

Al distribution and structure stability of H-BEA zeolite at different Si/Al ratios and temperatures: a first-principles study

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Supporting Information

Since zeolite is not a high-entropy alloy structure, its configurational entropy and the contribution of electrons to entropy can be ignored. Therefore, the contribution of entropy in zeolite system mainly comes from vibrational entropy. The standard Gibbs free energy for each structure (H-BEA(n), RAl-BEA(n), and BEA) is calculated by Equation S1 [1, 2]:

$$G^\theta = E_{\text{DFT}} + E_{\text{ZPE}} + U_{\text{vib}}^\theta - T * S_{\text{vib}}^\theta \quad (1)$$

In Equation S1, E_{DFT} is the total energy obtained directly from DFT calculations, T is the temperature of the temperature at which the H-BEA(n) zeolites are synthesized. E_{ZPE} is the zero-point-energy (ZPE) correction of the total energy:

$$E_{\text{ZPE}} = \sum_i \frac{h\nu_i}{2} \quad (2)$$

where h is Planck constant, ν_i is the vibration frequency of each atom (cm^{-1}). The small vibrational modes ($< 50 \text{ cm}^{-1}$) associated with the frustrated motions of the surface bound species may have little effect on ZPE and entropy value. De Moor et al. [3] studied the entropy contributions of these frequencies for alkanes and alkenes in FAU and suggested their replacement with 50 cm^{-1} . Therefore, in order to obtain consistent results, the immobile adsorbate approach was used for all surface species and the low-lying frequencies were replaced by normal modes of 50 cm^{-1} . U_{vib}^θ and S_{vib}^θ is the standard vibrational internal energy and vibrational entropy, respectively, which can be calculated based on the harmonic oscillator approximation:

$$U_{\text{vib}}^\theta = \sum_i \frac{h\nu_i}{e^{\frac{h\nu_i}{k_B T}} - 1} \quad (3)$$

$$S_{\text{vib}}^\theta = k_B \sum_i \left[\frac{h\nu_i}{k_B T \left(e^{\frac{h\nu_i}{k_B T}} - 1 \right)} - \ln \left(1 - e^{-\frac{h\nu_i}{k_B T}} \right) \right] \quad (4)$$

where k_B is Boltzmann constant. The standard Gibbs free energy for each gaseous species (H, Al, and Si) is calculated by Equation S5:

$$G^\theta = E_{\text{DFT}} + E_{\text{ZPE}} + \int_0^T C_p dT - T^* S^\theta \quad (5)$$

The integral of heat capacity C_p can be separable into translational, rotational and vibrational parts:

$$\int_0^T C_p dT = \int_0^T (k_B + C_{V,\text{trans}} + C_{V,\text{rot}} + C_{V,\text{vib}}) dT \quad (6)$$

The standard entropy S^θ can also be calculated by the translational, rotational, and vibrational components, given by:

$$S^\theta = S_{\text{trans}} + S_{\text{rot}} + S_{\text{vib}} \quad (7)$$

$$S_{\text{trans}} = \frac{5}{2} k_B + k_B \ln \left[\left(\frac{2\pi M k_B T}{h^2} \right)^{\frac{3}{2}} \frac{k_B T}{p^\theta} \right] \quad (8)$$

$$S_{\text{rot}} = k_B \ln \left[\left(\frac{8\pi^2 I k_B T}{\sigma h^2} \right) + 1 \right] \quad (9)$$

where M is the mass of the molecule, I is the degenerate moment of inertia for a linear molecule, σ is the symmetry number of the molecule.

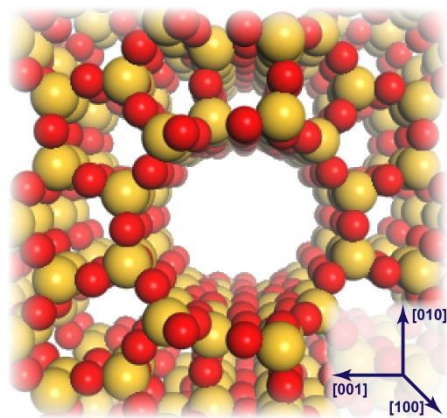


Fig. 1S. The unit cell structure of BEA zeolite. Up along the paper is the [010] axis. Perpendicular to the paper facing outwards is the [010] axis. All the other structures are the same orientation. The unit cell is composed of Si and O. O and Si atoms are depicted as red and yellow spheres.

Table 1S

Al-O and Si-O bond distances near H atom, O-H bond distances, hydrogen bond distances and O-Al-O angles for the nine Brønsted acid sites of H-BEA zeolite.

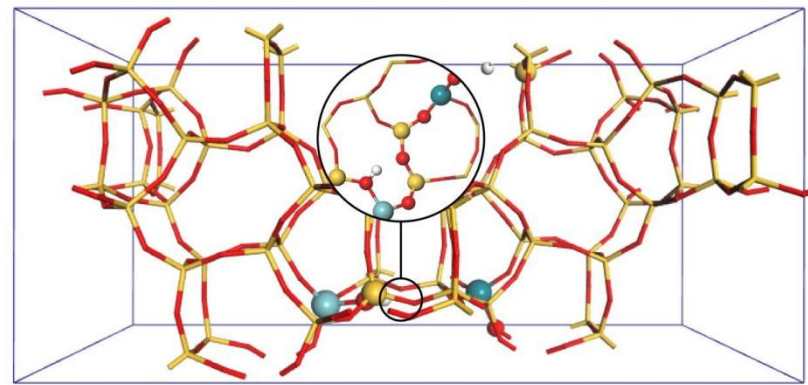
T site	The most stable Brønsted acid sites	d_{Al-O} (Å)	d_{Si-O} (Å)	d_{O-H} (Å)	$d_{O...H}$ (Å)	$\angle_{Al/Si-O-Si}$ (°)
Si-BEA	-	-	1.60~1.63	-	-	140~160
T1	Al(T1)-OH-Si(T3)	1.901	1.704	0.977	-	132.378
T2	Al(T2)-OH-Si(T4)	1.900	1.704	0.976	-	131.721
T7	Al(T7)-OH-Si(T5)	1.924	1.697	0.991	1.974	131.448
T9	Al(T9)-OH-Si(T1X)	1.884	1.695	0.975	-	130.649
T3	Al(T3)-OH-Si(T5)	1.936	1.699	0.994	1.968	131.902
T4	Al(T4)-OH-Si(T6)	1.922	1.691	1.000	1.851	130.548
T5	Al(T5)-OH-Si(T7)	1.891	1.710	0.992	1.934	132.768
T6	Al(T6)-OH-Si(T8)	1.891	1.708	0.996	1.856	131.842
T8	Al(T8)-OH-Si(T6Y)	1.923	1.697	0.995	1.896	132.667

