

## Supporting Information

### Predictions of Chemical Shifts for Reactive Intermediates in CO<sub>2</sub>

#### Reduction under *operando* Conditions

Hao Yang<sup>a,†</sup>, Fabio Ribeiro Negreiros<sup>b,c,†</sup>, Qintao Sun<sup>a</sup>, Miao Xie<sup>a</sup>, Luca Sementa<sup>b</sup>,  
Mauro Stener<sup>d</sup>, Yifan Ye<sup>e</sup>, Alessandro Fortunelli<sup>b,f,\*</sup>, William A. Goddard, III<sup>f,\*</sup>, Tao  
Cheng<sup>a,\*</sup>

<sup>a</sup>*Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, Suzhou, 215123, Jiangsu, PR China;*

<sup>b</sup>*CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche, Pisa, 56124, Italy;*

<sup>c</sup>*INFIQC, CONICET, Universidad Nacional de Córdoba, Córdoba, 5000, Argentina;*

<sup>d</sup>*Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, Trieste, 34127, Italy;*

<sup>e</sup>*National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, 230029, China;*

<sup>f</sup>*Materials and Process Simulation Center, California Institute of Technology, Pasadena, CA 91125, U.S.A.*

\*To whom correspondence should be addressed.

E-mail: Alessandro Fortunelli: [alessandro.fortunelli@cnr.it](mailto:alessandro.fortunelli@cnr.it);

William A. Goddard, III: [wag@caltech.edu](mailto:wag@caltech.edu);

Tao Cheng: [tcheng@suda.edu.cn](mailto:tcheng@suda.edu.cn);

Electronic structure calculations were performed within the density functional framework, as implemented in the Vienna ab initio simulation program (VASP), a plane-wave pseudopotential package. The exchange and correlation energies were calculated using the Perdew, Burke, and Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). Spin polarization did not have an appreciable effect on the overall energies. For example, the total energies are different by less than 0.01 eV for adsorbed hydrogen (H\*) on Cu(100) surface. The calculations were therefore carried out without spin polarization to reduce computational demands. The vdW corrections has been applied to all elements.

We used plane-wave cutoff energy of 400 eV and the First order Methfessel-Paxton scheme with a smearing width of 0.2 eV. Dipole corrections were applied along the z-axis. The PBE-D3 method was employed to correct van der Waals interaction of water-water and water-Cu.

For the vacuum Quantum Mechanics (v-QM) calculations, we employed a  $4 \times 4 \times 3$  Cu(100) surface slab with the bottom two layers fixed with vacuum layers of at least 15 Å. We investigated 22 reactive intermediates during carbon dioxide reduction reactions (CO<sub>2</sub>RR) and carbon monoxide reductions (CORR). The convergence criteria were  $1 \times 10^{-5}$  eV energy differences for solving the electronic wave function. All geometries (atomic coordinates) were converged to within  $1 \times 10^{-3}$  eV/Å. The Hessian matrix and vibrational modes of surface species were computed with finite differences methods as implemented in VASP.

For the explicit solvation calculations, we simulate the water/Cu(100) interface using 48 explicit water molecules (5 layers, 1.21 nm thick) on a  $4 \times 4$  Cu (100) surface slab (3 layers) with an area of 1.02 nm<sup>2</sup> with the bottom two layers fixed. The simulation box is 40 Å along the z-axis with a vacuum of 24 Å. The lateral dimensions of the slab were fixed using the 3.61 Å lattice constant.

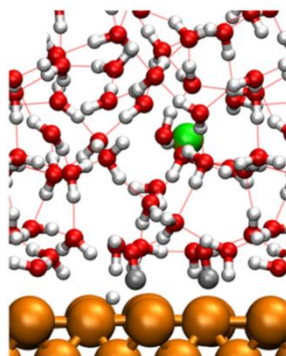
We calculate the potential of zero charge (PZC) of Cu(100) in contact with explicit water to be 3.61 V, which corresponds to -0.38 V (RHE) ( $3.61 - 4.40 + 0.0592 \times 7 = -$

0.38 V), close to the onset potential [ -0.30 V (RHE)] of CO production at pH 6.8. (7) We find that including one extra Na solvated in the solution leads to a work function of 3.40 ( $\pm 0.25$ ) eV, which corresponds to -0.59 V (RHE) ( $3.40 - 4.40 + 0.0592 \times 7 = -0.59$  V), close to the potential [-0.60 V (RHE)] with maximum C<sub>2</sub>H<sub>4</sub> production at pH 7.

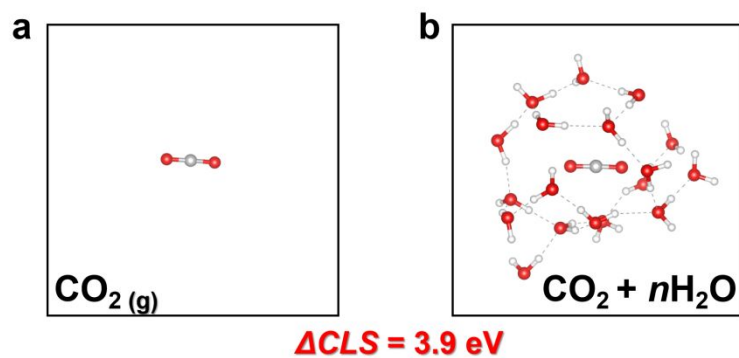
To equilibrate the interface, we first carried out 2 ns reactive force field (ReaxFF) Molecular Dynamics (MD) simulations at 298K as we did in our previous work. The ReaxFF MD (RMD) simulations were carried out using LAMMPS with a version of 22 Aug 2018. The time step of RMD simulation is 0.25 fs, and the temperature was controlled by coupling a Nose-Hoover thermostat with a temperature damping parameter of 25 fs. In QM-MD, the convergence criteria were  $1 \times 10^{-5}$  eV energy differences for solving the electronic wave function. From the 2ns RMD generated the interface, we carried out 22 ps QM-MD simulation (2ps for equilibration and 20 ps for production) at 298K with a time step of 1.0 only using the gamma point of the Brillouin zone with no consideration of symmetry. The temperature was controlled by coupling a Nose-Hoover thermostat with a temperature damping parameter of 100 fs. The simulated potential energies of 2ns QM-MD and 20 ps QM-MD simulation are shown in Figure S1. The potential energies of 20 ps QM-MD production oscillated around the average values indicates an equilibration of interface structure from the simulations that combines 2ns RMD and 2 + 20 ps QM-MD simulation.

The calculations with the ADF program were performed employing Slater Type Orbitals (STO) as basis functions, with Triple Zeta plus Polarization (TZP) quality for all the atoms. Except that the atom carrying the core hole uses a much larger STO basis set with even-tempered exponents of size 6S 4P 2D 1F. This is designated as ET-QZ3P in the ADF database. This large basis set for the core-hole atom is crucial for a complete description of relaxation/polarization effects following core-hole formation, especially for the relatively shallow core the 1s orbital of carbon. Binding energies are calculated via a  $\Delta$ SCF approach, as total energy differences between the ion and the ground state configuration. Calculations were always performed using spin-unrestricted wavefunctions for open shell electron configurations. The computational effort of these

small-molecule simulations is negligible compared to the simulations on the large electro-catalytic system.



**Figure S1.** Snapshot of the atomic structure of the water/Cu(100) electrode. The colors are C in gray, H in white, O in red, Cu in orange, and Na in green. Hydrogen bonds are shown with the red dashed line.



**Figure S2.** The optimized structures of (a) CO<sub>2</sub> gas, (b) CO<sub>2</sub> gas surrounded by a large number of water molecules (denoted as CO<sub>2</sub> + nH<sub>2</sub>O), the color code are same as Fig. S1. Note that the CLS of CO<sub>2</sub> + nH<sub>2</sub>O is lowered than CO<sub>2(g)</sub> about 3.9 eV.

**Table S1.** The calculated binding energy of  $C_{1s}$  for several species on Cu(100) is referred to as a vacuum. Note that the change of core-level shifts (CLS) due to the work function's effect can be neglected.

Species	$C_{1s}$	Vacuum-level	total ( $C_{1s}$ + vacuum)	delta ( $C_{1s}$ )	delta (total)
<i>l</i> -CO <sub>2</sub>	-271.90	2.72	-269.18	-1.67	-1.67
<i>b</i> -CO <sub>2</sub>	-270.23	2.72	-267.51	0	0
*CH <sub>3</sub>	-267.03	2.79	-264.24	3.21	3.27
*CO	-270.04	2.76	-267.28	0.19	0.24
*CCO	-267.47	2.73	-264.74	2.76	2.77
*CCO	-269.42	2.73	-266.69	0.81	0.82

**Table S2.** Calculated work function and Applied potential (U) for each species on Cu(100) surface.

Species	Work function / eV	U / V
* <i>l</i> -CO <sub>2</sub>	4.3323	-0.3477
* <i>b</i> -CO <sub>2</sub>	4.4011	-0.2789
*COOH	4.4230	-0.257
*CO	4.4016	-0.2784
*CHO	4.4133	-0.2667
*CHOH	4.3870	-0.293
*CH	4.4373	-0.2427
*CH <sub>2</sub>	4.2944	-0.3856
*CH <sub>3</sub>	4.4659	-0.2141
*CH <sub>4</sub>	4.4648	-0.2152
*OC-CO	4.4540	-0.226
*OCCOH	4.5301	-0.1499
*HOC-COH	4.3234	-0.3566
*C=C=O	4.2720	-0.408
*CCOH	4.2684	-0.4116
*CHCOH	4.3221	-0.3579
*CCH	4.3418	-0.3382
*CCH <sub>2</sub>	4.3506	-0.3294
*CHCH <sub>2</sub>	4.3285	-0.3515
*C <sub>2</sub> H <sub>4</sub>	4.3020	-0.378



**Table S3.** The changes of charge (e-), work function (W), and CLS (eV).

	*I-CO <sub>2</sub>		*COOH		*CO	
	CLS	Work Function	CLS	Work Function	CLS	Work Function
+0.4 e	278.88	5.547	277.67	5.6675	277.57	5.4605
+0.2 e	278.71	4.7124	277.40	4.8379	277.27	4.6887
0 e	278.50	4.3038	277.12	4.3883	276.97	4.374
-0.2 e	278.19	4.1348	276.83	4.2685	276.64	4.2056
-0.4 e	277.81	3.9933	276.52	4.1423	276.29	4.0833

Note here '+' is referred to withdraw electrons, and '-' is giving electrons to the systems, respectively.

**Table S4.** Comparison of calculated C 1s binding energy for important reactive intermediates in CO<sub>2</sub>RR. Note that we chose CO as the reference here.

Species	C 1s binding energy (eV)	Relative difference (eV)
CO <sub>(g)</sub>	280.68	0
* <i>l</i> -CO <sub>2</sub>	278.50	2.18
* <i>b</i> -CO <sub>2</sub>	277.27	3.41
*CO	276.99	3.69
*CHO	276.63	4.05
*OC-CO	275.51	5.17

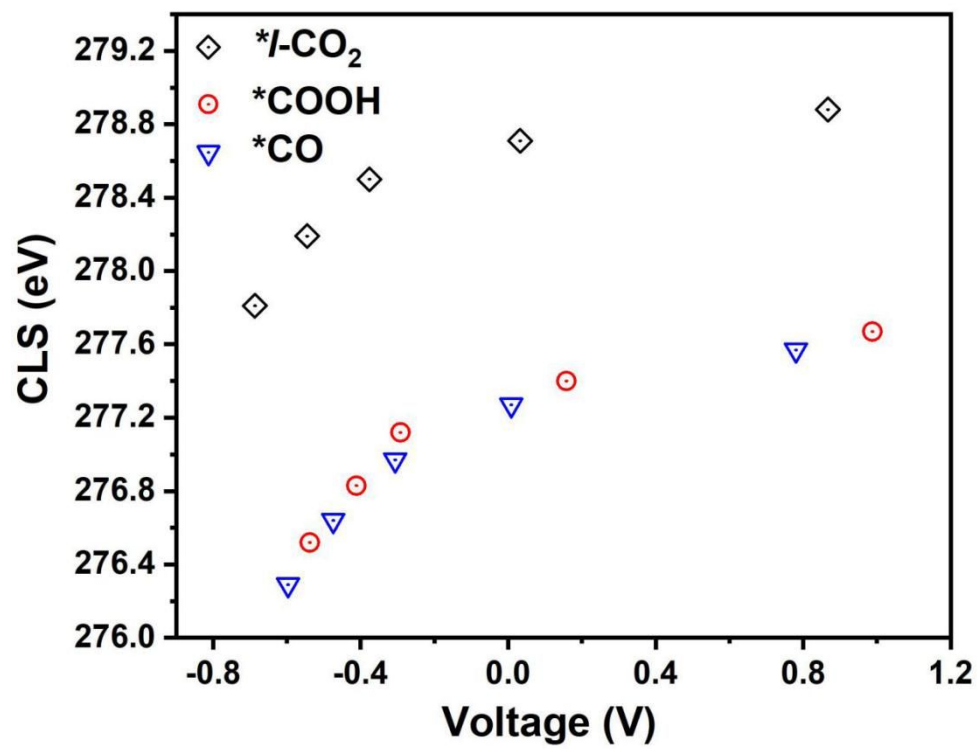


Figure S3. The changes of CLS (eV) as a function of Voltage (V)

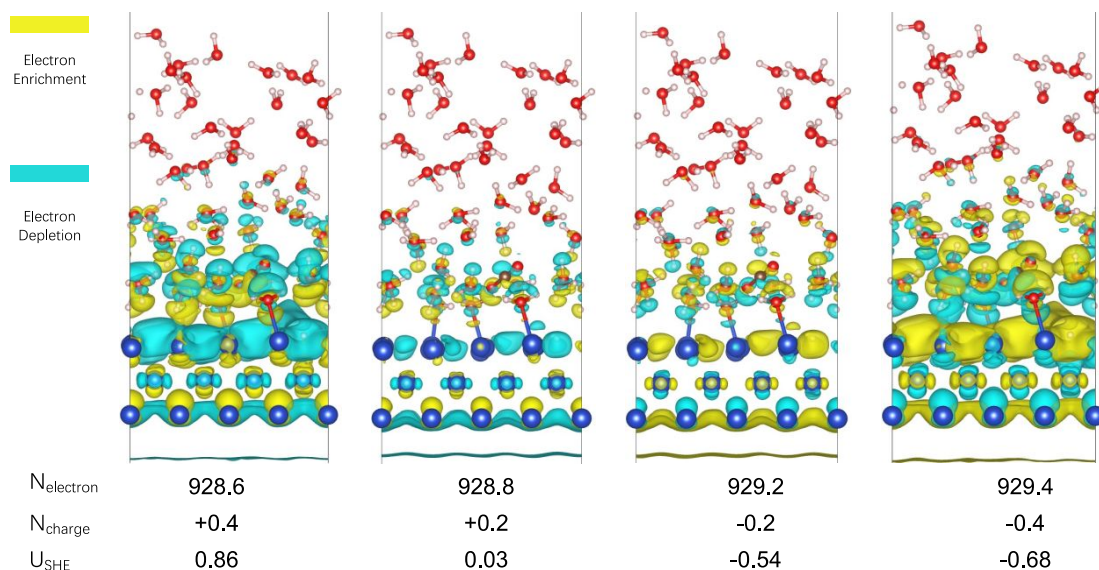


Figure S4. The charge density differences of different number of total electrons ( $N_{\text{electron}}$ ) of *l*-CO<sub>2</sub> adsorption on Cu(100) surface. The neutral case with  $N_{\text{electron}}$  of 929 is taken as reference.  $N_{\text{electron}}$  of 928.6, 928.8, 929.2 and 929.4 are considered with net charge ( $N_{\text{charge}}$ ) of +0.4, +0.2, -0.2 and -0.4 and applied voltage ( $U_{\text{SHE}}$ ) of 0.86, 0.03, -0.54, -0.68. The yellow color represents electron enrichment, and the light blue color represents electron depletion.

