	0.2452287935144735
0.3046990164806375	0.0530077140114660	0.2466651428079134
0.3731996553497962	0.9891804690892000	0.2463863441543806
0.5066188828460464	0.0563905942121187	0.2431627177483862
0.5739134951678305	0.9915518377253348	0.2487156741102403
0.7072154601647572	0.0584604053749106	0.2446496782542898
0.7753589086328814	0.9942173844389348	0.2455756678809380
0.9076950054566476	0.0580474588691901	0.2456949104234047
0.9739067177372345	0.1908462683147093	0.2528412081797783
0.1045292263944595	0.2552089731165310	0.2681330747401633
0.1718694186576496	0.1875246402961839	0.2648212637876055
0.3029232504534199	0.2467618192482980	0.2699787512030788
0.3714025433148074	0.1862048214796151	0.2482058611576830
0.5005090661975853	0.2476357251999934	0.2262158816575961
0.5724756718075407	0.1884035390262118	0.2281745501601577
0.7073310136738385	0.2555245801933488	0.2211961350409557
0.7737882437978989	0.1910407217500786	0.2353587663262847
0.9073052294675065	0.2574901999045303	0.2429986920855594
0.9738652899564035	0.3902411751844982	0.2417782052924395
0.1048156153942797	0.4567634213521805	0.2589268407081114
0.1673992484437827	0.3884243636686735	0.2766722504675981
0.2948039503071977	0.4590231743117986	0.2996379540877595
0.7195306658995912	0.4588960643338195	0.1908361973581968
0.7775892655435536	0.3883766242629387	0.2104339748985999
0.9093467031128042	0.4567623807767697	0.2247319434026061
0.9762391242397692	0.5905311983844441	0.2245586616286379
0.1072687233697067	0.6570392582567597	0.2416697339983676
0.1716519421512469	0.5905111671134635	0.2589370503850529
0.3025727001920271	0.6588761692579749	0.2767853933151840
0.3594986614223230	0.5884403938519548	0.2997676656632042
0.7842189275776332	0.5881097850010619	0.1904369195111663
0.9128263874917779	0.6588585442951959	0.2099679739559677
0.9754460231662292	0.7918034055790180	0.2205953679548850
0.1062888099941633	0.8561929379971088	0.2353936843390705
0.1733626043058740	0.7897491474084534	0.2431401446499299
0.3066037278862019	0.8563202898845678	0.2530081737707027
0.3729273453828514	0.7920053190489518	0.2680786480793719
0.5079353569526862	0.8597226304532272	0.2642765210079911
0.5796678330083903	0.8004053204673225	0.2687987770893700
0.7086818642371026	0.8610165036974095	0.2467793048352251
0.7765025955114130	0.7997344703931327	0.2248015953440381
0.9077316172604631	0.8590331422819825	0.2271882796859450

0.3846029139317279   0.3884982848576458   0.3282110450347678
0.5201172533308005   0.6593201611381858   0.3277841587327984
0.6924475065918799   0.6581652355019003   0.1669151938941801
0.5576100177320193   0.3887655655790910   0.1677013801909670
0.5373529742844496   0.5237087269223110   0.2461986515638770

OH@FeS$_4$C

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    0.0000000000000000   0.0000000000000000   15.0000000000000000

  C   S   Fe   O   H
  44   4   1   1   1

Direct

0.9725631325097726   0.9923766804075665   0.2375936189180659
0.1048246380275178   0.0572207987703940   0.2425658935279849
0.1708638501792618   0.9898562517883079   0.2397014180917192
0.3031454060842818   0.0541978590479531   0.2419072330736148
0.3717823519405500   0.9902315338464112   0.2405707600927136
0.5050369118330399   0.0573700959111733   0.2380487230609646
0.5724824938593430   0.9924876966939868   0.2424837220737520
0.7058767420513211   0.0598166048713354   0.2395370248283827
0.7738215658095005   0.9954489503117506   0.2415309276517118
0.9064353737225324   0.0594779914427995   0.2403491361742606
0.9728095906214940   0.1924351724423577   0.2454989309050035
0.1037400274226829   0.2570938743988234   0.2597860382393900
0.1705083108518945   0.1890331176480058   0.2575117223329124
0.3014714309305970   0.2485567583923400   0.2663808717556040
0.3696113945568129   0.1871333493438659   0.2461475901461026
0.4992597949891182   0.2489773714306422   0.2259695911717080
0.5713406424035169   0.1900362305802440   0.2260720568919700
0.7059451840835217   0.2571161187514174   0.2181095944995571
0.7724908371642417   0.1923302015636787   0.2305906346855145
0.9060086520767495   0.2587547252849876   0.2363773567041595
0.9729592713618533   0.3914588555380129   0.2339718051899427
0.1044860225186244   0.4580401572346108   0.2499211434998110
0.1675279153017706   0.3902633497461314   0.2678816791118703
0.2949835553113580   0.4603475803440626   0.2930052570250942
0.7168524229899041   0.4600081688444697   0.1892606417318113
0.7756423060788662   0.3895235815150411   0.2063161175788436
0.9082030597684683   0.4579983948502092   0.2179300140614511
0.9750629344210809   0.5917674247826213   0.2177384696961875
0.1063266068437367   0.6582534337305970   0.2336637739254460