Table 2S shows the results of 23 structures in which T sites are occupied by 2 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

Table 2S

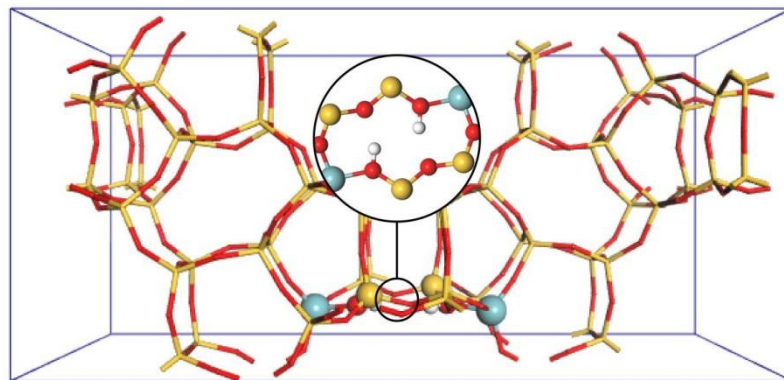
Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA(2).

T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)				
		323K	373K	423K	473K	
T1T1	5	-87.3	-80.1	-77.0	-70.4	
T1T2	6	-92.3	-84.9	-81.7	-75.0	
T1T7	6	-94.2	-86.6	-83.3	-76.5	
T1T9	4	-88.1	-80.9	-77.8	-71.1	
T2T2	6	-91.1	-83.9	-80.7	-74.1	
T2T7	6	-97.5	-90.1	-86.8	-80.1	
T2T9	3	-93.8	-86.6	-83.4	-76.8	
T7T7	7	-105.4	-97.5	-93.7	-86.4	
T7T9	3	-101.1	-93.6	-90.1	-83.2	
T9T9	3	-88.6	-81.2	-77.9	-71.1	
AlSiAl-	T1T1	1	-68.0	-60.6	-57.2	-50.4
	T1T2	1	-54.8	-47.3	-44.0	-37.2
	T1T7	2	-85.9	-79.3	-76.7	-70.6
	T1T9	2	-77.1	-70.1	-67.1	-60.7
	T2T7	1	-85.3	-78.1	-74.9	-68.3
	T2T9	1	-87.3	-80.2	-77.2	-70.7
	T7T9	1	-97.2	-89.6	-86.2	-79.2
	T9T9	1	-46.1	-39.5	-37.0	-31.1
AlAl-	T1T1	1	-27.8	-21.0	-18.3	-12.1
	T1T9	2	-37.4	-30.0	-26.6	-19.8
	T2T2	1	-41.6	-34.2	-31.0	-24.3
	T2T7	1	-62.4	-54.8	-51.3	-44.4
	T7T7	1	-72.6	-65.2	-62.0	-55.2



T7T9

(a)



T7T7 in the same 6MR

(b)

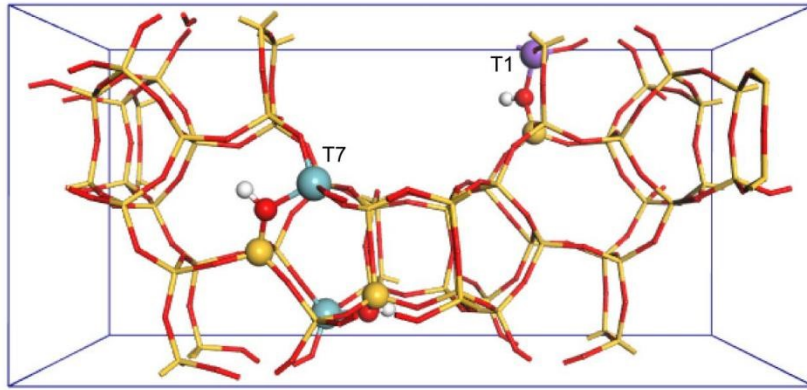
Fig. 2S. The unit cell of (a) T7T9 and (b) T7T7 in the same 6MR in H-BEA(2). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

Table 3S shows the results of 28 structures in which T sites are occupied by 3 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

Table 3S

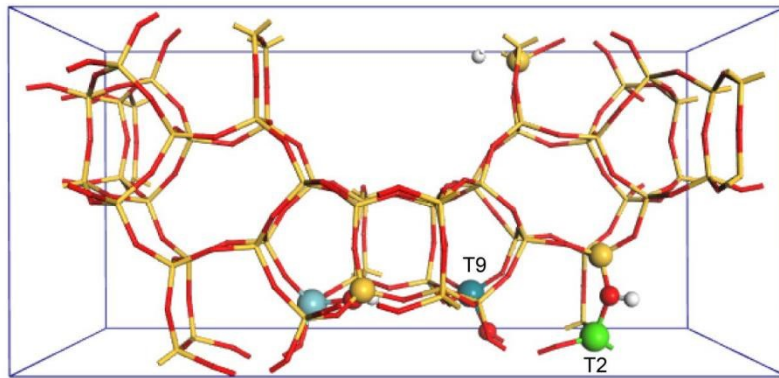
Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA(3).