We carried out analysis of charge density differences to investigate the electron redistribution at different number of total electrons by taking the neutral case as reference. The plots of *l*-CO<sub>2</sub> are shown in Figure S4. As expected, the electron enrichment and depletion mainly occur in Cu electrode, but slightly leaks to the first layer of water and adsorbent. Such leakage increases as the number of electrons included increasing, which might correspond to a physical effect or might be due to a flaw of PBE-PW that requires further investigation.

We also carried out Bader charge analysis to quantitatively estimate the number of electron transfer in Cu electrode. As shown in Figure S5, charge transfer follows a non-linear trend, which well agrees with the non-linear trend of CLS as a function of  $U_{\text{SHE}}$ , as shown in Figure S3.

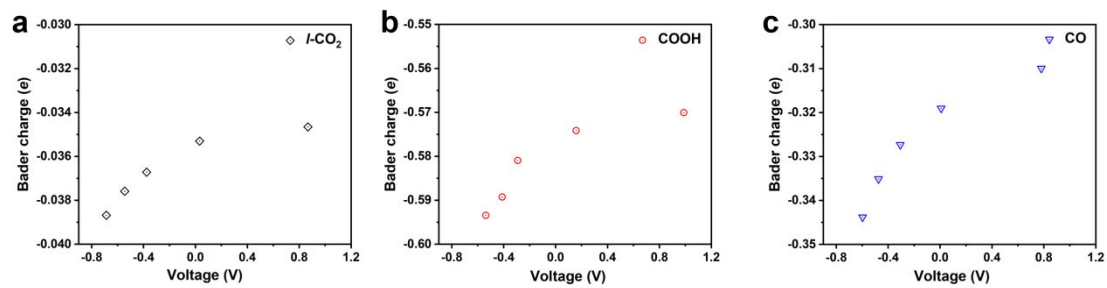


Figure S5. The changes of charge difference ( $e$ ) as a function of Voltage (V) for (a)  $l$ -CO<sub>2</sub>, (b) COOH, and (c) CO, respectively.

## Structural information: coordinates for all predicted intermediates

01-CO<sub>2</sub>

xyzjob

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10.227000000000000  0.000000000000000  0.000000000000000
0.000000000000001  10.225000000000000  0.000000000000000
0.000000000000002  0.000000000000002  40.000000000000000

Cu    O    H    C
48    50   97   1
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Selective dynamics

Direct

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0.299140326917639	0.431926946115413	0.398954270000000	T	T	T
0.883219570424504	0.711858836559814	0.635702110000000	T	T	T
0.755750937476787	0.775008488915961	0.628191420000000	T	T	T
0.134385573107676	0.494045728433095	0.606576760000000	T	T	T
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0.027284720630957	0.923864204469848	0.541120730000000	T	T	T
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02-b-CO<sub>2</sub>

xyzjob

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0.000000000000002	0.000000000000002	40.000000000000000			
Cu	O	H	C		
48	50	97	1		

Selective dynamics

Direct

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0.034532130798553	0.789076679440851	0.418890710000000	T	T	T
0.144871133350151	0.825542500801418	0.392195980000000	T	T	T

0.694030346049496	0.089800543350504	0.479380390000000	T	T	T
0.619769164332199	0.998438907252264	0.505911810000000	T	T	T
-0.014782330341840	0.899026153543130	0.610983840000000	T	T	T
0.874152450214833	0.932071054776049	0.583209200000000	T	T	T
0.214827764967908	0.795569059683090	0.539465260000000	T	T	T
0.240711415566461	0.962720255919589	0.535919060000000	T	T	T
0.759296847558785	0.571680291329682	0.639101190000000	T	T	T
0.611268194135612	0.525191139595149	0.648515650000000	T	T	T
0.885605560479681	1.062816299654220	0.376098410000000	T	T	T
0.929443061493429	0.999503967292000	0.409380080000000	T	T	T
0.540678132503217	0.813658650358024	0.404096170000000	T	T	T
0.487395801271057	0.900993083616509	0.373590650000000	T	T	T
0.188888334368055	0.943415165199306	0.628209010000000	T	T	T
0.103629422396441	0.905518323785350	0.661930260000000	T	T	T
0.351297418123770	0.876706402710367	0.700761280000000	T	T	T
0.783043148107920	0.613331132883697	0.426407340000000	T	T	T
0.713797316506610	0.907658023865183	0.360430790000000	T	T	T
0.687615465901154	0.706199996348684	0.442362710000000	T	T	T
0.742136087161944	0.447877466710533	0.387973800000000	T	T	T
0.384057308881353	0.575979431490083	0.388919370000000	T	T	T
0.565029533066344	0.324551792109193	0.371865250000000	T	T	T
0.324438307502659	0.533777839915521	0.557555880000000	T	T	T
0.408260419441048	0.614363902922230	0.669777100000000	T	T	T

03-COOH

xyzjob

1.000000000000000

10.227000000000000	0.000000000000000	0.000000000000000	
0.000000000000001	10.225000000000000	0.000000000000000	
0.000000000000002	0.000000000000002	40.000000000000000	
Cu	O	H	C
48	50	98	1

Selective dynamics

Direct

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0.500050021563684	-0.000000000000000	0.800000010000000	T	T	T
0.750069997345419	-0.000000000000000	0.800000010000000	T	T	T
-0.000000000000000	0.249980009326885	0.800000010000000	T	T	T
0.250020005781725	0.249980009326885	0.800000010000000	T	T	T
0.500050021563684	0.249980009326885	0.800000010000000	T	T	T
0.750069997345419	0.249980009326885	0.800000010000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000010000000	T	T	T
0.250020005781725	0.499950008653389	0.800000010000000	T	T	T
0.500050021563684	0.499950008653389	0.800000010000000	T	T	T
0.750069997345419	0.499950008653389	0.800000010000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000010000000	T	T	T
0.250020005781725	0.750020057983628	0.800000010000000	T	T	T
0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T

0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
0.625010024453398	0.374960013989946	0.754830000000000	T	T	T
0.875040020235357	0.374960013989946	0.754830000000000	T	T	T
0.124960002889703	0.625040023320567	0.754830000000000	T	T	T
0.374989998671663	0.625040023320567	0.754830000000000	T	T	T
0.625010024453398	0.625040023320567	0.754830000000000	T	T	T
0.875040020235357	0.625040023320567	0.754830000000000	T	T	T
0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
-0.003787420087582	1.009312647657975	0.713571450000000	T	T	T
0.250406185790662	-0.001671660062367	0.712596080000000	T	T	T
0.504057601656360	1.005721167523971	0.711647920000000	T	T	T
0.744464117215782	-0.011910360444382	0.707242730000000	T	T	T
0.008026090185607	0.232498888674650	0.704281240000000	T	T	T
0.251242345809993	0.253849879471266	0.712210300000000	T	T	T
0.482040251147208	0.247919719250015	0.708444690000000	T	T	T
0.744673587220622	0.250787669357017	0.710793330000000	T	T	T
-0.003559550082312	0.510698269054416	0.705887370000000	T	T	T
0.238203815508477	0.487276798180548	0.708093480000000	T	T	T
0.501311841592862	0.508702078979931	0.705859830000000	T	T	T
0.743832627201173	0.497375948557349	0.712111620000000	T	T	T
0.009705130224435	0.761070038395912	0.710362940000000	T	T	T
0.245084945667605	0.755841288200821	0.709150890000000	T	T	T
0.490483421342456	0.754962708168049	0.708959500000000	T	T	T
0.739825707108516	0.737043747499482	0.710872560000000	T	T	T
0.309530227157905	0.525863069620225	0.652794970000000	T	T	T

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0.472012790915322	0.896774253459110	0.483393040000000	T	T	T
0.543553852569717	-0.005539780206690	0.599885150000000	T	T	T
0.719919466648186	0.982314176650640	0.655322260000000	T	T	T
0.421550959748391	0.570134541272010	0.572797700000000	T	T	T
0.411476839515430	0.967562296100244	0.369871220000000	T	T	T
0.788796328240960	0.263683809838181	0.347864820000000	T	T	T
0.169470133919008	0.580273161650288	0.570787500000000	T	T	T
0.020066890464046	0.094291653518073	0.444768500000000	T	T	T
0.223690725172866	0.636146113734934	0.394905150000000	T	T	T
0.249638325772905	0.408788805252117	0.490954430000000	T	T	T
0.417197719647727	0.341431752738993	0.541762680000000	T	T	T
0.694988426071653	0.151993585670963	0.558191380000000	T	T	T
0.847026039587533	0.384141814332528	0.582082860000000	T	T	T
0.805323408623154	0.990391776952020	0.468860260000000	T	T	T
0.888658740550288	0.584905831823139	0.528285100000000	T	T	T
0.089277972064554	0.800558129869232	0.364803790000000	T	T	T
0.502824261627838	0.715888096710152	0.388433600000000	T	T	T
0.415411449606414	0.404763495101936	0.372901390000000	T	T	T
0.825280369084658	0.757194688251325	0.625815240000000	T	T	T
0.042240170976806	0.199570077446063	0.574893880000000	T	T	T
0.104473402415958	0.847672751627100	0.536177340000000	T	T	T
0.078392251812829	0.605768612601535	0.481272430000000	T	T	T
0.769660317798445	0.783759679242474	0.563007050000000	T	T	T
0.514052201887484	0.809408910199462	0.546063770000000	T	T	T
0.715825146553495	0.526673799650464	0.477689150000000	T	T	T
0.272197026294573	1.017392947959453	0.310300240000000	T	T	T
0.278583776442270	0.263763959841164	0.586559130000000	T	T	T

0.593484083724357	0.111089084144792	0.456281980000000	T	T	T
0.636843314727036	0.773417818856616	0.444141930000000	T	T	T
0.824972419077540	0.698331846055120	0.380979080000000	T	T	T
0.243080555621257	0.811392420273467	0.472318760000000	T	T	T
0.076801541776044	0.704785126295892	0.626858730000000	T	T	T
0.090496662092745	0.188413537029809	0.505725820000000	T	T	T
0.872307340172162	-0.013660580509682	0.534100080000000	T	T	T
0.232875455385255	0.386886924434953	0.421146670000000	T	T	T
0.575641003311734	0.555909570741271	0.329461510000000	T	T	T
0.211761974897008	0.949660605432323	0.413032070000000	T	T	T
0.611386754138359	0.300562311214132	0.505253190000000	T	T	T
-0.065754581520583	0.093566203491002	0.626171020000000	T	T	T
0.146501533387855	0.950182055451775	0.645667860000000	T	T	T
0.769352737791327	0.498456258597662	0.641959010000000	T	T	T
-0.005283030122167	0.284087090599433	0.404305980000000	T	T	T
0.557438742890809	0.183834826858973	0.383911710000000	T	T	T
0.369061338534565	0.098983733693134	0.637611600000000	T	T	T
0.905440530938369	0.501472268710191	0.432085580000000	T	T	T
0.861499689922235	0.263256089822220	0.664757430000000	T	T	T
0.295184746826166	1.070624229945535	0.536770390000000	T	T	T
0.520050732026205	0.567762441183511	0.635961830000000	T	T	T
0.248942645756810	0.212721397936743	0.321751400000000	T	T	T
0.173968784023037	0.341896562756332	0.313816060000000	T	T	T
0.508575931760849	0.830712690994318	0.467426840000000	T	T	T
0.384211918884922	0.870363302473702	0.480342480000000	T	T	T
0.470739260885871	0.040230931501037	0.612824840000000	T	T	T
0.513010541863401	0.924064914477340	0.585808930000000	T	T	T
0.942405491793185	0.419346485646034	0.419392560000000	T	T	T



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0.782270598090056	0.027172411013819	0.640238280000000	T	T	T
0.323891207490007	0.578289561576284	0.567614630000000	T	T	T
0.461254060666530	0.647871274172411	0.560397150000000	T	T	T
0.475299120991317	0.045616831701985	0.372879910000000	T	T	T
0.755965047481734	0.333739362451990	0.331975290000000	T	T	T
0.235097005436628	1.003366257436108	0.540703440000000	T	T	T
0.155290213591092	0.614289962919472	0.593603580000000	T	T	T
0.050123711159118	0.135280385047384	0.466527130000000	T	T	T
0.936200251649692	0.046735841743736	0.452067580000000	T	T	T
0.211735604896402	0.551401240573066	0.407296410000000	T	T	T
0.305218947058209	0.678549495317027	0.401593910000000	T	T	T
0.199055284603168	0.339161102654279	0.501447680000000	T	T	T
0.322804757464877	0.416476795538963	0.507259350000000	T	T	T
0.492748021394827	0.331858262381799	0.525898810000000	T	T	T
0.445069150292256	0.425573755878376	0.553875330000000	T	T	T
0.643472914880346	0.089073473323374	0.572709750000000	T	T	T
0.730814376900127	0.225417618410445	0.571390830000000	T	T	T
0.826097259103549	0.422073415747775	0.603770890000000	T	T	T
0.844328359525149	0.451433946843227	0.564260940000000	T	T	T
0.862086739935807	0.663748344764792	0.543136380000000	T	T	T
0.139285803220993	0.533296299897555	0.488513820000000	T	T	T
0.142098843286047	0.856069701940401	0.350050410000000	T	T	T
0.140961293259734	0.726354127100645	0.372107030000000	T	T	T
0.471631930906512	0.805486850053125	0.380413620000000	T	T	T
0.339170127843326	0.387064544441574	0.358262420000000	T	T	T
0.376988618717884	0.430400596058464	0.393418040000000	T	T	T

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0.818079818918148	0.840439131357213	0.639420200000000	T	T	T
0.967435052371996	0.610326942771609	0.515139560000000	T	T	T
0.998519793090828	0.286279400681232	0.578086410000000	T	T	T
0.140520453249545	0.832416261057878	0.512893900000000	T	T	T
0.126218912918823	0.643185203997565	0.555142070000000	T	T	T
0.029530040682888	0.571977801340782	0.462114360000000	T	T	T
0.781857618080502	0.786824259356812	0.588394050000000	T	T	T
0.811342898762354	0.866054132312919	0.553406360000000	T	T	T
0.610778464124288	0.793880109620078	0.552892540000000	T	T	T
0.513544431875750	0.827726350882895	0.521044820000000	T	T	T
0.783554968119752	0.501287518703296	0.461453070000000	T	T	T
0.779225548019634	0.547248200418112	0.497894610000000	T	T	T
0.321860917443053	0.972896106299257	0.292066430000000	T	T	T
0.330659557646524	1.002880617417985	0.329046050000000	T	T	T
0.320741707417170	0.256458019568577	0.564098220000000	T	T	T
0.141836883279984	0.223219448328430	0.579693100000000	T	T	T
0.544974692602571	0.045088411682269	0.470413290000000	T	T	T
0.582987433481617	0.192244847172753	0.468402290000000	T	T	T
0.662294595315606	0.698120396047227	0.458243160000000	T	T	T
0.616636044259744	0.746497177852195	0.420442040000000	T	T	T
0.900759170830106	0.726381767101672	0.369005420000000	T	T	T
0.243739405636491	0.867067812350748	0.452605110000000	T	T	T
0.190545844406385	0.731589817295990	0.469770910000000	T	T	T
0.475278530990847	0.570911411300998	0.612104630000000	T	T	T
0.365235218446084	1.041633718863882	0.521807650000000	T	T	T
0.109048102521746	0.797190939743599	0.632118500000000	T	T	T
0.101583012349115	0.664953954809770	0.650449640000000	T	T	T