0.1712899460550086	0.5916957856460623	0.2497607801660365
0.3020422014811331	0.6595130913000267	0.2677712890319774
0.3594917427470157	0.5895791285666285	0.2931341946629801
0.7816568948227614	0.5896255745361413	0.1891653507615229
0.9109244963406650	0.6601688214734335	0.2060285277257386
0.9736918564043743	0.7926102669494595	0.2176358291367631
0.1049142861491010	0.8573140439889332	0.2303693359169263
0.1720828705549882	0.7909572408783190	0.2361213957503689
0.3051752877301427	0.8572706598832790	0.2454386060384726
0.3715119946783149	0.7926682347063359	0.2597502935420825
0.5063914101292002	0.8605979265444469	0.2572804026925362
0.5777807977868370	0.8010032079930245	0.2661484591862183
0.7073915247959360	0.8625231512553776	0.2456183824053145
0.7753152213707079	0.8010393337817315	0.2251216160319919
0.9062633038653056	0.8598030262744931	0.2253025828769225
0.3731087526702233	0.3837694093794095	0.3330160805050444
0.5137479052180373	0.6668513831832487	0.3341418597508378
0.6841345175622737	0.6540361354815253	0.1791519727565426
0.5548318299274292	0.3949087602545348	0.1778838904159334
0.5794017715089356	0.5246515104015776	0.3138394963107362
0.6918066133220263	0.5407214850956307	0.3996047073140746
0.6961025241661707	0.4692003959125804	0.4224733253754305

O@FeS₄C

1.00000000000000

12.3236999512000001	0.0000000000000000	0.0000000000000000
-6.1625538564999998	10.6730391195000003	0.0000000000000000
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C	S	Fe	O
44	4	1	1

Direct

0.9730906229551148	0.9913774854224433	0.2388257822183740
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0.3721009528126797	0.9887569316668882	0.2417736465565826
0.5053655023381647	0.0559243282857949	0.2388694778440644
0.5728550542805511	0.9910779125807211	0.2436244078253504
0.7062392992453513	0.0586785184057966	0.2410483151890346
0.7743722192181095	0.9943820770257854	0.2426353913336964
0.9069986457855530	0.0585644388378823	0.2417111431177840
0.9732759708521461	0.1914542681147207	0.2476244164828853
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0.3702021236889123	0.1859539435683811	0.2457935564054726
0.4994067072302913	0.2474011476772333	0.2244469773780789
0.5715000410165555	0.1884957920370355	0.2259928061356837
0.7063025365539616	0.2560128912033980	0.2195112389083102
0.7728427116333880	0.1913481250675780	0.2327836046096413
0.9063515377491727	0.2577701653506093	0.2392641845950153
0.9730270529356316	0.3904581300696798	0.2377034755100340
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0.2957797096091940	0.4589968404296361	0.2947389977876115
0.7172748598267621	0.4587983344299931	0.1897089068521495
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0.1062247014253441	0.6568481889310204	0.2377257120101620
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0.3025115979416829	0.6582245502492616	0.2704872753165166
0.3604405004781963	0.5882920249590115	0.2947076474247736
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0.9110841728514965	0.6588359918506260	0.2082314712520801
0.9739328799218750	0.7912763442429949	0.2195252330364801
0.1051429087544252	0.8559606679640999	0.2328204603530178
0.1722304057680306	0.7895407354128167	0.2393074812623363
0.3054842793406002	0.8558701179029755	0.2476540738841258
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    0.3718481561362137   0.9911911727405839   0.2400185217239538
    0.5051596196904088   0.0583904288427686   0.2373474354230709
    0.5725736929518930   0.9935165114291464   0.2421863881566854
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    0.4993190736168752   0.2499141470416766   0.2258004396154577
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    0.1673242525573808   0.3911647105639916   0.2686455992448537
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    0.3022308070520251   0.6604795791479221   0.2677282397744880
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    0.3053376781967191   0.8582509764817359   0.2450283035782261
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    0.5065037731718935   0.8616373502268169   0.2570489958480662

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0.9064403937251420	0.8608258431790645	0.2253090336503118
0.3722770217481154	0.3842297310358720	0.3347309727968792
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0.6852660902419362	0.6559529860190758	0.1767890875738726
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0.5777675643253337	0.5259097837830777	0.3133370590050827
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0.6906157153320942	0.4229097486240364	0.4088288582618149
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   C    S    Fe    O    H
   44    4    1    2    1
Direct
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0.3718481561362137	0.9911911727405839	0.2400185217239538
0.5051596196904088	0.0583904288427686	0.2373474354230709
0.5725736929518930	0.9935165114291464	0.2421863881566854
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0.7740469441063427	0.9966622628604693	0.2415217388126899
0.9066099055261693	0.0606099583461734	0.2404347444428905
0.9729008330574148	0.1935509302187325	0.2455939284257215
0.1037457205242932	0.2580563696569322	0.2605511177261394
0.1705964221526793	0.1899369690875235	0.2583324275375590
0.3015403139353829	0.2493365615940243	0.2674090373408369
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0.9731570871584245	0.3925511904580266	0.2332403684301433
0.1045271347678031	0.4590291088166626	0.2497853210752858

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