T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)				
		323K	373K	423K	473K	
T1T1T1	3	-119.6	-110.1	-100.2	-90.7	
T1T1T2	4	-130.1	-120.6	-110.8	-101.3	
T1T1T7	3	-129.3	-119.6	-109.6	-99.9	
T1T1T9	1	-111.0	-101.5	-91.6	-82.0	
T1T2T2	4	-127.8	-118.3	-108.5	-99.0	
T1T2T7	4	-136.5	-126.9	-116.8	-107.1	
T1T2T9	4	-136.3	-126.7	-116.8	-107.2	
T1T7T7	5	-140.8	-130.6	-120.0	-109.7	
T1T7T9	3	-131.2	-120.8	-110.2	-99.8	
T1T9T9	1	-111.9	-102.1	-91.9	-82.1	
T2T2T2	4	-120.3	-110.5	-100.3	-90.4	
T2T2T7	4	-137.8	-127.8	-117.4	-107.4	
T2T2T9	5	-134.0	-124.1	-113.9	-104.0	
T2T7T7	4	-147.7	-137.5	-126.9	-116.6	
T2T7T9	4	-142.0	-132.1	-121.8	-111.9	
T2T9T9	2	-128.4	-118.4	-108.0	-98.0	
T7T7T7	4	-145.9	-135.4	-124.6	-114.1	
T7T7T9	3	-145.4	-135.2	-125.1	-115.4	
T7T9T9	1	-135.4	-125.4	-115.5	-105.4	
T9T9T9	2	-118.7	-108.6	-98.5	-88.3	
	T1T2T7	3	-122.0	-112.1	-102.3	-92.3
	T1T7T7	2	-120.7	-110.5	-100.4	-90.1
	T1T7T9	3	-128.1	-118.1	-108.1	-98.1
	T2T2T7	1	-104.6	-98.1	-86.5	-78.3
AlSiAl-	T2T7T7	2	-97.7	-87.4	-77.2	-66.9
	T2T7T9	3	-127.7	-117.7	-107.8	-97.8
	T7T7T9	6	-154.0	-143.6	-132.9	-122.5
	T7T9T9	1	-139.8	-129.7	-119.2	-109.1



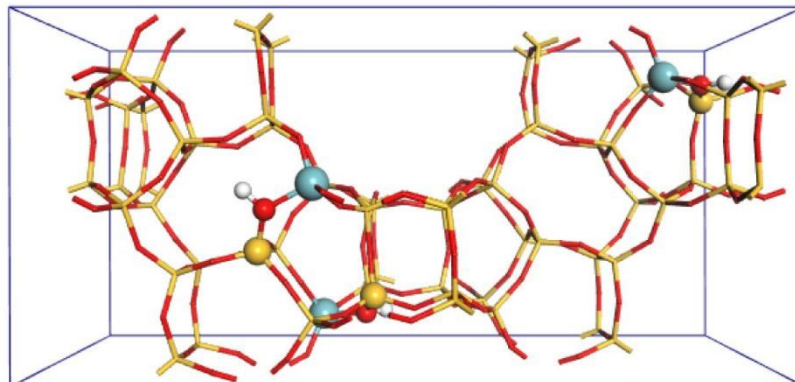
T1T7T7

(a)



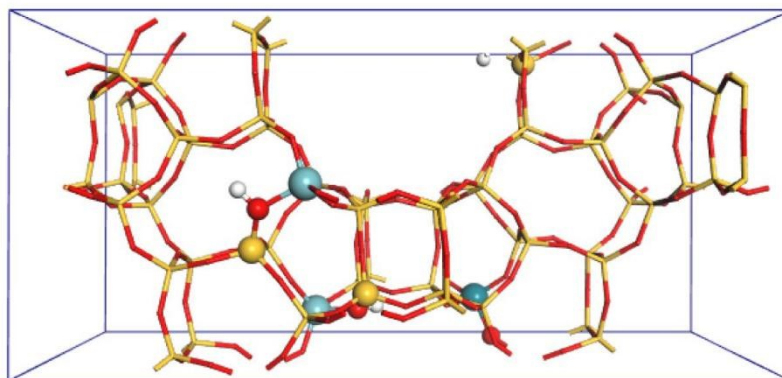
T2T7T9

(b)



T7T7T7

(c)



T7T7T9

(d)

Fig. 3S. The unit cell of (a) T1T7T7, (b) T2T7T9, (c) T7T7T7 and (d) T7T7T9 in H-BEA(3). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

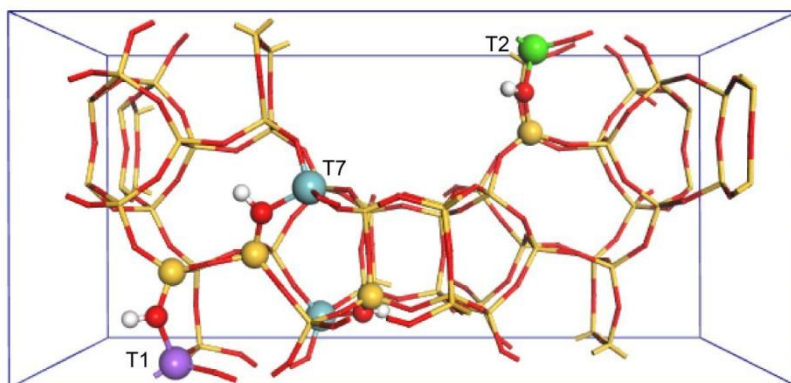
Table 4S shows the results of 43 structures in which T sites are occupied by 4 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

Table 4S

Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA(4).

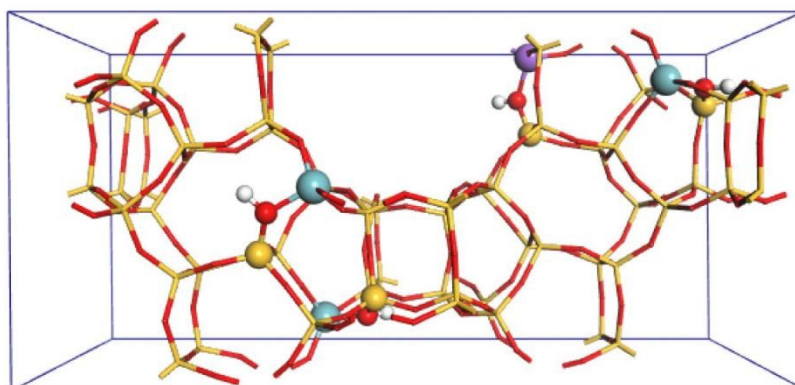
T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)			
		323K	373K	423K	473K
T1T1T1T1	1	-161.2	-148.4	-135.1	-122.2
T1T1T1T2	2	-164.5	-151.7	-138.4	-125.6
T1T1T1T7	1	-159.7	-146.8	-133.5	-120.5
T1T1T2T2	2	-158.5	-145.2	-131.4	-118.1
T1T1T2T7	3	-168.9	-155.9	-142.5	-129.5
T1T1T2T9	2	-170.8	-158.0	-144.7	-131.9
T1T1T7T7	3	-169.4	-155.2	-140.5	-126.3
T1T1T7T9	1	-167.7	-154.7	-141.2	-128.1
T1T2T2T2	2	-155.3	-142.5	-129.3	-116.5
T1T2T2T7	2	-170.3	-157.4	-144.0	-131.1
T1T2T2T9	3	-170.2	-157.8	-145.1	-132.7
T1T2T7T7	4	-185.4	-172.0	-158.2	-144.9
T1T2T7T9	3	-175.0	-161.4	-147.4	-133.8
T1T2T9T9	2	-151.1	-138.1	-124.7	-111.6
T1T7T7T7	4	-182.6	-168.9	-154.0	-140.2
T1T7T7T9	3	-178.5	-164.9	-150.8	-137.2
T1T7T9T9	1	-153.1	-139.7	-125.9	-112.4
T2T2T2T2	2	-146.9	-133.7	-120.0	-106.7
T2T2T2T7	2	-163.1	-149.7	-136.0	-122.6
T2T2T2T9	3	-161.6	-148.5	-134.8	-121.6
T2T2T7T7	2	-186.0	-172.6	-158.8	-145.4
T2T2T7T9	3	-178.5	-165.0	-150.9	-137.4
T2T2T9T9	1	-174.2	-161.2	-147.6	-134.6
T2T7T7T7	3	-177.4	-163.7	-149.7	-136.0
T2T7T7T9	2	-189.9	-176.2	-162.3	-148.8
T2T7T9T9	1	-180.4	-167.2	-153.5	-140.2
T2T9T9T9	1	-155.9	-142.5	-128.7	-115.2
T7T7T7T7	2	-188.4	-173.2	-157.3	-141.1