0.045288561047296	0.185564066923491	0.527927090000000	T	T	T
0.176707524086369	0.142237595306953	0.508909120000000	T	T	T
0.851219969684511	0.347424782962592	0.653239050000000	T	T	T
0.892994180650542	0.197814057380548	0.648310130000000	T	T	T
0.819759418956986	0.060264242248489	0.545343290000000	T	T	T
0.855268439778136	0.993444507065927	0.509829130000000	T	T	T
0.250889135801828	0.381560804236225	0.444722730000000	T	T	T
0.153221863543268	0.341396222737672	0.416129170000000	T	T	T
0.530082282258189	0.557492130800313	0.308915080000000	T	T	T
0.511321761824347	0.509502999009819	0.345250580000000	T	T	T
0.141323453268114	0.005484710204636	0.423455430000000	T	T	T
0.159754823694338	0.893086613321516	0.397509090000000	T	T	T
0.656974585192578	0.378439184119755	0.496048520000000	T	T	T
0.662597995322616	0.246447199195071	0.519537730000000	T	T	T
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0.231444425352166	1.002852517416939	0.642244650000000	T	T	T
0.135920803143180	0.940067335074396	0.670469500000000	T	T	T
0.800665828515449	0.588217831946709	0.646357470000000	T	T	T
0.673025855563762	0.511390229080235	0.639958930000000	T	T	T
0.932098621554835	0.266474459942298	0.384204860000000	T	T	T
0.000416090009621	0.199823767455530	0.417443480000000	T	T	T
0.560353002958199	0.172190006424499	0.408567380000000	T	T	T
0.502220131613875	0.265562949908293	0.381153670000000	T	T	T
0.349384958079544	0.186188396946787	0.626910370000000	T	T	T
0.383721838873589	0.116496614346552	0.661016720000000	T	T	T
0.359762488319527	0.872185082541672	0.691815780000000	T	T	T
0.775642707936785	0.895596753415169	0.463287660000000	T	T	T

0.710050816419967	0.230220148589633	0.360098850000000	T	T	T
0.731330676912066	0.049098041831873	0.464152160000000	T	T	T
0.759375067560594	0.702440436208411	0.363322560000000	T	T	T
0.344753067972436	0.980302756575599	0.386943170000000	T	T	T
0.516500291944099	0.664500244792841	0.368031390000000	T	T	T
0.019671010454894	0.890779863235452	0.536666440000000	T	T	T
0.270586786257338	0.357918253354112	0.590408080000000	T	T	T
0.430368419952293	0.535870259993594	0.659758630000000	T	T	T

04-CO

xyzjob

1.000000000000000		
10.227000000000000	0.000000000000000	0.000000000000000
0.000000000000001	10.225000000000000	0.000000000000000
0.000000000000002	0.000000000000002	40.000000000000000

Cu	O	H	C
48	49	97	1

Selective dynamics

Direct

-0.000000000000000	-0.000000000000000	0.800000010000000	T	T	T
0.250020005781725	-0.000000000000000	0.800000010000000	T	T	T
0.500050021563684	-0.000000000000000	0.800000010000000	T	T	T
0.750069997345419	-0.000000000000000	0.800000010000000	T	T	T
-0.000000000000000	0.249980009326885	0.800000010000000	T	T	T
0.250020005781725	0.249980009326885	0.800000010000000	T	T	T
0.500050021563684	0.249980009326885	0.800000010000000	T	T	T
0.750069997345419	0.249980009326885	0.800000010000000	T	T	T

-0.000000000000000	0.499950008653389	0.800000010000000	T	T	T
0.250020005781725	0.499950008653389	0.800000010000000	T	T	T
0.500050021563684	0.499950008653389	0.800000010000000	T	T	T
0.750069997345419	0.499950008653389	0.800000010000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000010000000	T	T	T
0.250020005781725	0.750020057983628	0.800000010000000	T	T	T
0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
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0.770791847824611	0.192298647174758	0.434630520000000	T	T	T
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0.911322021074381	0.244395569118523	0.472237380000000	T	T	T
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0.057176051322196	0.981336236614161	0.413101140000000	T	T	T
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0.058781941359333	0.978198716497095	0.551158010000000	T	T	T
0.281554226510961	0.554237810678895	0.663834130000000	T	T	T

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xyzjob

1.000000000000000				
10.227000000000000	0.000000000000000	0.000000000000000		
0.000000000000001	10.225000000000000	0.000000000000000		
0.000000000000002	0.000000000000002	40.000000000000000		
Cu	O	H	C	Na

48 50 98 2 1

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.8000000100000000	T	T	T
0.250020005781725	-0.0000000000000000	0.8000000100000000	T	T	T
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0.703460646267566	0.630257733515237	0.621536900000000	T	T	T
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0.605726064007451	0.562828770999433	0.563563600000000	T	T	T
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0.744238957210570	0.971269326238553	0.319873260000000	T	T	T
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0.486867921258854	0.557856150813897	0.462370530000000	T	T	T

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0.636256304713464	0.868511222404597	0.346154990000000	T	T	T
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0.084803941961093	0.326460592180411	0.652450080000000	T	T	T
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0.828742869164731	0.457214947058924	0.524622220000000	T	T	T
0.706049986327447	0.394064604702748	0.503319970000000	T	T	T
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0.636681124723291	-0.058366582177682	0.605804770000000	T	T	T
0.774236887904273	0.836615091214533	0.487271620000000	T	T	T
0.705161906306913	0.838832811297281	0.450153490000000	T	T	T
0.771713827845927	0.633284513628166	0.453190830000000	T	T	T
0.733114396953319	0.566723611144753	0.421462650000000	T	T	T
0.963283172275985	0.643889134023834	0.375768380000000	T	T	T
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0.075006901734536	0.782964429212802	0.617201440000000	T	T	T
0.030452920704224	0.666878924881594	0.642483290000000	T	T	T
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0.732247106933255	0.491728988346660	0.643295050000000	T	T	T
0.841020799448655	0.380143714183354	0.644762610000000	T	T	T
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0.336076827771800	0.088463173300606	0.407560490000000	T	T	T
0.264188676109377	0.119833234471041	0.370971410000000	T	T	T
0.090547312093908	0.023356080871423	0.616138520000000	T	T	T

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0.138258133197223	0.620477703150337	0.687246060000000	T	T	T
0.894254000679681	0.888012593132205	0.690047080000000	T	T	T
0.374513038660633	0.213181177953897	0.670044370000000	T	T	T
0.402440619306463	0.495723548495697	0.671014490000000	T	T	T
0.093075972152391	0.519748069392068	0.492316190000000	T	T	T

06-CHOH

xyzjob

1.000000000000000		
10.227000000000000	0.000000000000000	0.000000000000000
0.000000000000001	10.225000000000000	0.000000000000000
0.000000000000002	0.000000000000002	40.000000000000000

Cu	O	H	C	Na
48	50	99	2	1

Selective dynamics

Direct

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0.750069997345419	-0.000000000000000	0.800000010000000	T	T	T
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0.250020005781725	0.249980009326885	0.800000010000000	T	T	T
0.500050021563684	0.249980009326885	0.800000010000000	T	T	T
0.750069997345419	0.249980009326885	0.800000010000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000010000000	T	T	T
0.250020005781725	0.499950008653389	0.800000010000000	T	T	T

0.500050021563684	0.499950008653389	0.800000010000000	T	T	T
0.750069997345419	0.499950008653389	0.800000010000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000010000000	T	T	T
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0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
0.625010024453398	0.374960013989946	0.754830000000000	T	T	T
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0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
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0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
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0.519780692019957	0.499982878654621	0.707352510000000	T	T	T
0.760599497588911	0.499852298649741	0.713031930000000	T	T	T
0.995737673026498	0.742789087713838	0.709140060000000	T	T	T
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0.112023672590554	0.312665091665692	0.372662460000000	T	T	T
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xyzjob

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Cu O H C Na

48 49 98 2 1

Selective dynamics

Direct

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0.664410965364545	0.647398784154777	0.472041750000000	T	T	T
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0.597502893817287	0.903850043723110	0.384490110000000	T	T	T
0.231258115347854	0.172078876420352	0.439449840000000	T	T	T



0.231965515364212	0.096061083584088	0.473528570000000	T	T	T
0.692436206012633	0.686180915601760	0.521094200000000	T	T	T
0.703055706258208	0.820398650609496	0.497539360000000	T	T	T
0.834697069302425	0.702288116202729	0.654610640000000	T	T	T
0.860208649892373	0.594610182185213	0.628858300000000	T	T	T
0.505269111684374	0.922171184406680	0.528690570000000	T	T	T
0.644607494906590	0.900663893604235	0.550057050000000	T	T	T
0.670193415498259	0.218556468154455	0.598314960000000	T	T	T
0.667655675439581	0.274224620231462	0.636708750000000	T	T	T
0.889007890558365	0.181020386753966	0.448552820000000	T	T	T
0.830867309213855	1.038840588759677	0.461654170000000	T	T	T
0.030265590699892	0.923879724470425	0.460578640000000	T	T	T
1.005300303247629	0.806236450081095	0.434318040000000	T	T	T
0.157281843637156	0.886435273073350	0.312726990000000	T	T	T
0.164695363808595	0.883322212957203	0.352472660000000	T	T	T
0.070892041639386	0.296652321068254	0.414721450000000	T	T	T
0.223309075164036	0.310629491589741	0.398338060000000	T	T	T
0.949795591964085	0.126526064720753	0.506929760000000	T	T	T
0.875213130239356	0.075040772799814	0.539481860000000	T	T	T
0.153212133543043	0.755325328181574	0.652841840000000	T	T	T
0.030145460697115	0.763379808482093	0.628144990000000	T	T	T
0.217437035028249	0.450616696812743	0.491888870000000	T	T	T
0.192954934462090	0.540215000155697	0.459509690000000	T	T	T
0.478232801059167	0.598177992318328	0.624688000000000	T	T	T
0.416323649627505	0.610899202792958	0.661069740000000	T	T	T
0.896481090731182	0.473033687649125	0.359850850000000	T	T	T
0.958042392154786	0.472537477630611	0.396745750000000	T	T	T
0.641161524826899	0.297256691090797	0.398533890000000	T	T	T

0.534718652365405	0.372081803882562	0.381189920000000	T	T	T
0.362702208387513	1.040475388820665	0.649184800000000	T	T	T
0.256087005922030	0.121286074525242	0.632147580000000	T	T	T
0.354139068189488	0.879265162805829	0.693407300000000	T	T	T
0.605815934009533	0.876706702710377	0.657397450000000	T	T	T
0.122064752822753	0.379398924155570	0.680552230000000	T	T	T
0.613150754179153	0.885129693024646	0.683437160000000	T	T	T
0.119029422752567	0.559381540870807	0.539119710000000	T	T	T

08-CH<sub>2</sub>

xyzjob

1.000000000000000					
10.227000000000000	0.000000000000000	0.000000000000000			
0.000000000000001	10.225000000000000	0.000000000000000			
0.000000000000002	0.000000000000002	40.000000000000000			
Cu	O	H	C	Na	
48	49	99	2	1	

Selective dynamics

Direct

-0.000000000000000	-0.000000000000000	0.800000100000000	T	T	T
0.250020005781725	-0.000000000000000	0.800000100000000	T	T	T
0.500050021563684	-0.000000000000000	0.800000100000000	T	T	T
0.750069997345419	-0.000000000000000	0.800000100000000	T	T	T
-0.000000000000000	0.249980009326885	0.800000100000000	T	T	T
0.250020005781725	0.249980009326885	0.800000100000000	T	T	T
0.500050021563684	0.249980009326885	0.800000100000000	T	T	T
0.750069997345419	0.249980009326885	0.800000100000000	T	T	T

-0.000000000000000	0.499950008653389	0.800000010000000	T	T	T
0.250020005781725	0.499950008653389	0.800000010000000	T	T	T
0.500050021563684	0.499950008653389	0.800000010000000	T	T	T
0.750069997345419	0.499950008653389	0.800000010000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000010000000	T	T	T
0.250020005781725	0.750020057983628	0.800000010000000	T	T	T
0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
0.625010024453398	0.374960013989946	0.754830000000000	T	T	T
0.875040020235357	0.374960013989946	0.754830000000000	T	T	T
0.124960002889703	0.625040023320567	0.754830000000000	T	T	T
0.374989998671663	0.625040023320567	0.754830000000000	T	T	T
0.625010024453398	0.625040023320567	0.754830000000000	T	T	T
0.875040020235357	0.625040023320567	0.754830000000000	T	T	T
0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
0.003347000077403	0.992794297041662	0.708191370000000	T	T	T
0.251290205811098	0.013813140515374	0.713802580000000	T	T	T
0.499510171551207	0.002840170105966	0.707058950000000	T	T	T
0.746750667268651	-0.006099780227589	0.712410220000000	T	T	T

1.019897163585186	0.253874439472186	0.710377010000000	T	T	T
0.265974386150670	0.247935609250601	0.709308720000000	T	T	T
0.512429571849966	0.253208159447325	0.709246370000000	T	T	T
0.770475747817297	0.235770238796704	0.707293480000000	T	T	T
1.014501633460408	0.493069168396665	0.710537590000000	T	T	T
0.246432845698778	0.496632778529623	0.712690870000000	T	T	T
0.496909841491072	0.508398428968606	0.708863810000000	T	T	T
0.753065587414686	0.494039088432851	0.710279740000000	T	T	T
0.998715583095355	0.749721467972489	0.712086820000000	T	T	T
0.251082845806307	0.750812368013193	0.709270060000000	T	T	T
0.510083521795717	0.763361108481398	0.709474700000000	T	T	T
0.754343267444236	0.737800137527697	0.711092960000000	T	T	T
0.376072628696705	0.503593858789340	0.644610430000000	T	T	T
0.568015053135387	-0.265668029912206	0.365596100000000	T	T	T
0.154838973580659	0.591561152071452	0.516263910000000	T	T	T
0.861042019911645	0.646584084124381	0.618110680000000	T	T	T
0.108424482507324	0.370668493829829	0.350551910000000	T	T	T
0.651436655064515	0.501736418720039	0.614733160000000	T	T	T
0.211605374893390	0.048509741809927	0.495401010000000	T	T	T
-0.012949060299452	-0.315529911772587	0.321395610000000	T	T	T
0.816182988874284	-0.130304624861731	0.321674400000000	T	T	T
1.067326314681989	-0.152036925672577	0.519753410000000	T	T	T
0.251610075818500	-0.037345891393399	0.386803810000000	T	T	T
0.718648876618803	0.571175181310836	0.402701300000000	T	T	T
0.367109468489430	0.392975564662122	0.349907610000000	T	T	T
0.397801619199188	0.150031285597741	0.620961370000000	T	T	T
0.842805489489929	0.760116668360342	0.551575310000000	T	T	T
0.317649207345654	0.126009934701496	0.551822720000000	T	T	T

0.139205563219135	0.753921618129203	0.421852240000000	T	T	T
0.687527225899110	0.182455506807511	0.503448030000000	T	T	T
0.546015362626635	0.764043508506856	0.441654130000000	T	T	T
0.920807431293732	0.826112390822680	0.456214360000000	T	T	T
0.435184620063674	0.144584675394533	0.350668840000000	T	T	T
0.560443062960281	0.527111169666787	0.554127510000000	T	T	T
0.857969729840598	-0.091993783432333	0.631855440000000	T	T	T
0.775215257926899	0.573318521390807	0.507849050000000	T	T	T
1.002337083179104	0.412557815392743	0.499854980000000	T	T	T
0.260879196032844	0.573353851392127	0.577531980000000	T	T	T
0.457217050573169	0.783355269227384	0.530776500000000	T	T	T
0.073300141695072	0.149744485587041	0.385876160000000	T	T	T
0.272841716309485	0.060294892249633	0.291395200000000	T	T	T
1.043308604126576	0.103602033865447	0.579032450000000	T	T	T
0.832183469244294	0.028837381075941	0.420907800000000	T	T	T
0.118369882737313	0.277071240337672	0.446607230000000	T	T	T
-0.037510870867439	0.596665812261907	0.381748110000000	T	T	T
0.600703993891317	0.145076595412880	0.441915400000000	T	T	T
0.289409656692617	-0.167123666235472	0.588752810000000	T	T	T
0.880641380364887	0.248654559277428	0.543925700000000	T	T	T
0.476369341016065	0.324749752116577	0.517470420000000	T	T	T
0.630120784571585	0.048458601808019	0.604740220000000	T	T	T
0.316356467315762	0.676602385244381	0.465417230000000	T	T	T
0.351157228120534	0.413900725442846	0.460656310000000	T	T	T
0.405074229367371	0.608200522692274	0.312007330000000	T	T	T
0.389891479016261	-0.013694580510954	0.448651510000000	T	T	T
0.671008275517111	-0.057585972148558	0.542700970000000	T	T	T
0.090575602094563	0.520689679427198	0.627829360000000	T	T	T

0.515210821914286	0.369230453776176	0.406728510000000	T	T	T
0.783372428115537	0.283613020581750	0.610696410000000	T	T	T
0.226928855247746	-0.184883716898103	0.326439970000000	T	T	T
0.629349834553750	0.005523320206073	0.364788010000000	T	T	T
0.013574060313904	0.259792419692988	0.634856110000000	T	T	T
0.608539214072504	0.670584425019843	0.379832690000000	T	T	T
0.597522823817747	-0.176313156578338	0.369452760000000	T	T	T
0.097822382262149	0.515336179227452	0.510887280000000	T	T	T
0.222654305148890	0.574993741453311	0.533477950000000	T	T	T
0.863051279958111	0.738729877562386	0.628180050000000	T	T	T
0.948100691924885	0.606160562616156	0.614364910000000	T	T	T
0.209612644847306	0.375090203994807	0.349637690000000	T	T	T
0.075090871736482	0.385771424393330	0.327814770000000	T	T	T
0.600189223879417	0.556021320745438	0.629703870000000	T	T	T
0.734875826994045	0.552311220607012	0.613061000000000	T	T	T
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0.271877296287181	0.059477322219129	0.514940980000000	T	T	T
0.073584831701652	-0.281068290486797	0.327529920000000	T	T	T
0.919919881273198	-0.241065368994269	0.322379460000000	T	T	T
0.822936669030458	-0.072882842719296	0.301988760000000	T	T	T
0.737667497058609	-0.092896563466015	0.333940200000000	T	T	T
0.090616372095512	0.749603597968098	0.516543980000000	T	T	T
0.990566022906903	-0.155932755817927	0.534378350000000	T	T	T
0.195587844522978	0.038369501431589	0.381078440000000	T	T	T
0.195867864529461	-0.106528713974641	0.397988220000000	T	T	T
0.811808218773110	0.574641501440166	0.392024730000000	T	T	T
0.676599885646416	0.487285558180870	0.398487700000000	T	T	T
0.406173979392793	0.392935074660606	0.373808790000000	T	T	T

0.388454368983035	0.471909797607198	0.335921100000000	T	T	T
0.364287688424171	0.129051204814963	0.643942430000000	T	T	T
0.396776749175486	0.247845239247237	0.621115190000000	T	T	T
0.786060908177706	-0.156472435838064	0.549951600000000	T	T	T
0.859086119866422	0.737225947506279	0.574944450000000	T	T	T
0.365664488456018	0.204657457635873	0.541122030000000	T	T	T
0.851985649702219	0.273553500206425	0.628314610000000	T	T	T
0.093761932168251	0.691445255798181	0.407029240000000	T	T	T
0.062738801450836	0.784967329287530	0.435758870000000	T	T	T
0.604485053978752	0.237348258855589	0.509523940000000	T	T	T
0.761564347611225	0.228647228530944	0.515959520000000	T	T	T
0.538360142449614	0.765836158573741	0.416787640000000	T	T	T
0.458140350594524	-0.255247239523404	0.452913530000000	T	T	T
0.949734331962667	-0.136648685098435	0.476842030000000	T	T	T
0.884158070446211	-0.102829793836636	0.442596860000000	T	T	T
0.381194308815146	0.110168444110445	0.367680560000000	T	T	T
0.408118619437773	0.233997978730582	0.345246600000000	T	T	T
0.548772702690398	0.618792543087462	0.549353080000000	T	T	T
0.767167937740804	-0.064811392418142	0.631839850000000	T	T	T
0.896688020735963	0.935459774902484	0.654494540000000	T	T	T
0.798092318455930	0.649716034241242	0.523719400000000	T	T	T
0.717110976583231	0.538064880075472	0.524453380000000	T	T	T
0.982205852713572	0.326479952181134	0.511518010000000	T	T	T
0.912570611103246	0.455355356989545	0.503234730000000	T	T	T
0.354471338197174	0.557255190791472	0.578291370000000	T	T	T
0.256925335941410	0.670292385008949	0.579415060000000	T	T	T
0.446523720325892	0.770098698732773	0.506869050000000	T	T	T
0.526193162168251	-0.148334235534426	0.529092520000000	T	T	T

0.085459211976249	0.219988798207892	0.367545830000000	T	T	T
0.100060452313904	0.195566177296675	0.406080250000000	T	T	T
0.319247917382624	0.051157941908733	0.270272840000000	T	T	T
0.342709527925178	0.077099382876616	0.308371520000000	T	T	T
0.130125983009172	0.124089304629838	0.569854930000000	T	T	T
1.036674853973169	0.155928075817760	0.600419760000000	T	T	T
0.754507367448029	0.080597913007149	0.423958790000000	T	T	T
0.893857800670519	0.070259312621408	0.404646090000000	T	T	T
0.130733943023232	0.212549457930328	0.463511550000000	T	T	T
0.059831071383592	0.340074932688372	0.457396010000000	T	T	T
0.008878650205319	0.513127339145046	0.378960050000000	T	T	T
-0.034703740802523	0.634956423690552	0.357278080000000	T	T	T
0.522661712086584	0.082945953094758	0.444106380000000	T	T	T
0.634364144669707	0.156909535854376	0.465523710000000	T	T	T
0.365705358456957	-0.155305575794533	0.575331300000000	T	T	T
0.218413725050826	-0.121132034519501	0.577434170000000	T	T	T
0.830711419210247	0.280281270457438	0.563643850000000	T	T	T
0.950043011969805	0.186884706972763	0.553289360000000	T	T	T
0.424042749806013	0.362801833536323	0.498260200000000	T	T	T
0.498080491518138	0.395572844759022	0.533375040000000	T	T	T
0.352786798158218	0.128216974783843	0.575671740000000	T	T	T
0.542996982556840	0.071735182676479	0.612430220000000	T	T	T
0.260759876030087	0.653118604368186	0.483940560000000	T	T	T
0.249461845768818	0.706121046345741	0.447885010000000	T	T	T
0.341700567901848	0.518534109346777	0.461674010000000	T	T	T
0.260036636013366	0.379419474156332	0.455119050000000	T	T	T
0.480884871120495	0.656118964480137	0.321222670000000	T	T	T
0.332792747695854	0.662122144704117	0.318332930000000	T	T	T



0.319959777399091	0.005783330215775	0.465568250000000	T	T	T
0.354267538192461	-0.022904340854572	0.426913870000000	T	T	T
0.672632215554659	0.026670910995110	0.528172410000000	T	T	T
0.650746035048538	-0.017233620642993	0.565801090000000	T	T	T
0.110065772545282	0.576940231525936	0.646622610000000	T	T	T
0.172013653977823	0.515198679222328	0.613955330000000	T	T	T
0.541610922524787	0.285142630638817	0.418010590000000	T	T	T
0.473267180944334	0.426056125896372	0.424504200000000	T	T	T
0.590923813665151	0.522373049490005	0.578399960000000	T	T	T
0.732434676937596	0.368207083737995	0.613636470000000	T	T	T
0.227692025265395	-0.106855063986817	0.312502550000000	T	T	T
0.248363885743434	-0.142441175314553	0.347480770000000	T	T	T
0.688530795922313	0.041209681537555	0.381147080000000	T	T	T
0.566343163096724	0.073344842736538	0.355944480000000	T	T	T
0.040590520938662	0.356279253292958	0.635823790000000	T	T	T
0.054706541265092	0.217143288101731	0.654422410000000	T	T	T
0.328182367589234	0.947397955347902	0.662198720000000	T	T	T
0.412132799530595	0.800575889869897	0.666129550000000	T	T	T
0.689939335954894	0.129571854834396	0.607237380000000	T	T	T
0.882129310399296	0.120186414484215	0.697067450000000	T	T	T
0.383530008869150	0.524586409572587	0.673461280000000	T	T	T
0.366278458470216	0.883810172975413	0.682227600000000	T	T	T
0.747350897282536	0.674972495183570	0.452282910000000	T	T	T

09-CH<sub>3</sub>

xyzjob

1.000000000000000

10.227000000000000	0.000000000000000	0.000000000000000	
0.0000000000000001	10.225000000000000	0.000000000000000	
0.0000000000000002	0.000000000000002	40.000000000000000	
Cu	O	H	C
48	50	102	2

Selective dynamics

Direct

-0.000000000000000	-0.000000000000000	0.800000010000000	T	T	T
0.250020005781725	-0.000000000000000	0.800000010000000	T	T	T
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0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
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0.522798822089752	0.743972397757995	0.708271180000000	T	T	T
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0.780096318039777	0.274900390256675	0.651800760000000	T	T	T
0.971838342473824	0.936431654938748	0.575596930000000	T	T	T
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0.521762892065796	0.804486570015804	0.573453630000000	T	T	T
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0.398934529225384	0.974195956347746	0.458221140000000	T	T	T

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0.553541402800675	0.785249289298054	0.423072060000000	T	T	T
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0.148335803430273	0.435356236243364	0.448262550000000	T	T	T
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0.535079292373746	0.334576642483227	0.589116590000000	T	T	T
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0.934703011615068	0.424680125845037	0.500665310000000	T	T	T
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0.866134410029412	0.240193288961731	0.646953020000000	T	T	T
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0.889799050576660	0.938729705024489	0.563825260000000	T	T	T
0.159384773685783	0.721839956932215	0.537738980000000	T	T	T
0.071672751657436	0.847459631619149	0.552707740000000	T	T	T
0.523410632103901	0.796654269723579	0.599342090000000	T	T	T
0.452302610459529	0.878318532770513	0.571568990000000	T	T	T
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0.502243331614403	0.478835387865594	0.446253580000000	T	T	T
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0.347837948043776	0.065228372433702	0.539823490000000	T	T	T
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0.750439037353945	0.901851533648538	0.515448050000000	T	T	T
0.675195495613934	0.864653802260675	0.549539060000000	T	T	T
0.500029501563215	0.672815105103081	0.459017490000000	T	T	T
0.579900123410228	0.252575549423726	0.638891910000000	T	T	T
0.613264954181793	0.162974786080675	0.480495180000000	T	T	T
0.558631852918392	0.276349720310748	0.453005940000000	T	T	T
0.812707648793918	0.968457846133662	0.457533060000000	T	T	T
0.700926836208976	0.851838951782543	0.458129930000000	T	T	T
0.554698802827447	1.119302291761741	0.391564790000000	T	T	T
0.637326104738203	1.203988174921418	0.366030870000000	T	T	T
0.742885557179270	0.481233007955051	0.423531400000000	T	T	T
0.837075339357416	0.592826412118660	0.411170590000000	T	T	T
0.825467829088990	0.220546848228714	0.453742620000000	T	T	T
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0.950399911978058	0.871288022508205	0.613482190000000	T	T	T
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0.201211514653026	0.656456004492714	0.400015510000000	T	T	T
0.068016031572876	0.715152646682709	0.387892120000000	T	T	T
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0.250378455790016	0.455928177010914	0.630352000000000	T	T	T
0.674743175603481	0.879274902806200	0.652801060000000	T	T	T
0.538833522460555	0.975303626389076	0.659321270000000	T	T	T
0.421590119749301	0.302543481288049	0.637047150000000	T	T	T
1.152305506647130	0.125105964667765	0.393543260000000	T	T	T
0.682990415794192	1.063212649669007	0.648501520000000	T	T	T
0.405685289381500	0.879935202830836	0.700060210000000	T	T	T
0.509163681774440	0.602596602483188	0.666052840000000	T	T	T
0.650105575033734	0.975949296413164	0.662598550000000	T	T	T

10-CO-CO

xyzjob

1.000000000000000		
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0.000000000000001	10.225000000000000	0.000000000000000
0.000000000000002	0.000000000000002	40.000000000000000

Cu	O	H	C	Na
48	50	97	2	1

Selective dynamics

Direct

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0.750069997345419	-0.000000000000000	0.800000010000000	T	T	T
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0.250020005781725	0.249980009326885	0.800000010000000	T	T	T
0.500050021563684	0.249980009326885	0.800000010000000	T	T	T
0.750069997345419	0.249980009326885	0.800000010000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000010000000	T	T	T
0.250020005781725	0.499950008653389	0.800000010000000	T	T	T
0.500050021563684	0.499950008653389	0.800000010000000	T	T	T
0.750069997345419	0.499950008653389	0.800000010000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000010000000	T	T	T
0.250020005781725	0.750020057983628	0.800000010000000	T	T	T
0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
0.625010024453398	0.374960013989946	0.754830000000000	T	T	T
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0.124960002889703	0.625040023320567	0.754830000000000	T	T	T
0.374989998671663	0.625040023320567	0.754830000000000	T	T	T
0.625010024453398	0.625040023320567	0.754830000000000	T	T	T
0.875040020235357	0.625040023320567	0.754830000000000	T	T	T
0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
0.625010024453398	0.875010042647071	0.754830000000000	T	T	T