T7T7T7T9	2	-189.3	-175.6	-161.3	-147.5
T7T7T9T9	2	-178.6	-164.9	-150.7	-137.0
T7T9T9T9	1	-164.2	-150.7	-136.9	-123.4
T9T9T9T9	1	-147.7	-134.4	-120.7	-107.4
T1T2T7T7	3	-157.0	-143.5	-129.5	-115.9
T1T2T7T9	2	-165.8	-152.4	-138.6	-125.1
T1T7T7T7	4	-164.1	-150.3	-136.1	-122.2
T1T7T7T9	3	-165.5	-151.9	-137.8	-124.2
T2T2T7T7	2	-137.4	-123.1	-108.4	-94.1
AlSiAl- T2T2T7T9	2	-148.9	-135.4	-121.6	-108.1
T2T7T7T7	1	-137.4	-123.7	-109.6	-95.9
T2T7T7T9	2	-189.4	-175.7	-161.6	-147.8
T2T7T9T9	1	-179.8	-165.2	-149.8	-134.7
T7T7T7T9	2	-181.6	-167.0	-151.7	-136.7
T7T7T9T9	1	-188.0	-174.3	-160.1	-146.3



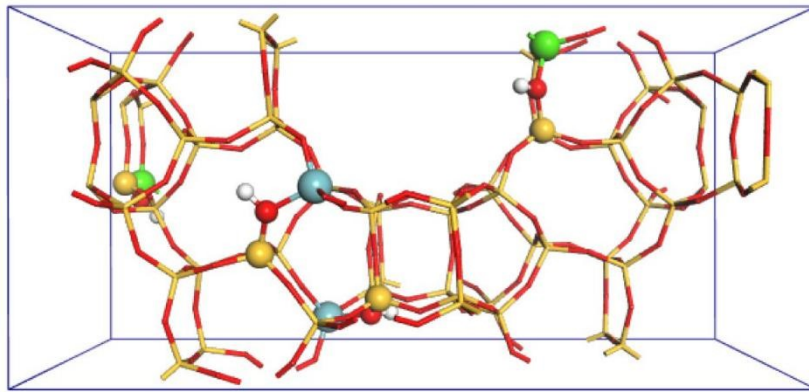
T1T2T7T7

(a)



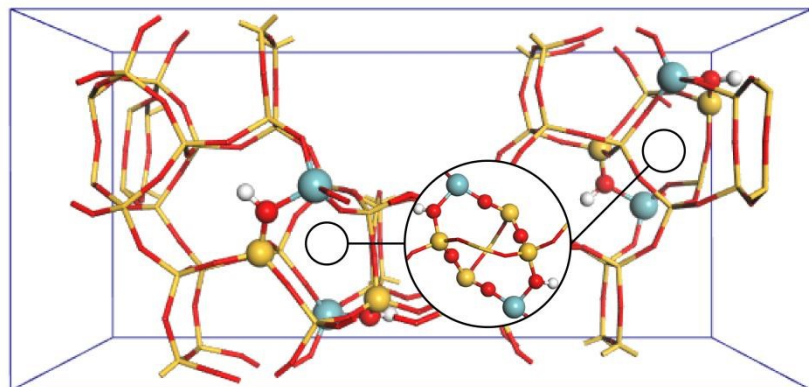
T1T7T7T7

(b)



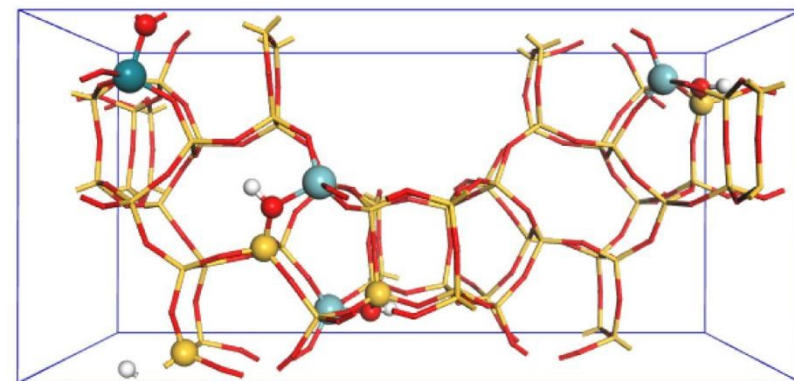
T2T2T7T7

(c)



T7T7T7T7

(d)



T7T7T7T9

(e)