0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
1.000927943146524	1.004191057466885	0.709626540000000	T	T	T
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0.501917831606883	0.987955506861125	0.704346590000000	T	T	T
0.760080977576914	-0.015728560586836	0.712411110000000	T	T	T
0.001022790023653	0.239547008937623	0.710400140000000	T	T	T
0.250878885801594	0.261349219751071	0.711495470000000	T	T	T
0.498007571516456	0.241306329003266	0.712183450000000	T	T	T
0.746953417273345	0.239025938918181	0.709538090000000	T	T	T
0.005980860138310	0.492836318387971	0.710969430000000	T	T	T
0.270584786257289	0.500095778658826	0.707717200000000	T	T	T
0.509867731790720	0.494012198431843	0.712343440000000	T	T	T
0.743575707195238	0.498407598595843	0.706559070000000	T	T	T
0.991193302921404	0.750499448001516	0.709486920000000	T	T	T
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0.203542864706942	0.222889988316137	0.387839640000000	T	T	T
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0.480872601120211	0.491612208342308	0.558786430000000	T	T	T
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11-COH-CO

xyzjob

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0.0000000000000001	10.2250000000000000	0.0000000000000000		
0.0000000000000002	0.0000000000000002	40.0000000000000000		
Cu	O	H	C	Na
48	50	98	2	1

Selective dynamics

Direct

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0.124960002889704	0.124990004663442	0.7548300000000000	T	T	T

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0.086995112011763	0.063595732372792	0.427511420000000	T	T	T
0.011698700270529	0.922716324427022	0.558122940000000	T	T	T
0.018057890417590	0.944991015258103	0.623983300000000	T	T	T
0.220409545096988	0.331633412373408	0.454617150000000	T	T	T
0.916419621192256	0.356069153285125	0.637415340000000	T	T	T
0.199527184614080	0.635260903701907	0.417980540000000	T	T	T
0.557830992899873	0.228880448539648	0.389549070000000	T	T	T
0.280130906478048	0.010831940404147	0.642201170000000	T	T	T
0.900440990822753	0.262796919805086	0.325259180000000	T	T	T
0.869443780105935	0.270831390104861	0.364892090000000	T	T	T
0.616904954265962	0.603530692518044	0.534506530000000	T	T	T

0.601819503917111	0.605051682574787	0.492901430000000	T	T	T
0.563002313019458	0.837799051258709	0.628152140000000	T	T	T
0.445824420309719	0.787184119370239	0.606906720000000	T	T	T
0.796399778416789	0.485659788120215	0.407387260000000	T	T	T
0.778131227994329	0.640292703889653	0.414793460000000	T	T	T
0.097434692253183	0.782914529210944	0.635130750000000	T	T	T
0.138503753202904	0.680862175403315	0.661488370000000	T	T	T
0.293857846795482	0.140363405237027	0.562997960000000	T	T	T
0.442901620242124	0.108766204058122	0.565083330000000	T	T	T
0.537937742439845	0.012594270469897	0.384983800000000	T	T	T
0.436277110088931	0.947811095363315	0.363621690000000	T	T	T
0.690115265958961	0.279583850431413	0.392765040000000	T	T	T
0.820042448963528	0.266400229939530	0.415703210000000	T	T	T
0.500898521583309	0.762854168462484	0.513811050000000	T	T	T
0.349921008091943	0.789470239455540	0.523437050000000	T	T	T
0.884157800446201	0.218990958170660	0.474612490000000	T	T	T
0.803650768584472	0.112044424180430	0.455412460000000	T	T	T
0.427707139890750	0.825718200807971	0.416445760000000	T	T	T
0.466252130782106	0.776635758976675	0.452273530000000	T	T	T
0.287915626658062	0.366886983688743	0.407630620000000	T	T	T
0.316026147308125	0.480902797942729	0.386599910000000	T	T	T
0.703163506260702	0.032800451223804	0.565062320000000	T	T	T
0.775870457942055	0.104613243903178	0.592166870000000	T	T	T
0.117096832707871	0.834956771152665	0.542538550000000	T	T	T
0.224945415201877	0.729016757199990	0.555299900000000	T	T	T
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0.716811776576317	0.923177604444225	0.442238720000000	T	T	T

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0.260938066034213	0.478503537853213	0.487987400000000	T	T	T
0.089993012081089	0.188382357028645	0.356247290000000	T	T	T
0.220794235105876	0.250125169332293	0.371670350000000	T	T	T
0.955369422092979	0.630975213542005	0.625449450000000	T	T	T
0.797297078437547	0.627426503409604	0.625589440000000	T	T	T
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0.594948503758218	0.510881899061262	0.585392210000000	T	T	T
0.974650912538858	0.586294311874944	0.532565120000000	T	T	T
0.927509951448724	0.574731671443530	0.571707560000000	T	T	T
0.767440247747101	0.243575939087941	0.553096770000000	T	T	T
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0.496135901473169	0.556979790781203	0.449383350000000	T	T	T
0.806825768657896	0.851687781776909	0.389286530000000	T	T	T
0.659798495257876	0.807701090135746	0.396729490000000	T	T	T
0.207123184789733	0.010006330373340	0.463138810000000	T	T	T
0.306432827086281	0.931249724745408	0.482597570000000	T	T	T
0.528901232230869	0.930628614722230	0.585181570000000	T	T	T
0.495691421462892	0.926569104570768	0.544600060000000	T	T	T
0.405741279382790	0.580183711646953	0.611501060000000	T	T	T
0.280321586482458	0.662542214719785	0.611574450000000	T	T	T
0.994505822998005	0.384923104361682	0.510504290000000	T	T	T
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0.729145606861533	0.050292371876430	0.649603330000000	T	T	T
0.733788126968896	0.893297493329389	0.647620450000000	T	T	T
0.771963747851706	0.746862747865829	0.512089240000000	T	T	T
0.793675828353799	0.870618012483208	0.486811720000000	T	T	T
0.965931302337215	0.694646075917604	0.481455200000000	T	T	T
0.946097071878557	0.595003472199883	0.454458070000000	T	T	T
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0.239036695527740	0.897075793470357	0.351343230000000	T	T	T
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0.124776872885470	0.110071434106826	0.406359110000000	T	T	T
0.936004051645155	0.912245494036342	0.543428160000000	T	T	T
-0.011040310255305	0.946932805330553	0.581974310000000	T	T	T
0.095115032199540	0.990747236965291	0.631894930000000	T	T	T
0.940191061741977	0.966112176046142	0.636943200000000	T	T	T
0.272021756290515	0.269755550064714	0.467908190000000	T	T	T

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0.902724550875564	0.450622676812958	0.628020440000000	T	T	T
0.927403561446260	0.376196984036098	0.663300660000000	T	T	T
0.124195772872035	0.631641383566865	0.432220390000000	T	T	T
0.267408716183846	0.693079655859159	0.428438110000000	T	T	T
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0.484766501210257	0.286648350694993	0.381617760000000	T	T	T
0.318826737372885	0.086998573245966	0.656632710000000	T	T	T
0.355923828230761	0.950620185468127	0.636521660000000	T	T	T
0.374047388649868	0.611212992804665	0.702039960000000	T	T	T
0.521314222055422	0.417172765564929	0.635220260000000	T	T	T
0.601318453905524	0.551119530562552	0.669036830000000	T	T	T
0.654037975124670	0.677276795269545	0.670312920000000	T	T	T
0.376056628696333	0.399750224914885	0.546184050000000	T	T	T

12-COH-COH

xyzjob

1.000000000000000				
10.227000000000000	0.000000000000000	0.000000000000000		
0.000000000000001	10.225000000000000	0.000000000000000		
0.000000000000002	0.000000000000002	40.000000000000000		
Cu	O	H	C	Na
48	50	99	2	1

Selective dynamics

Direct

-0.000000000000000	-0.000000000000000	0.800000010000000	T	T	T
0.250020005781725	-0.000000000000000	0.800000010000000	T	T	T



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0.750069997345419	-0.0000000000000000	0.8000000100000000	T	T	T
-0.0000000000000000	0.249980009326885	0.8000000100000000	T	T	T
0.250020005781725	0.249980009326885	0.8000000100000000	T	T	T
0.500050021563684	0.249980009326885	0.8000000100000000	T	T	T
0.750069997345419	0.249980009326885	0.8000000100000000	T	T	T
-0.0000000000000000	0.499950008653389	0.8000000100000000	T	T	T
0.250020005781725	0.499950008653389	0.8000000100000000	T	T	T
0.500050021563684	0.499950008653389	0.8000000100000000	T	T	T
0.750069997345419	0.499950008653389	0.8000000100000000	T	T	T
-0.0000000000000000	0.750020057983628	0.8000000100000000	T	T	T
0.250020005781725	0.750020057983628	0.8000000100000000	T	T	T
0.500050021563684	0.750020057983628	0.8000000100000000	T	T	T
0.750069997345419	0.750020057983628	0.8000000100000000	T	T	T
0.124960002889704	0.124990004663442	0.7548300000000000	T	T	T
0.374989998671663	0.124990004663442	0.7548300000000000	T	T	T
0.625010024453398	0.124990004663442	0.7548300000000000	T	T	T
0.875040020235357	0.124990004663442	0.7548300000000000	T	T	T
0.124960002889704	0.374960013989946	0.7548300000000000	T	T	T
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0.625010024453398	0.374960013989946	0.7548300000000000	T	T	T
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0.875040020235357	0.625040023320567	0.7548300000000000	T	T	T
0.124960002889703	0.875010042647071	0.7548300000000000	T	T	T
0.374989998671663	0.875010042647071	0.7548300000000000	T	T	T

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0.000597360013816	0.257709749615286	0.710639160000000	T	T	T
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0.491140111357641	0.254271059486983	0.709893730000000	T	T	T
0.749989817343561	0.234425808746543	0.710273870000000	T	T	T
0.000120130002777	0.503493858785613	0.709891350000000	T	T	T
0.248711705751471	0.496182118512812	0.711115680000000	T	T	T
0.514255361892187	0.486602818155403	0.709647810000000	T	T	T
0.763530817656693	0.506448098895834	0.710621130000000	T	T	T
-0.000456950010570	0.751656658044694	0.711775980000000	T	T	T
0.248386855743962	0.762546438451002	0.712035110000000	T	T	T
0.490523161343375	0.733214667356616	0.701719450000000	T	T	T
0.746203447255999	0.749448797962318	0.710434780000000	T	T	T
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0.683895665815127	0.747658337895511	0.636589390000000	T	T	T
0.881731490390095	0.261425899753936	0.334664930000000	T	T	T
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0.502588141622382	0.807736010137046	0.588313110000000	T	T	T
0.750368827352322	0.618195603065193	0.399881020000000	T	T	T
0.116912002703598	0.008418810314112	0.623022350000000	T	T	T
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0.005791390133930	0.984420216729222	0.414665620000000	T	T	T
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0.212106984904987	0.781672729164606	0.482697560000000	T	T	T
0.118464052739484	0.677656935283726	0.470022100000000	T	T	T
0.025403720587464	0.265232679895971	0.352407050000000	T	T	T
0.111776112584834	0.366018623656342	0.371733210000000	T	T	T
0.924958441389723	0.605119452577320	0.579183310000000	T	T	T
0.795373488393057	0.651914654323266	0.601800390000000	T	T	T
-0.007787200180082	0.334284372472323	0.618341060000000	T	T	T
0.068056271573804	0.195442307292049	0.611291010000000	T	T	T

0.040729410941869	0.770263788738934	0.565099130000000	T	T	T
0.102152252362276	0.678471235314112	0.590393600000000	T	T	T
0.408622799449428	0.552728960622601	0.560463670000000	T	T	T
0.422226279764007	0.698530286062523	0.563766680000000	T	T	T
0.767338767744754	0.504424038820323	0.551547950000000	T	T	T
0.662449435319184	0.543605020282181	0.524591630000000	T	T	T
0.745031017228884	0.186515146958973	0.500075470000000	T	T	T
0.720149346653496	0.352538803153398	0.509315080000000	T	T	T
0.480218371105075	0.363508673562699	0.462041000000000	T	T	T
0.554731342828200	0.264243279859051	0.485034480000000	T	T	T
0.866920190047580	0.095159423550445	0.349841860000000	T	T	T
0.915095801161650	0.963013235930513	0.369133100000000	T	T	T
0.289739916700254	0.442495996509750	0.606775030000000	T	T	T
0.201953844670196	0.372090363882885	0.630617830000000	T	T	T
0.312390557224054	0.012607120470376	0.465829470000000	T	T	T
0.394967319133646	0.140963315259413	0.456179000000000	T	T	T
0.611906524150376	0.584855071821242	0.437068690000000	T	T	T
0.465391090762198	0.602674412486093	0.433174580000000	T	T	T
0.718757166621306	0.887838143125692	0.357996320000000	T	T	T
0.561722942989880	0.853438751842240	0.361039650000000	T	T	T
0.026494760612692	0.149794585588909	0.473540840000000	T	T	T
0.943084971808898	0.101909193802288	0.502922570000000	T	T	T
0.511186191821208	0.903871053723892	0.553486180000000	T	T	T
0.527383662195776	0.955060015633780	0.515922010000000	T	T	T
0.120038972775907	0.695494605949261	0.661435310000000	T	T	T
0.181439894195805	0.575063011455892	0.640057890000000	T	T	T
0.923846251363997	0.599773912377868	0.471818290000000	T	T	T
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0.641894844843854	0.795313999673575	0.494611410000000	T	T	T
0.672104445542456	0.903554333712078	0.465574620000000	T	T	T
0.817522738905260	0.758789378310816	0.459070380000000	T	T	T
0.847820879605906	0.688559555690513	0.424350610000000	T	T	T
0.111101632569228	0.831952451040567	0.325529980000000	T	T	T
0.109744432537851	0.837001931228968	0.365315780000000	T	T	T
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0.022031410509475	0.204797067641085	0.408879610000000	T	T	T
0.775546247934555	0.957085685709359	0.506869990000000	T	T	T
0.759835987571252	0.029188541089037	0.543537970000000	T	T	T
0.386519668938291	0.860010422087433	0.660067020000000	T	T	T
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0.271703076283152	0.359602383416949	0.481978270000000	T	T	T
0.849889129653740	0.480193347916264	0.618848380000000	T	T	T
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0.295549576834604	0.092431623448675	0.404698470000000	T	T	T
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0.398352619211929	0.272384480162807	0.636600090000000	T	T	T
0.437855110125423	0.157543705878034	0.659125410000000	T	T	T
0.362774138389175	0.615071362948626	0.702886190000000	T	T	T
0.479506051088608	0.454253436948430	0.638305990000000	T	T	T
0.734443656984052	0.825832670812244	0.645226300000000	T	T	T
0.576253403325892	0.571676141329526	0.666195420000000	T	T	T

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0.161613243737313	0.558642690843247	0.525049780000000	T	T	T

13-C-COH

xyzjob

1.000000000000000					
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0.000000000000001	10.225000000000000	0.000000000000000			
0.000000000000002	0.000000000000002	40.000000000000000			
Cu	O	H	C	Na	
48	49	98	2	1	

Selective dynamics

Direct

-0.000000000000000	-0.000000000000000	0.800000100000000	T	T	T
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0.500050021563684	-0.000000000000000	0.800000100000000	T	T	T
0.750069997345419	-0.000000000000000	0.800000100000000	T	T	T
-0.000000000000000	0.249980009326885	0.800000100000000	T	T	T
0.250020005781725	0.249980009326885	0.800000100000000	T	T	T
0.500050021563684	0.249980009326885	0.800000100000000	T	T	T
0.750069997345419	0.249980009326885	0.800000100000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000100000000	T	T	T
0.250020005781725	0.499950008653389	0.800000100000000	T	T	T
0.500050021563684	0.499950008653389	0.800000100000000	T	T	T
0.750069997345419	0.499950008653389	0.800000100000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000100000000	T	T	T
0.250020005781725	0.750020057983628	0.800000100000000	T	T	T



0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
0.625010024453398	0.374960013989946	0.754830000000000	T	T	T
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0.875040020235357	0.625040023320567	0.754830000000000	T	T	T
0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
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0.243243925625032	0.976276296425369	0.709883710000000	T	T	T
0.497921591514471	-0.007796880290905	0.708986990000000	T	T	T
0.767322637744382	0.006731710251159	0.712271550000000	T	T	T
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0.511406191826303	0.242284709039765	0.707524930000000	T	T	T
0.751458007377510	0.253173979446054	0.710936950000000	T	T	T
-0.005856540135436	0.502884828762895	0.709634920000000	T	T	T
0.244302365649506	0.494346518444323	0.709574880000000	T	T	T

0.478418981063469	0.496326748518200	0.709772240000000	T	T	T
0.737156807046797	0.495892698502015	0.710623430000000	T	T	T
0.986105332803745	0.767200598624645	0.705854190000000	T	T	T
0.244045945643580	0.731792317303550	0.707120120000000	T	T	T
0.494562541436785	0.745453557813252	0.707759230000000	T	T	T
0.736398737029265	0.761370618407129	0.711242430000000	T	T	T
0.752235657395492	0.542738050249839	0.639152200000000	T	T	T
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0.898931040787836	0.192857637195619	0.334729470000000	T	T	T
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0.129612092997291	0.184771486893917	0.432395020000000	T	T	T
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0.594309053743434	0.522841399507482	0.424267230000000	T	T	T
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0.983469252742788	0.957736765733653	0.423503850000000	T	T	T
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0.221468355121472	0.695956935966513	0.361832760000000	T	T	T
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0.921770001315987	0.320479441957252	0.529908370000000	T	T	T
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0.731355816912643	0.023535670878132	0.438810560000000	T	T	T
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0.385905058924073	0.892158843286905	0.635940080000000	T	T	T
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0.143581013320319	0.619825893126024	0.426310570000000	T	T	T
0.545477202614197	0.913809564094699	0.273307410000000	T	T	T
0.692743456019732	0.918122574255618	0.266520680000000	T	T	T
0.296901596865865	0.159862415964548	0.433637080000000	T	T	T
0.432269189996255	0.208876307793281	0.417843710000000	T	T	T
0.138790593209543	0.930075764701604	0.516682470000000	T	T	T
0.073473341699071	0.929600864683883	0.550596920000000	T	T	T
0.334489297735083	0.959955285816421	0.627149400000000	T	T	T

0.362989278394152	0.886590573079149	0.660948790000000	T	T	T
0.566917643110003	0.287850910739863	0.489724400000000	T	T	T
0.441612420212310	0.225529648414631	0.474260320000000	T	T	T
0.049167701137010	0.571430181320352	0.615566910000000	T	T	T
1.045309774172856	0.434243886201858	0.658832090000000	T	T	T
0.008291670191747	0.275857060292372	0.357738190000000	T	T	T
0.070995241641772	0.272710970174983	0.394888020000000	T	T	T
0.729675256873785	0.080788063014240	0.402770330000000	T	T	T
0.661410285295150	0.171717236406856	0.377997220000000	T	T	T
0.352608528154092	0.136210735082093	0.591304900000000	T	T	T
0.333871047720788	0.232073008658768	0.621796040000000	T	T	T
0.641767424840911	0.296059421046132	0.683978890000000	T	T	T
0.901668440851139	0.458784997117506	0.642733770000000	T	T	T
0.696906146115997	0.587504231920088	0.665079120000000	T	T	T
0.603310833951599	0.638012663804577	0.681930130000000	T	T	T
0.343189177936267	0.408222385230983	0.520397280000000	T	T	T

14-CH-COH

xyzjob

1.000000000000000				
10.227000000000000	0.000000000000000	0.000000000000000		
0.000000000000001	10.225000000000000	0.000000000000000		
0.000000000000002	0.000000000000002	40.000000000000000		
Cu	O	H	C	Na
48	49	99	2	1

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.8000000100000000	T	T	T
0.250020005781725	-0.0000000000000000	0.8000000100000000	T	T	T
0.500050021563684	-0.0000000000000000	0.8000000100000000	T	T	T
0.750069997345419	-0.0000000000000000	0.8000000100000000	T	T	T
-0.0000000000000000	0.249980009326885	0.8000000100000000	T	T	T
0.250020005781725	0.249980009326885	0.8000000100000000	T	T	T
0.500050021563684	0.249980009326885	0.8000000100000000	T	T	T
0.750069997345419	0.249980009326885	0.8000000100000000	T	T	T
-0.0000000000000000	0.499950008653389	0.8000000100000000	T	T	T
0.250020005781725	0.499950008653389	0.8000000100000000	T	T	T
0.500050021563684	0.499950008653389	0.8000000100000000	T	T	T
0.750069997345419	0.499950008653389	0.8000000100000000	T	T	T
-0.0000000000000000	0.750020057983628	0.8000000100000000	T	T	T
0.250020005781725	0.750020057983628	0.8000000100000000	T	T	T
0.500050021563684	0.750020057983628	0.8000000100000000	T	T	T
0.750069997345419	0.750020057983628	0.8000000100000000	T	T	T
0.124960002889704	0.124990004663442	0.7548300000000000	T	T	T
0.374989998671663	0.124990004663442	0.7548300000000000	T	T	T
0.625010024453398	0.124990004663442	0.7548300000000000	T	T	T
0.875040020235357	0.124990004663442	0.7548300000000000	T	T	T
0.124960002889704	0.374960013989946	0.7548300000000000	T	T	T
0.374989998671663	0.374960013989946	0.7548300000000000	T	T	T
0.625010024453398	0.374960013989946	0.7548300000000000	T	T	T
0.875040020235357	0.374960013989946	0.7548300000000000	T	T	T
0.124960002889703	0.625040023320567	0.7548300000000000	T	T	T
0.374989998671663	0.625040023320567	0.7548300000000000	T	T	T
0.625010024453398	0.625040023320567	0.7548300000000000	T	T	T
0.875040020235357	0.625040023320567	0.7548300000000000	T	T	T



0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
-0.003286280075995	1.002486457403286	0.712889820000000	T	T	T
0.250898955802053	1.006402987549408	0.709234720000000	T	T	T
0.504181451659225	1.006755567562562	0.709894930000000	T	T	T
0.746194997255803	0.012402460462738	0.707636250000000	T	T	T
-0.001699880039308	0.243274369076694	0.712768810000000	T	T	T
0.247209945716750	0.254681489502298	0.708999600000000	T	T	T
0.493574731413943	0.251099259368645	0.707660660000000	T	T	T
0.738768337084062	0.247963919251658	0.710957350000000	T	T	T
0.995018543009866	0.494885248464420	0.710049570000000	T	T	T
0.242677635611939	0.497367398557037	0.715504100000000	T	T	T
0.491040331355334	0.502184118736743	0.707624740000000	T	T	T
0.752421437399794	0.497710008569819	0.708766140000000	T	T	T
1.005105473243121	0.750675658008098	0.711410710000000	T	T	T
0.264287266111655	0.751558258041027	0.711270610000000	T	T	T
0.491479421365493	0.745860917828450	0.707306900000000	T	T	T
0.756294557489361	0.773488188859237	0.708918060000000	T	T	T
0.766299677720729	0.678787255325897	0.635493530000000	T	T	T
0.033295450769962	0.076524622855169	0.313060710000000	T	T	T
0.462431640693761	0.478061727836724	0.495754870000000	T	T	T
0.575092893299061	0.883279772955619	0.632044940000000	T	T	T
0.866336350034076	0.427119945936068	0.396256330000000	T	T	T
0.300469776948382	0.634394683669594	0.592559790000000	T	T	T
0.648318384992402	0.262507459794288	0.592374770000000	T	T	T
0.563154743022988	0.698474036060420	0.355537150000000	T	T	T

0.643646494884365	0.211769977901242	0.332817980000000	T	T	T
0.532084662304488	0.599545772369359	0.549165450000000	T	T	T
0.959221072182047	0.041318181541604	0.419882270000000	T	T	T
0.480520921112076	0.503062708769526	0.395855350000000	T	T	T
0.405697189381774	0.360614553454709	0.347126220000000	T	T	T
1.010288933362990	0.772693558829594	0.633476670000000	T	T	T
0.132077693054307	0.595715462226445	0.550212510000000	T	T	T
0.810500468742877	0.262850409807081	0.641512890000000	T	T	T
0.797678538446367	0.817962230518592	0.424307740000000	T	T	T
0.983863522751902	0.039091721458533	0.538451120000000	T	T	T
0.170953163953300	0.698616356065731	0.371186080000000	T	T	T
0.316692527323536	0.555930060742034	0.441478850000000	T	T	T
0.276935256404146	0.091315243407022	0.342365380000000	T	T	T
0.980642812677422	0.390945424586376	0.555151620000000	T	T	T
0.142605583297761	0.189217547059804	0.581368290000000	T	T	T
0.262507516070500	0.342377582774279	0.532177120000000	T	T	T
0.738214517071252	0.503619098790288	0.577209020000000	T	T	T
0.845521709552743	0.362325093518533	0.497372860000000	T	T	T
0.682643045786164	0.092417533448147	0.536505810000000	T	T	T
0.565453433076141	0.155441195799589	0.472337630000000	T	T	T
0.969507842419927	0.797502229755218	0.322309280000000	T	T	T
0.382642038848616	0.268643900023237	0.601895320000000	T	T	T
0.550289682725482	-0.024693600921330	0.423105410000000	T	T	T
0.662207555313591	0.375025213992381	0.436666570000000	T	T	T
0.810301168738261	0.664346284787100	0.367404820000000	T	T	T
0.328406247594417	0.841458471395247	0.447053340000000	T	T	T
0.641358834831465	0.844530591509868	0.566668350000000	T	T	T
0.227934035270988	0.414404145461633	0.631636020000000	T	T	T

1.027951063771428	0.223482768338259	0.466482840000000	T	T	T
1.013162233429441	0.081802733052098	0.635861330000000	T	T	T
0.766052717715019	0.689551775727531	0.482121060000000	T	T	T
1.056924554441449	0.488360378220978	0.434704530000000	T	T	T
0.338337217824073	0.621394673184557	0.321479330000000	T	T	T
0.198556754591640	-0.050087181868782	0.394352490000000	T	T	T
0.912743521107245	0.770496388747618	0.541593650000000	T	T	T
0.266863966171243	0.829265740940332	0.634987800000000	T	T	T
0.310441477178977	-0.003703400138171	0.502630610000000	T	T	T
0.976957412592197	0.457205897058582	0.646024680000000	T	T	T
0.886119320491561	0.188624557037682	0.363053960000000	T	T	T
0.515522121921482	-0.034033271269800	0.356169590000000	T	T	T
0.376840398714462	0.058759622192352	0.640185390000000	T	T	T
0.973661342515977	0.107697844018259	0.330961340000000	T	T	T
-0.020860820482409	0.090892563391247	0.293175860000000	T	T	T
0.486941391260545	0.528142019705252	0.516710580000000	T	T	T
0.539691512480395	0.433631306179002	0.486427220000000	T	T	T
0.518774741996695	0.953718335583716	0.642254480000000	T	T	T
0.619489224325726	0.857444001991677	0.653872560000000	T	T	T
0.875930340255940	0.346424692925281	0.384441050000000	T	T	T
0.846879109584130	0.503698008793232	0.382246010000000	T	T	T
0.300715686954072	0.715149326682592	0.607119070000000	T	T	T
0.283505866556087	0.548609170468890	0.607511340000000	T	T	T
0.666215545406277	0.204163927617457	0.573508700000000	T	T	T
0.719619226641234	0.258720979653017	0.610186770000000	T	T	T
0.577421583352909	0.792601129572352	0.354331300000000	T	T	T
0.478776781071741	0.686805275625056	0.343620000000000	T	T	T
0.600513113886897	0.125959474699609	0.328926100000000	T	T	T

0.563927583040862	0.263100109816401	0.333186870000000	T	T	T
0.610985214129070	0.566808711147922	0.561330940000000	T	T	T
0.461006180660800	0.604730572562807	0.566114030000000	T	T	T
0.987124332827310	0.080897453018328	0.441905360000000	T	T	T
0.910655581058961	-0.040966711528489	0.424843360000000	T	T	T
0.508854491767292	0.583654531776450	0.384555560000000	T	T	T
0.415047479597995	0.535335609973643	0.413944850000000	T	T	T
0.430540769956282	0.398306024860997	0.369634810000000	T	T	T
0.375769188689684	0.439639206403169	0.335934970000000	T	T	T
0.995307053016534	0.777255458999795	0.657700220000000	T	T	T
1.100776855455529	0.788425209416548	0.630167020000000	T	T	T
1.067031634675173	0.661646494686367	0.550357890000000	T	T	T
0.192898954460800	0.620090673135902	0.569473100000000	T	T	T
0.863870589977061	0.178217176649379	0.642591040000000	T	T	T
0.877805700299306	0.333028762425477	0.645749910000000	T	T	T
0.799262188482986	0.746865267865927	0.407709640000000	T	T	T
0.712893766485714	0.866553352331550	0.424119740000000	T	T	T
0.953433162048196	-0.053152101983130	0.541069240000000	T	T	T
1.007094993289136	0.066582312484225	0.559804830000000	T	T	T
0.174625634038232	0.789471029455570	0.379753490000000	T	T	T
0.140543933250083	0.635537213712215	0.386785950000000	T	T	T
0.351192668121355	0.534450999940636	0.465299790000000	T	T	T
0.230917505339982	0.516801639282132	0.439466970000000	T	T	T
0.203635244709074	0.111970544177682	0.326915160000000	T	T	T
0.314255007267165	0.176248356575912	0.345011900000000	T	T	T
1.032895883885782	0.477579817818748	0.554824320000000	T	T	T
0.902367330867302	0.406972125184342	0.569923560000000	T	T	T
1.088299925166999	0.264450119866768	0.573474310000000	T	T	T

1.096611985359216	0.179092876682044	0.603571440000000	T	T	T
0.229948455317571	0.429202886013780	0.539865050000000	T	T	T
0.327961027584120	0.361427923485056	0.515318730000000	T	T	T
0.709034166396460	0.406253745157535	0.581540150000000	T	T	T
0.745585927241723	0.562990261005457	0.596191390000000	T	T	T
0.889821180577168	0.361311593480724	0.520387380000000	T	T	T
0.826391929110365	0.454317466950817	0.494596330000000	T	T	T
0.668508405459294	-0.000128420004792	0.546525790000000	T	T	T
0.777647027983133	0.090148203363472	0.532849970000000	T	T	T
0.620533284349868	0.218843588165164	0.459199990000000	T	T	T
0.609191294087582	0.137660125136166	0.493646810000000	T	T	T
0.984295842761905	-0.118421454418367	0.311962020000000	T	T	T
1.051885094324905	0.776437578969281	0.335220760000000	T	T	T
0.481909171144177	0.279178700416303	0.596242640000000	T	T	T
0.325631397530243	0.268388690013721	0.581543140000000	T	T	T
0.492277211383944	0.916160064182406	0.434901550000000	T	T	T
0.546017372626684	0.053372901991374	0.438085710000000	T	T	T
0.749911787341752	0.391901394622044	0.425574940000000	T	T	T
0.600558893887963	0.419046215634826	0.420589830000000	T	T	T
0.853681869741449	0.709118796457584	0.349219700000000	T	T	T
0.713659786503422	0.658061794552626	0.361331380000000	T	T	T
0.280274656481373	-0.123637044612959	0.426766080000000	T	T	T
0.299726166931182	0.749854007977438	0.448386420000000	T	T	T
0.594102383738652	0.767348978630181	0.559216610000000	T	T	T
0.629519454557671	0.865184212280469	0.591245900000000	T	T	T
0.247712715728376	0.413977395445711	0.655915100000000	T	T	T
0.297818926887083	0.352394923148039	0.624018570000000	T	T	T
1.059840584508879	0.292829210925604	0.451521480000000	T	T	T