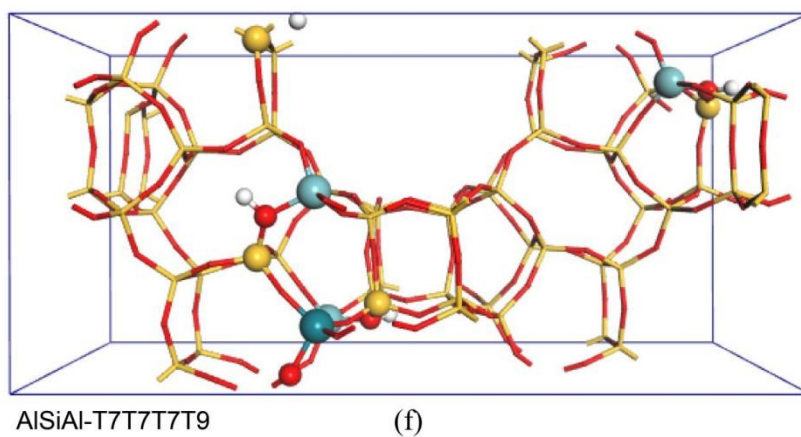


Fig. 4S. The unit cell of (a) T1T2T7T7, (b) T1T7T7T7, (c) T2T2T7T7, (d) T7T7T7T7, (e) T7T7T7T9, (f) AlSiAl-T7T7T7T9 and (g) AlSiAl-T7T7T9T9 in H-BEA(4). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

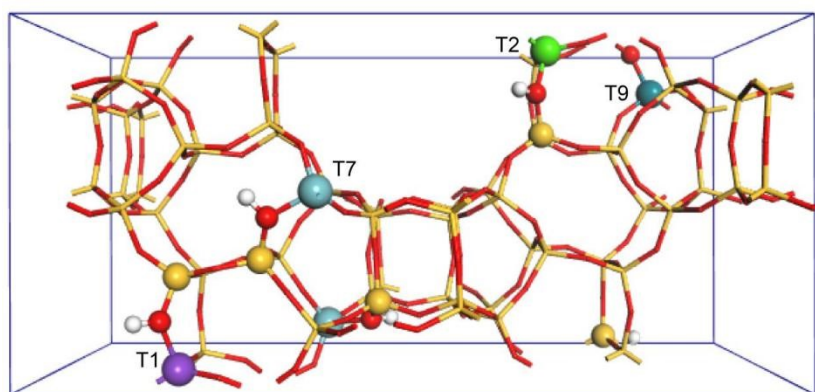
Table 5S shows the results of 41 structures in which T sites are occupied by 5 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

Table 5S

Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA(5).

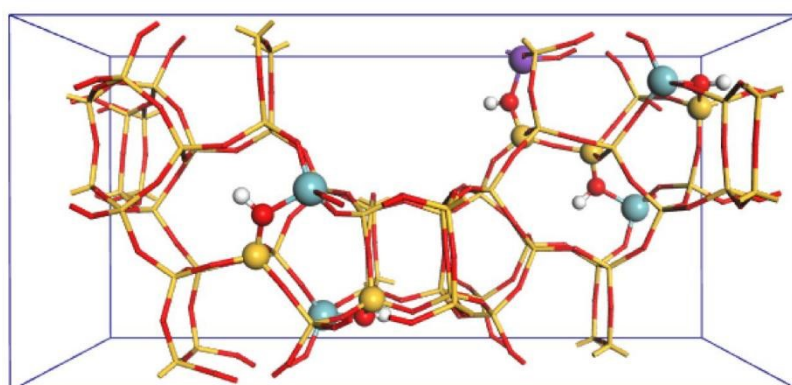
T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)			
		323K	373K	423K	473K
T1T1T1T2T7	1	-200.1	-184.0	-167.4	-151.3
T1T1T1T7T7	1	-209.2	-193.0	-176.1	-159.9
T1T1T2T2T7	2	-203.5	-187.3	-170.6	-154.4
T1T1T2T2T9	1	-195.4	-179.5	-163.0	-147.1
T1T1T2T7T7	1	-205.8	-189.5	-172.5	-156.2
T1T1T7T7T7	1	-207.3	-190.8	-173.8	-157.3
T1T2T2T2T7	2	-194.8	-178.7	-162.0	-145.8
T1T2T2T2T9	1	-190.6	-174.7	-158.3	-142.3
T1T2T2T7T7	2	-210.3	-194.1	-177.3	-161.1
T1T2T2T7T9	1	-212.2	-196.1	-179.4	-163.2
T1T2T7T7T7	2	-208.2	-191.8	-174.9	-158.6
T1T2T7T7T9	2	-217.7	-201.2	-184.1	-167.3
T1T7T7T7T7	1	-225.5	-208.3	-190.5	-173.3
T1T7T7T7T9	2	-225.9	-208.8	-191.1	-173.9
T2T2T2T2T9	1	-172.8	-156.8	-140.2	-124.1
T2T2T2T7T9	1	-205.0	-188.9	-172.1	-156.0
T2T2T7T7T7	2	-205.2	-188.9	-172.1	-155.8
T2T2T7T7T9	1	-225.1	-208.6	-191.7	-175.3
T2T2T7T9T9	1	-210.3	-193.9	-177.1	-160.8
T2T2T9T9T9	1	-184.2	-168.0	-151.4	-135.4
T2T7T7T7T7	2	-196.5	-179.7	-162.5	-145.9
T2T7T7T7T9	2	-228.0	-211.0	-193.4	-176.4
T2T7T7T9T9	1	-227.3	-210.6	-193.4	-176.8
T7T7T7T7T9	2	-229.5	-212.1	-194.0	-176.6
T7T7T7T9T9	1	-226.2	-208.9	-191.0	-173.6
T7T7T9T9T9	1	-211.8	-195.1	-177.8	-161.0
T1T1T1T7T7	2	-197.1	-180.4	-163.1	-146.3
AlSiAl- T1T1T2T7T7	2	-184.4	-167.8	-150.6	-133.9
T1T1T7T7T7	2	-197.8	-181.2	-164.0	-147.4

T1T1T7T7T9	1	-226.1	-209.2	-191.8	-174.9
T1T2T2T7T7	3	-199.0	-182.4	-165.2	-148.6
T1T2T7T7T9	3	-204.2	-187.6	-170.4	-153.7
T1T7T7T7T7	4	-212.3	-195.6	-178.3	-161.6
T1T7T7T7T9	3	-219.0	-202.0	-184.3	-167.3
T2T2T7T7T7	2	-179.0	-162.0	-144.4	-127.4
T2T2T7T7T9	3	-193.0	-176.2	-158.9	-142.1
T2T7T7T7T7	4	-194.2	-177.1	-159.5	-142.4
T2T7T7T7T9	5	-202.8	-185.9	-168.3	-151.4
T2T7T7T9T9	2	-233.9	-217.0	-199.6	-182.7
T7T7T7T7T9	2	-239.5	-222.0	-203.9	-186.4
T7T7T7T9T9	2	-222.9	-205.5	-187.6	-170.3