0.950437041978918	0.269459760053682	0.477978060000000	T	T	T
0.999813213120739	-0.005453040203452	0.628324240000000	T	T	T
1.042342084104224	0.079510702966582	0.659656070000000	T	T	T
0.687648655901916	0.634831143685878	0.479268650000000	T	T	T
0.776947777966960	0.732869417343736	0.460518160000000	T	T	T
1.019497913575956	0.526042919626934	0.456400070000000	T	T	T
0.976482782581226	0.469504277517447	0.419959440000000	T	T	T
0.332099577679818	0.647047614141682	0.297227960000000	T	T	T
0.260895446033226	0.651772724317976	0.335552180000000	T	T	T
0.120335272782761	-0.013750630513047	0.407408270000000	T	T	T
0.238106685506228	0.014374400536313	0.378485070000000	T	T	T
0.859096209866657	0.732581807332997	0.524084240000000	T	T	T
0.848686429625921	0.768285818665134	0.559980240000000	T	T	T
0.300899856958326	0.917319444225662	0.632527730000000	T	T	T
0.305301627060115	0.803795819990034	0.656244380000000	T	T	T
0.386273518932600	0.040263371502249	0.496300220000000	T	T	T
0.292602096766442	-0.067748362527726	0.483107940000000	T	T	T
0.066955711548352	0.428649005993115	0.642509410000000	T	T	T
0.978496502627789	0.541902710218670	0.633442150000000	T	T	T
0.797559398443610	0.199429237440812	0.352901120000000	T	T	T
0.892971560650024	0.130791054879883	0.381273790000000	T	T	T
0.536252902400880	-0.024359450908861	0.380209250000000	T	T	T
0.421236329741117	-0.010231240381731	0.352407460000000	T	T	T
0.361565958361230	0.130815134880782	0.622743700000000	T	T	T
0.341347747893683	0.089600193343032	0.661514170000000	T	T	T
0.640389284809044	0.377897564099550	0.709681650000000	T	T	T
0.849190159637577	0.728400217176988	0.633148720000000	T	T	T
0.550316072726088	0.557009530782308	0.651800480000000	T	T	T

0.712717116481627	0.669553314981379	0.668402340000000	T	T	T
0.591444483677188	0.604615422558513	0.672957380000000	T	T	T
0.170101683933607	0.134828865030533	0.518771780000000	T	T	T

15-CH-C

xyzjob

1.000000000000000					
10.227000000000000	0.000000000000000	0.000000000000000			
0.000000000000001	10.225000000000000	0.000000000000000			
0.000000000000002	0.000000000000002	40.000000000000000			
Cu	O	H	C	Na	
48	48	98	2	1	

Selective dynamics

Direct

-0.000000000000000	-0.000000000000000	0.800000100000000	T	T	T
0.250020005781725	-0.000000000000000	0.800000100000000	T	T	T
0.500050021563684	-0.000000000000000	0.800000100000000	T	T	T
0.750069997345419	-0.000000000000000	0.800000100000000	T	T	T
-0.000000000000000	0.249980009326885	0.800000100000000	T	T	T
0.250020005781725	0.249980009326885	0.800000100000000	T	T	T
0.500050021563684	0.249980009326885	0.800000100000000	T	T	T
0.750069997345419	0.249980009326885	0.800000100000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000100000000	T	T	T
0.250020005781725	0.499950008653389	0.800000100000000	T	T	T
0.500050021563684	0.499950008653389	0.800000100000000	T	T	T
0.750069997345419	0.499950008653389	0.800000100000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000100000000	T	T	T

0.250020005781725	0.750020057983628	0.800000010000000	T	T	T
0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
0.625010024453398	0.374960013989946	0.754830000000000	T	T	T
0.875040020235357	0.374960013989946	0.754830000000000	T	T	T
0.124960002889703	0.625040023320567	0.754830000000000	T	T	T
0.374989998671663	0.625040023320567	0.754830000000000	T	T	T
0.625010024453398	0.625040023320567	0.754830000000000	T	T	T
0.875040020235357	0.625040023320567	0.754830000000000	T	T	T
0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
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0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
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0.747092607276562	-0.002096280078210	0.708026030000000	T	T	T
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0.253756275868133	0.244635089127462	0.710066220000000	T	T	T
0.509712751787142	0.248029979254122	0.709061640000000	T	T	T
0.740420797122274	0.243119109070895	0.708534240000000	T	T	T
0.010461420241918	0.508706788980107	0.710832470000000	T	T	T



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0.440688670190955	0.487286458180909	0.426252040000000	T	T	T
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0.051743391196568	0.308176521498220	0.546627070000000	T	T	T
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0.286107986616261	0.696001995968196	0.457054240000000	T	T	T
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0.736803827038633	0.637480373784724	0.594694710000000	T	T	T

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0.029073330672318	0.659378024601731	0.501320650000000	T	T	T
0.504343711662980	0.767987048653985	0.586367740000000	T	T	T
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0.834722019303002	0.397250464821614	0.459144660000000	T	T	T
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0.822618259023095	0.978049246491521	0.352623440000000	T	T	T
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0.245651245680698	0.174990726528997	0.572165430000000	T	T	T
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0.852685409718402	0.966151796047619	0.471944250000000	T	T	T
0.011217780259411	0.781452189156381	0.443065240000000	T	T	T
0.348147468050934	0.976218706423218	0.353253600000000	T	T	T
0.132412643062051	0.388298604487618	0.378023650000000	T	T	T
0.878391610312858	0.087054103248029	0.531309180000000	T	T	T
0.071113831644509	0.135067315039433	0.623480460000000	T	T	T
0.317941037352410	0.533977049922953	0.512850110000000	T	T	T
0.717197706585245	0.400423984940019	0.627717670000000	T	T	T
0.992400892949330	0.612031382835208	0.352319040000000	T	T	T
0.618457044301858	0.360945023467042	0.346243160000000	T	T	T
0.385388298912125	0.167084106233995	0.637996360000000	T	T	T
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0.375343628679847	0.852157321794425	0.659867210000000	T	T	T
0.368399478519262	0.986710066814660	0.636986790000000	T	T	T
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0.848399949619302	0.841360851391609	0.384120700000000	T	T	T
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0.908523241009651	0.730555907257418	0.657487460000000	T	T	T
0.267295366181226	0.521597429461066	0.603213740000000	T	T	T
0.282764676538946	0.540487930165878	0.562259720000000	T	T	T
0.588729923614413	1.182162504107091	0.356504070000000	T	T	T
0.498194221520768	1.057512879456342	0.358334370000000	T	T	T
0.734942706995590	0.443693396554425	0.324122060000000	T	T	T
0.742638827173570	0.589707462002288	0.311744040000000	T	T	T
0.324103387494915	0.942627485169917	0.526662810000000	T	T	T
0.164893943813181	0.941414645124665	0.529511540000000	T	T	T
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0.561294182979965	0.783152649219824	0.448341070000000	T	T	T
0.548307732679652	0.916193824183658	0.432872620000000	T	T	T
0.452431210462501	0.402553595019482	0.436477170000000	T	T	T
0.376619958709357	0.539842670141809	0.440019680000000	T	T	T
0.573505263262345	0.099273963703961	0.543914480000000	T	T	T
0.627292814506180	0.187518326996401	0.572165390000000	T	T	T
-0.027052750625599	0.944535405241095	0.546760260000000	T	T	T
0.075068731735973	0.847001731602063	0.569422150000000	T	T	T
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0.347832048043639	0.752226648065966	0.445383510000000	T	T	T
0.379133208767478	0.577646141552274	0.353414030000000	T	T	T
0.410596079495062	0.478763807862924	0.385018040000000	T	T	T
0.805336988623467	0.679949455369262	0.608213180000000	T	T	T
0.654037285124650	0.693359965869614	0.593791400000000	T	T	T
0.910829351062980	0.385821774395208	0.620974730000000	T	T	T
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0.012291300284238	0.711684646553320	0.479253660000000	T	T	T
0.044697701033636	0.717876206784332	0.519160430000000	T	T	T
0.442897030242016	0.694781335922650	0.583380350000000	T	T	T
0.460581490650973	0.822214400677242	0.603705200000000	T	T	T
0.740951017134536	0.855400151915413	0.485758750000000	T	T	T
0.691764445997096	0.733524207368166	0.504262890000000	T	T	T
0.585553743540970	0.319426951917985	0.529762520000000	T	T	T
0.628327764530116	0.470375657549956	0.518930590000000	T	T	T
0.789115288248343	0.435702686256293	0.439834170000000	T	T	T
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0.032228770745292	1.096281940902836	0.361077850000000	T	T	T
0.126000082913758	0.218791538163227	0.368230520000000	T	T	T
0.224800925198533	0.435089596233418	0.658904060000000	T	T	T

0.148574523435797	0.404568025094640	0.626943550000000	T	T	T
0.363554858407226	0.223334598332724	0.459864530000000	T	T	T
0.487096491264134	0.312928101675511	0.479418730000000	T	T	T
0.732567306940667	0.596738692264626	0.406155580000000	T	T	T
0.590652553658873	0.525402159603022	0.414307900000000	T	T	T
0.814533498836139	0.917692754239589	0.333778320000000	T	T	T
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0.229450465306052	0.078168262916499	0.450025770000000	T	T	T
0.235804845452997	0.098026683657428	0.487179200000000	T	T	T
0.248036195735856	0.101872763800929	0.555437180000000	T	T	T
0.193349594471223	0.145374785424010	0.591006640000000	T	T	T
0.199643034616759	0.702662116216685	0.596046860000000	T	T	T
0.213419914935347	0.836464851208929	0.619500780000000	T	T	T
0.837791869373990	0.600512592405428	0.520019890000000	T	T	T
0.749301307327642	0.604456402552577	0.553346290000000	T	T	T
0.775457827932512	0.058262812173819	0.635389440000000	T	T	T
0.847203369591630	0.919399374303257	0.647704120000000	T	T	T
0.865794520021551	1.007109997575785	0.495838230000000	T	T	T
0.798557818466696	1.014683317858357	0.455567060000000	T	T	T
-0.033547260775780	0.859277512060088	0.457577110000000	T	T	T
-0.067749351566706	0.754734028159511	0.429365460000000	T	T	T
0.364679538433235	0.954346485607159	0.377399420000000	T	T	T
0.274987376359098	1.040910918836919	0.352916200000000	T	T	T
0.122017602821668	0.400045644925907	0.401719750000000	T	T	T
0.224663705195365	0.415678875509193	0.372071730000000	T	T	T
0.928802021478605	0.169938966340508	0.529177610000000	T	T	T
0.788301638229520	0.108580104051178	0.540227330000000	T	T	T
0.125677942906307	0.132975954961398	0.643239760000000	T	T	T

0.990185452898103	1.097898280963149	0.631121380000000	T	T	T
0.406095629390984	0.487411568185575	0.511751350000000	T	T	T
0.318323507361249	0.614511262927726	0.499379470000000	T	T	T
0.697662916133499	0.480136087914122	0.613859530000000	T	T	T
0.697126066121081	0.428528755988626	0.650521280000000	T	T	T
0.925112201393272	0.575719501480391	0.338428850000000	T	T	T
1.040977854072680	0.528437759716283	0.361259880000000	T	T	T
0.666170845405241	0.387402644454191	0.367371280000000	T	T	T
0.538639412456067	0.418390865610376	0.348038280000000	T	T	T
0.334258047729735	0.240533078974416	0.629913140000000	T	T	T
0.369677048548802	0.173092986458191	0.662835520000000	T	T	T
0.347709518040804	0.654616424424078	0.692088340000000	T	T	T
0.595258553765386	0.806125450076948	0.646688760000000	T	T	T
0.640386534808976	0.624696643307755	0.680502130000000	T	T	T
0.603413703953975	0.734334117398386	0.666736590000000	T	T	T
0.107485902485616	0.444695136591804	0.501789960000000	T	T	T

16-CH<sub>2</sub>-C

xyzjob

1.000000000000000				
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0.000000000000001	10.225000000000000	0.000000000000000		
0.000000000000002	0.000000000000002	40.000000000000000		
Cu	O	H	C	Na
48	48	99	2	1

Selective dynamics

Direct

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-0.0000000000000000	0.249980009326885	0.8000000100000000	T	T	T
0.250020005781725	0.249980009326885	0.8000000100000000	T	T	T
0.500050021563684	0.249980009326885	0.8000000100000000	T	T	T
0.750069997345419	0.249980009326885	0.8000000100000000	T	T	T
-0.0000000000000000	0.499950008653389	0.8000000100000000	T	T	T
0.250020005781725	0.499950008653389	0.8000000100000000	T	T	T
0.500050021563684	0.499950008653389	0.8000000100000000	T	T	T
0.750069997345419	0.499950008653389	0.8000000100000000	T	T	T
-0.0000000000000000	0.750020057983628	0.8000000100000000	T	T	T
0.250020005781725	0.750020057983628	0.8000000100000000	T	T	T
0.500050021563684	0.750020057983628	0.8000000100000000	T	T	T
0.750069997345419	0.750020057983628	0.8000000100000000	T	T	T
0.124960002889704	0.124990004663442	0.7548300000000000	T	T	T
0.374989998671663	0.124990004663442	0.7548300000000000	T	T	T
0.625010024453398	0.124990004663442	0.7548300000000000	T	T	T
0.875040020235357	0.124990004663442	0.7548300000000000	T	T	T
0.124960002889704	0.374960013989946	0.7548300000000000	T	T	T
0.374989998671663	0.374960013989946	0.7548300000000000	T	T	T
0.625010024453398	0.374960013989946	0.7548300000000000	T	T	T
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0.124960002889703	0.625040023320567	0.7548300000000000	T	T	T
0.374989998671663	0.625040023320567	0.7548300000000000	T	T	T
0.625010024453398	0.625040023320567	0.7548300000000000	T	T	T
0.875040020235357	0.625040023320567	0.7548300000000000	T	T	T

0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
0.374989998671663	0.875010042647071	0.754830000000000	T	T	T
0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
0.875040020235357	0.875010042647071	0.754830000000000	T	T	T
-0.013663070315958	-0.011712810437008	0.707344040000000	T	T	T
0.255083105898817	1.002191367392274	0.709671380000000	T	T	T
0.510145251797144	0.994695237112587	0.708691750000000	T	T	T
0.759023387552459	-0.018776330700558	0.709573820000000	T	T	T
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0.237640145495443	0.235209558775785	0.710050650000000	T	T	T
0.504817211673931	0.269916650070728	0.713228570000000	T	T	T
0.734854216993546	0.217619728119501	0.707353580000000	T	T	T
-0.002829650065435	0.505525578861418	0.710681920000000	T	T	T
0.255763865914559	0.489075548247658	0.708373590000000	T	T	T
0.494549451436482	0.510520049047765	0.703068870000000	T	T	T
0.739223227094583	0.486246188142093	0.713628140000000	T	T	T
1.008898473330840	0.739513837591638	0.710155770000000	T	T	T
0.257967705965522	0.729000657199384	0.707693450000000	T	T	T
0.523179552098562	0.758285878292039	0.705040710000000	T	T	T
0.778558438004214	0.742014587684949	0.706094480000000	T	T	T
0.107536752486790	0.184292886876059	0.331665110000000	T	T	T
0.626331894483964	0.691053315783550	0.478300190000000	T	T	T
0.722940926718050	1.004042777461349	0.637377830000000	T	T	T
0.893556130663537	0.575021261454337	0.398051110000000	T	T	T
0.941987061783504	0.863133422203951	0.630127180000000	T	T	T
0.534721862365474	0.389353374526973	0.540981430000000	T	T	T
0.588771483615381	0.857741302002768	0.335103750000000	T	T	T
0.690408615965738	0.213760437975511	0.343359610000000	T	T	T