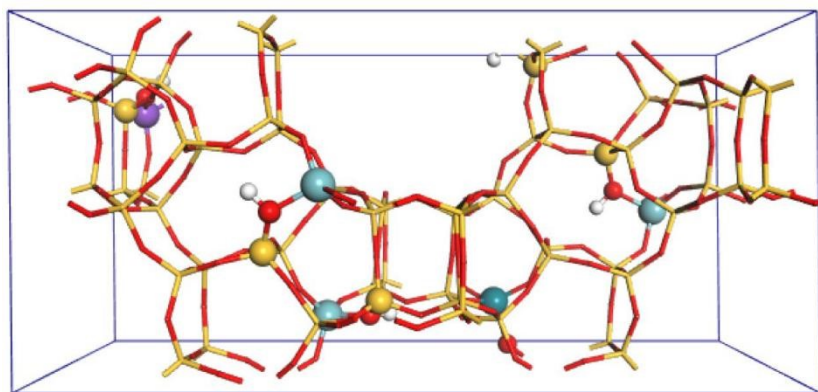
T1T2T7T7T9

(a)



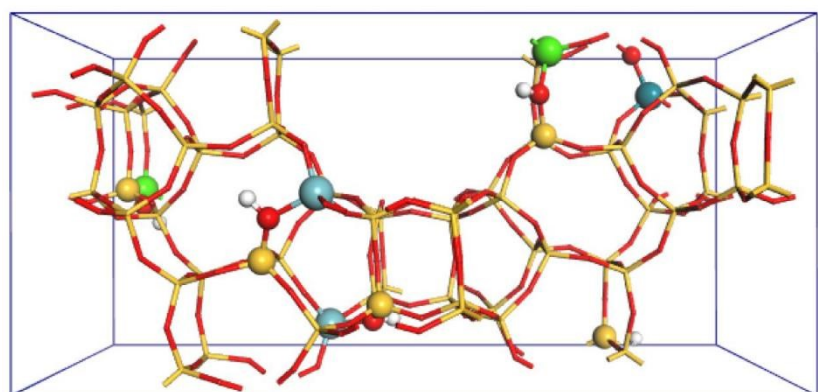
T1T7T7T7T7

(b)



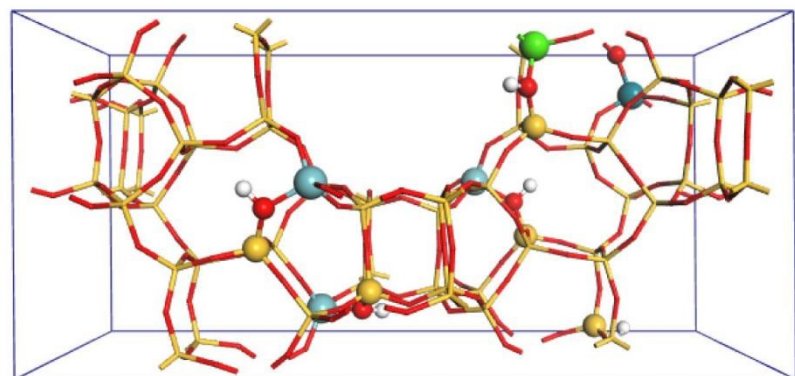
T1T7T7T9

(c)



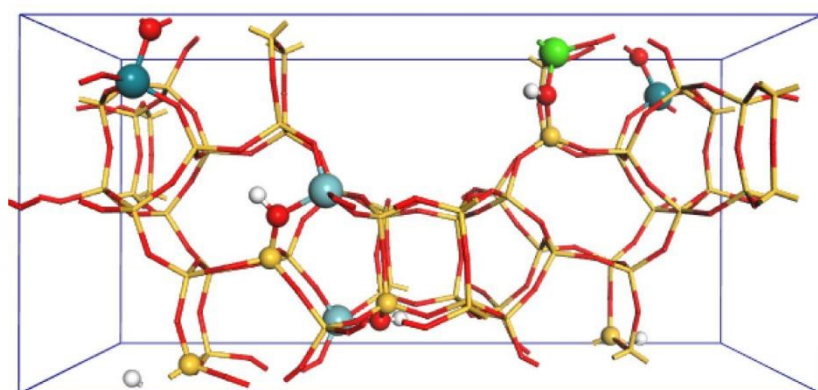
T2T2T7T9

(d)



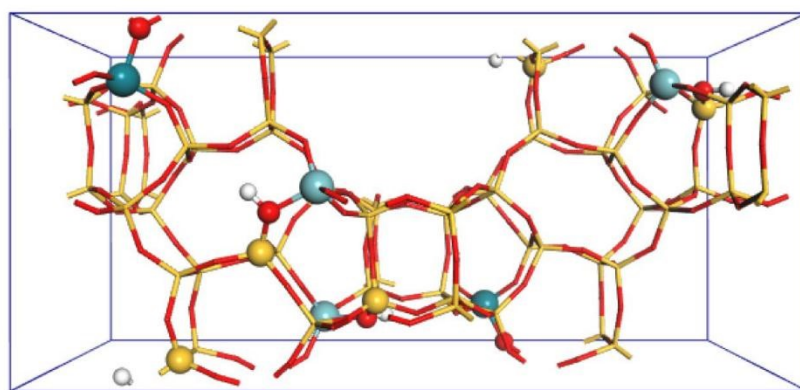
T2T7T7T9

(e)



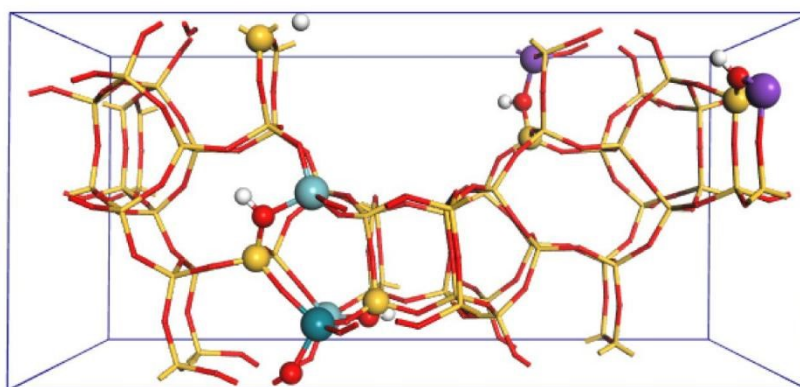
T2T7T7T9T9

(f)



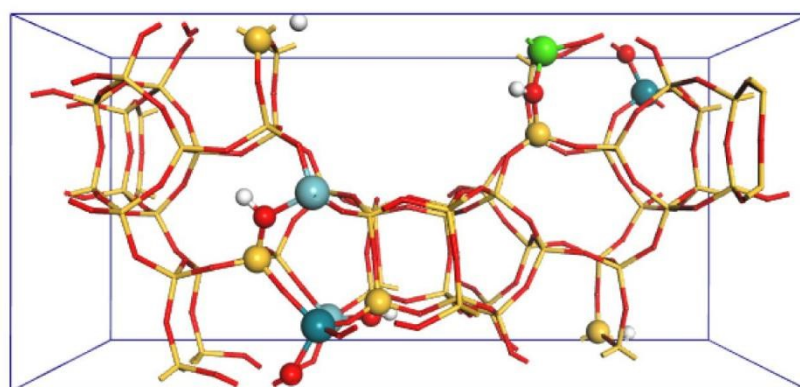
T7T7T7T9T9

(g)



AlSiAl-T1T1T7T7T9

(h)



AlSiAl-T2T7T7T9T9

(i)

Fig. 5S. The unit cell of (a) T1T2T7T7T9, (b) T1T7T7T7T7, (c) T1T7T7T7T9, (d) T2T2T7T7T9, (e) T2T7T7T7T9, (f) T2T7T7T9T9, (g) T7T7T7T9T9, (h) AlSiAl-T1T1T7T7T9 and (i) AlSiAl-T2T7T7T9T9 in H-BEA(5). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

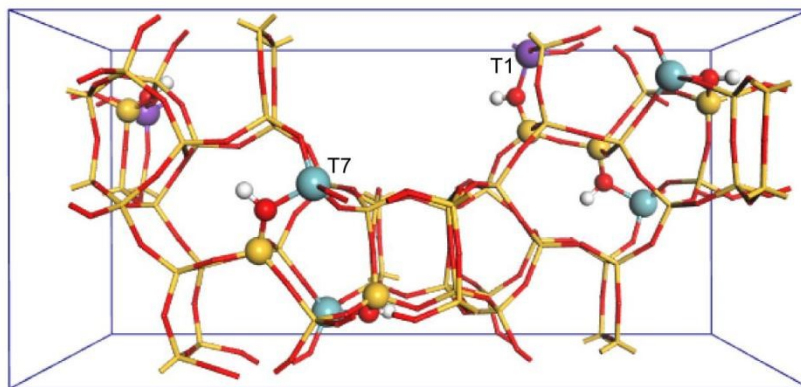
Table 6S shows the results of 33 structures in which T sites are occupied by 6 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

Table 6S

Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA(6).

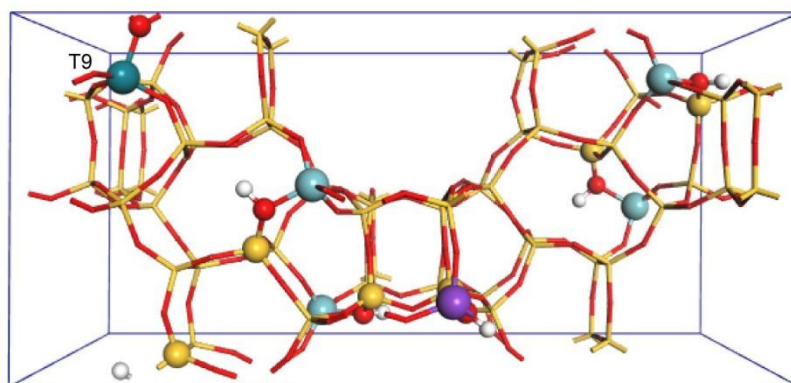
T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)			
		323K	373K	423K	473K
T1T1T2T2T7T7	1	-230.9	-211.3	-191.0	-171.4
T1T1T2T2T7T9	1	-226.0	-205.3	-184.8	-163.3
T1T1T2T7T7T7	1	-234.2	-213.6	-193.0	-171.4
T1T1T2T7T7T9	1	-237.6	-217.0	-196.5	-175.0
T1T1T7T7T7T7	2	-261.6	-241.3	-220.2	-199.9
T1T2T2T2T7T9	1	-236.5	-216.7	-196.3	-176.5
T1T2T2T7T7T7	1	-226.6	-206.7	-186.0	-166.1
T1T2T2T7T7T9	1	-246.4	-226.5	-205.8	-185.8
T1T2T7T7T7T7	1	-218.5	-198.2	-177.3	-157.1
T1T2T7T7T7T9	1	-245.8	-225.5	-204.6	-184.4
T1T2T7T7T9T9	1	-247.7	-227.7	-206.9	-186.8
T1T7T7T7T7T9	2	-264.6	-244.0	-222.7	-202.0
T2T2T2T7T9T9	1	-227.0	-206.9	-186.1	-165.9
T2T2T7T7T7T7	1	-223.7	-204.3	-184.2	-164.7
T2T2T7T7T7T9	1	-262.4	-244.9	-227.1	-210.3
T2T2T7T7T9T9	1	-253.1	-233.0	-212.3	-192.2
T2T7T7T7T7T9	1	-260.5	-240.4	-219.7	-199.6
T2T7T7T7T9T9	1	-260.7	-240.6	-219.8	-199.7
T7T7T7T7T9T9	1	-268.3	-247.4	-225.8	-204.8
T1T2T2T7T7T9	2	-235.5	-215.6	-195.1	-175.3
T1T2T7T7T7T7	3	-252.6	-232.5	-211.8	-191.7
T1T2T7T7T7T9	2	-266.7	-246.4	-225.4	-205.0
T1T2T7T7T9T9	1	-268.1	-247.3	-225.8	-205.0
AlSiAl- T1T7T7T7T7T9	2	-321.5	-298.9	-276.7	-255.2
T2T2T2T7T7T7	1	-210.9	-190.7	-170.0	-149.9
T2T2T7T7T7T7	2	-214.2	-193.0	-171.2	-150.0
T2T2T7T7T7T9	2	-241.5	-221.1	-200.1	-179.7
T2T2T7T7T9T9	4	-260.5	-240.3	-219.6	-199.5