0.477915161051814	0.143766085363990	0.536135650000000	T	T	T
0.954339722069160	0.203610037596792	0.430813100000000	T	T	T
0.363155958398005	0.713818336632929	0.355543970000000	T	T	T
0.436607910096587	0.508034548955032	0.387473370000000	T	T	T
0.897679950758903	0.155653645807521	0.529303950000000	T	T	T
0.264774466122929	0.140812875253799	0.574154740000000	T	T	T
1.037472503991610	0.270810040104059	0.629645400000000	T	T	T
0.860998189910638	0.956170685675218	0.421330160000000	T	T	T
0.216584015008516	0.405488545128988	0.529350200000000	T	T	T
0.255047605897995	0.921987884399843	0.395002250000000	T	T	T
0.171414283963968	0.736118987464978	0.537639940000000	T	T	T
0.286212756618686	0.248510389272049	0.374343050000000	T	T	T
0.966718432355422	0.670553585018699	0.580329430000000	T	T	T
0.402143029299579	0.201145377504841	0.629274840000000	T	T	T
0.379487458775672	0.743054157723736	0.576613470000000	T	T	T
0.423792539800225	0.613424762887188	0.514155710000000	T	T	T
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0.786768778194074	0.382525864272235	0.520721450000000	T	T	T
0.741205887140432	0.326514272182416	0.454012790000000	T	T	T
0.043795581012780	0.931547814756528	0.339972480000000	T	T	T
0.533749662342994	0.407253665194846	0.609659580000000	T	T	T
0.588176493601613	0.113854634247971	0.440599370000000	T	T	T
0.656241445175623	0.541417410200557	0.426993860000000	T	T	T
0.847851749606620	0.811498820277438	0.364027400000000	T	T	T
0.352413198149575	0.070130042616587	0.475864060000000	T	T	T
0.687849725906571	1.008919797643315	0.538923960000000	T	T	T
0.314325897268808	0.559914550890699	0.629779470000000	T	T	T
0.987161692828170	0.622481053225086	0.460659990000000	T	T	T

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0.699067076165972	0.921086374366200	0.474513590000000	T	T	T
0.073784641706277	0.852324011800645	0.442862210000000	T	T	T
0.236613455471702	0.809260440193917	0.301826700000000	T	T	T
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0.089002832058199	-0.018237690680460	0.501964420000000	T	T	T
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0.059241361369962	0.105252373927022	0.332844610000000	T	T	T
0.544985392602816	0.659769764616352	0.489335430000000	T	T	T
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0.627378314508164	0.979105146530914	0.641183230000000	T	T	T
0.726487306800058	0.101898613801887	0.636665430000000	T	T	T
0.917402331214980	0.487810898200479	0.389178040000000	T	T	T
0.930938521528014	0.591622482073741	0.421076350000000	T	T	T
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0.992996382963097	0.836555261212303	0.652088630000000	T	T	T
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0.671710645533353	0.812471810313741	0.343566710000000	T	T	T
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0.319875097397135	0.768801968684391	0.371994490000000	T	T	T
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0.810333678739014	0.121595344536782	0.533060080000000	T	T	T
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0.798923088475144	0.942473685164176	0.439528240000000	T	T	T
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0.452259620458531	0.277365470348645	0.624067090000000	T	T	T

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0.847290149593634	0.672981595109291	0.540105410000000	T	T	T
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0.849081329635054	0.317862741859618	0.530760050000000	T	T	T
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0.705288286309837	0.411232665343306	0.444309550000000	T	T	T
0.753974957435719	0.335330032511335	0.478795130000000	T	T	T
0.088177802039122	0.884298772993643	0.319873150000000	T	T	T
0.105677852443805	0.935781614914494	0.357964240000000	T	T	T
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0.502309251615928	0.099179763700450	0.452246600000000	T	T	T
0.627904594520328	0.198791157416997	0.444918400000000	T	T	T
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0.867989290072309	0.721218376909027	0.372114580000000	T	T	T
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0.694357436057055	0.938645835021359	0.555398760000000	T	T	T
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0.301920726981940	0.603137142503354	0.652541460000000	T	T	T
0.404966629364877	0.518640349350738	0.631456020000000	T	T	T
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0.648023274985577	0.829181360937183	0.474799820000000	T	T	T
0.644095134894739	-0.005961370222426	0.466248910000000	T	T	T
0.087959602034067	0.905165273772176	0.463752400000000	T	T	T
0.992639732954855	0.899424843558005	0.431207700000000	T	T	T
0.278885986449252	0.754088428135423	0.319143810000000	T	T	T
0.296086736847022	0.841686581403755	0.286308450000000	T	T	T
0.154426133571116	0.246620269201526	0.440723270000000	T	T	T
0.268893286218177	0.229992808581154	0.418010870000000	T	T	T
0.167480943873003	0.031653621181017	0.495722280000000	T	T	T
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0.426481529862413	0.029686141107609	0.636233200000000	T	T	T
0.452369180461064	0.903851693723169	0.658069720000000	T	T	T
0.403812879338193	0.462007327237731	0.461894270000000	T	T	T
0.279583966465395	0.409884175292988	0.443708560000000	T	T	T
0.062211901438652	0.531273369822083	0.593256820000000	T	T	T
0.206297704770646	0.497646838567462	0.607343380000000	T	T	T
0.832101999242407	0.282294820532567	0.363643110000000	T	T	T
0.941959301782869	0.270936840108792	0.391024680000000	T	T	T
0.545331542610824	0.095293543555452	0.400584520000000	T	T	T
0.427009189874616	0.151271055644000	0.380496390000000	T	T	T
0.868569420085724	0.319672821927159	0.633116450000000	T	T	T
0.754554877449125	0.335306532510455	0.660816050000000	T	T	T
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0.686878925884120	0.718198086796342	0.633886490000000	T	T	T
0.785703638169443	0.573756511407149	0.646187120000000	T	T	T
0.710325156426313	0.645402784080313	0.653182640000000	T	T	T

0.630453494579280	0.622184223214015	0.679826250000000	T	T	T
0.197733354572592	0.589007641976176	0.494146250000000	T	T	T

17-CH<sub>2</sub>-CH

xyzjob

1.000000000000000					
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Cu	O	H	C	Na	
48	48	100	2	1	

Selective dynamics

Direct

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0.500050021563684	0.249980009326885	0.800000100000000	T	T	T
0.750069997345419	0.249980009326885	0.800000100000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000100000000	T	T	T
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0.500050021563684	0.499950008653389	0.800000100000000	T	T	T
0.750069997345419	0.499950008653389	0.800000100000000	T	T	T
-0.000000000000000	0.750020057983628	0.800000100000000	T	T	T
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0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
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0.250941015803031	0.242871599061662	0.709777080000000	T	T	T
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0.244530965654796	0.494643518455403	0.709958960000000	T	T	T

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0.990565122906874	0.363982433580372	0.339869760000000	T	T	T
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0.423232179787269	0.314560821736430	0.562160340000000	T	T	T
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0.231581675355344	0.631769943571658	0.413376210000000	T	T	T
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0.916804881201173	-0.045314601690709	0.352729140000000	T	T	T
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0.482133811149369	0.590877662045946	0.437389760000000	T	T	T
0.664189685359431	0.870542602480391	0.359877760000000	T	T	T
0.248759875752586	-0.070640292635628	0.478182730000000	T	T	T
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0.986766562819038	0.996967387197359	0.512939840000000	T	T	T
0.328144987588374	0.780917849136440	0.638185950000000	T	T	T
0.221579255124034	0.292542970914924	0.487189560000000	T	T	T
0.933746661592950	0.640166873884958	0.636456420000000	T	T	T
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0.322269397452498	0.194719097265066	0.364356970000000	T	T	T
0.504753081672445	0.163571516102934	0.639284970000000	T	T	T
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0.703188346261269	0.759156698324528	0.391054380000000	T	T	T
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0.410110139483817	0.239928698951863	0.547121440000000	T	T	T
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0.653269035106884	0.240775268983452	0.647387270000000	T	T	T
0.782931638105339	0.337811482603922	0.653805080000000	T	T	T

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0.978216602621316	0.213854447979022	0.438532530000000	T	T	T
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18-CH<sub>2</sub>-CH<sub>2</sub>

xyzjob

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Cu	O	H	C	Na	
48	48	100	2	1	

Selective dynamics

Direct

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0.750069997345419	0.750020057983628	0.8000000100000000	T	T	T
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0.248492285746397	0.285332040645887	0.437821190000000	T	T	T
0.359017558302307	0.662054684701604	0.415242090000000	T	T	T
0.219628255078918	0.609773402750953	0.426067590000000	T	T	T
0.443769340262188	0.033039401232714	0.350179470000000	T	T	T
0.286485876625002	0.007897450294660	0.349912870000000	T	T	T
0.907252580980268	0.255775629543120	0.443550620000000	T	T	T
0.926886401434301	0.247549949236215	0.483803650000000	T	T	T
0.360080818326889	0.917166864219961	0.547746140000000	T	T	T
0.317675937346279	0.813983050370122	0.518546460000000	T	T	T
0.104728672421854	0.494390468445966	0.655715300000000	T	T	T
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0.660064405264026	0.727144727130142	0.458180800000000	T	T	T

0.634389314670294	0.654478554418934	0.492824490000000	T	T	T
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0.564327573050112	1.005255257506591	0.586581370000000	T	T	T
0.456135540548166	0.953229505565477	0.492767400000000	T	T	T
0.433697370029275	0.026938621005095	0.458928230000000	T	T	T
0.591523213679006	0.920299454336841	0.451130640000000	T	T	T
0.588313223604781	0.835738001181809	0.418527020000000	T	T	T
0.804644278607451	0.898719383531677	0.359073330000000	T	T	T
-0.265556506141009	0.951828055513193	0.329603800000000	T	T	T
0.758334247536521	0.299894481189213	0.412764430000000	T	T	T
0.877409330290144	0.295487351024782	0.391899290000000	T	T	T
0.727961486834155	0.209489387816156	0.512044850000000	T	T	T
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0.129594222996871	0.679357235347169	0.629089300000000	T	T	T
0.106163982455050	0.822547100689653	0.643339090000000	T	T	T
0.932140751555813	0.468137557466455	0.474333510000000	T	T	T
0.848776189628004	0.587935021936156	0.472672330000000	T	T	T
0.791181478296118	0.566792641147325	0.602087400000000	T	T	T
0.935148971625374	0.514696999203609	0.613628850000000	T	T	T
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0.077691301796617	0.356173593289017	0.365882190000000	T	T	T
0.391658079057113	0.106729823982142	0.655908440000000	T	T	T
0.372601268616427	0.202376957550787	0.622859090000000	T	T	T
0.653864775120661	0.527089309665975	0.650300700000000	T	T	T
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0.562337263004087	0.474712087711755	0.654863270000000	T	T	T
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19-CH<sub>4</sub>

xyzjob

1.000000000000000			
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0.000000000000001	10.225000000000000	0.000000000000000	
0.000000000000002	0.000000000000002	40.000000000000000	
Cu	O	H	C
48	50	102	2

Selective dynamics

Direct

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0.250020005781725	0.249980009326885	0.800000010000000	T	T	T
0.500050021563684	0.249980009326885	0.800000010000000	T	T	T
0.750069997345419	0.249980009326885	0.800000010000000	T	T	T
-0.000000000000000	0.499950008653389	0.800000010000000	T	T	T
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0.500050021563684	0.499950008653389	0.800000010000000	T	T	T
0.750069997345419	0.499950008653389	0.800000010000000	T	T	T

-0.000000000000000	0.750020057983628	0.800000010000000	T	T	T
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0.500050021563684	0.750020057983628	0.800000010000000	T	T	T
0.750069997345419	0.750020057983628	0.800000010000000	T	T	T
0.124960002889704	0.124990004663442	0.754830000000000	T	T	T
0.374989998671663	0.124990004663442	0.754830000000000	T	T	T
0.625010024453398	0.124990004663442	0.754830000000000	T	T	T
0.875040020235357	0.124990004663442	0.754830000000000	T	T	T
0.124960002889704	0.374960013989946	0.754830000000000	T	T	T
0.374989998671663	0.374960013989946	0.754830000000000	T	T	T
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0.124960002889703	0.625040023320567	0.754830000000000	T	T	T
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0.875040020235357	0.625040023320567	0.754830000000000	T	T	T
0.124960002889703	0.875010042647071	0.754830000000000	T	T	T
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0.625010024453398	0.875010042647071	0.754830000000000	T	T	T
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0.511570601830097	0.499229438626504	0.704476780000000	T	T	T
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-0.012186190281803	0.740037757611188	0.708107270000000	T	T	T
0.229269415301867	0.742512207703511	0.711792950000000	T	T	T
0.482273531152606	0.733514147367785	0.708940730000000	T	T	T
0.715657496549623	0.744552607779638	0.707273030000000	T	T	T
0.639038864777813	0.570472511284626	0.643752330000000	T	T	T
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0.395084419136355	0.655438404454738	0.500145420000000	T	T	T
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0.738321597073736	0.168176736274758	0.578097080000000	T	T	T
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0.635148204687836	0.371203123849780	0.540466510000000	T	T	T
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0.554952612833314	0.697686356031032	0.562850750000000	T	T	T
0.713728336505006	0.339764492676782	0.477995230000000	T	T	T
0.502143721612105	0.481895957979785	0.446002040000000	T	T	T
0.799049378478068	0.894336143368137	0.345999640000000	T	T	T
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0.327861197581813	0.276188040304714	0.435500120000000	T	T	T
0.369061838534575	0.816938250480381	0.447371040000000	T	T	T
0.399911869247990	0.846363631578259	0.381180170000000	T	T	T
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0.558524852915918	0.005546770206953	0.565235820000000	T	T	T
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0.768289697766745	0.587713181927883	0.538821160000000	T	T	T
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0.791911428312995	0.636089633732831	0.357461490000000	T	T	T
0.913328171120768	0.235088678771276	0.395640770000000	T	T	T
0.711402206451217	0.052534591960088	0.462694560000000	T	T	T
0.167810293880620	0.071448672665790	0.626480870000000	T	T	T
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0.816261348876093	0.861746542152205	0.626388170000000	T	T	T

20-CCO

xyzjob

1.000000000000000		
10.227000000000000	0.000000000000000	0.000000000000000

0.0000000000000001 10.225000000000000 0.000000000000000

0.0000000000000002 0.0000000000000002 40.000000000000000

Cu O H C Na

48 49 97 2 1

Selective dynamics

Direct

-0.000000000000000 -0.000000000000000 0.800000010000000 T T T

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