T2T7T7T7T7T9	1	-259.4	-238.8	-217.7	-197.2
T2T7T7T7T9T9	3	-295.9	-275.3	-254.2	-233.8
T2T7T7T9T9T9	2	-288.9	-268.6	-247.7	-227.4
T7T7T7T7T9T9	3	-337.3	-316.6	-295.2	-274.5
T7T7T7T9T9T9	2	-283.0	-262.5	-241.3	-220.8



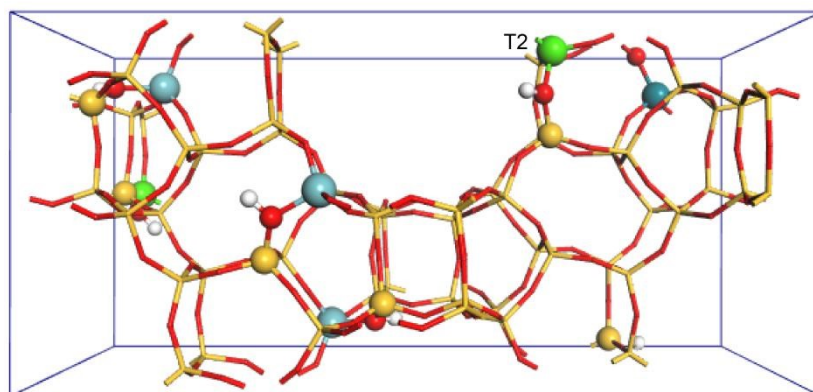
T1T1T7T7T7T7

(a)



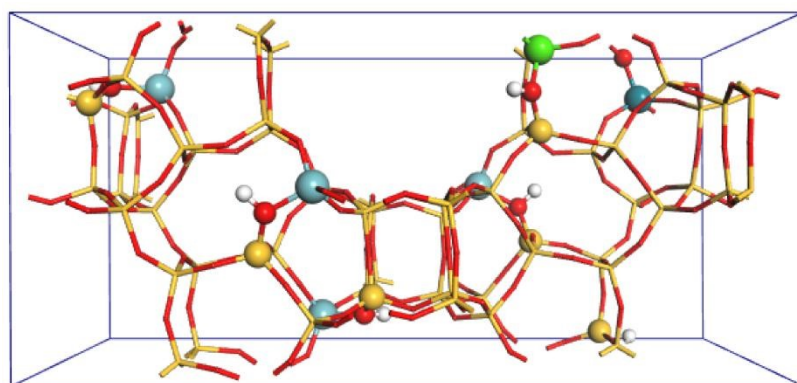
T1T7T7T7T7T9

(b)



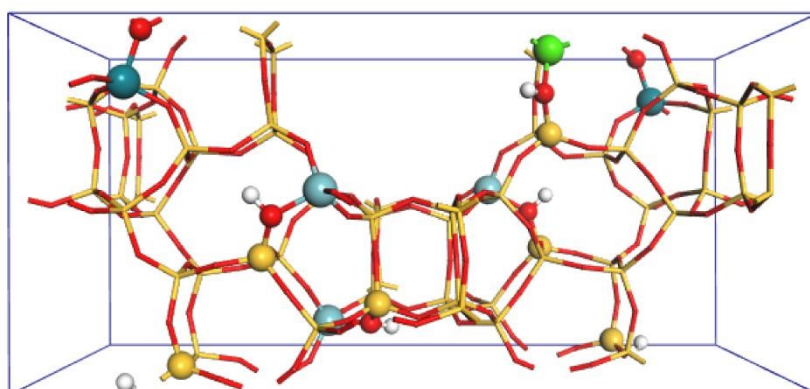
T2T2T7T7T7T9

(c)



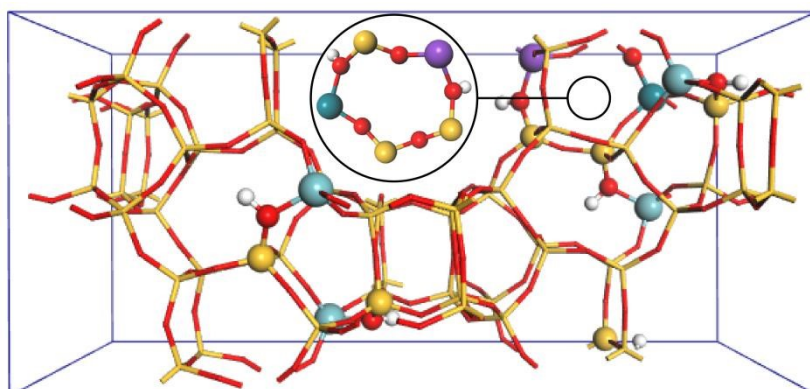
T2T7T7T7T7T9

(d)



T2T7T7T7T9T9

(e)



AlSiAl-T1T7T7T7T7T9

(f)

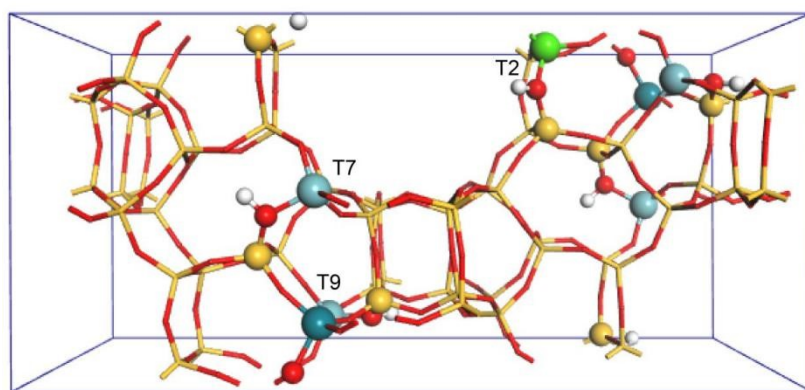
Fig. 6S. The unit cell of (a) T1T1T7T7T7T7, (b) T1T7T7T7T7T9, (c) T2T2T7T7T7T9, (d)T2T7T7T7T7T9, (e)T2T7T7T7T9T9 and (f)AlSiAl-T1T7T7T7T7T9 in H-BEA(6). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

Table 7S shows the results of 22 structures in which T sites are occupied by 7 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

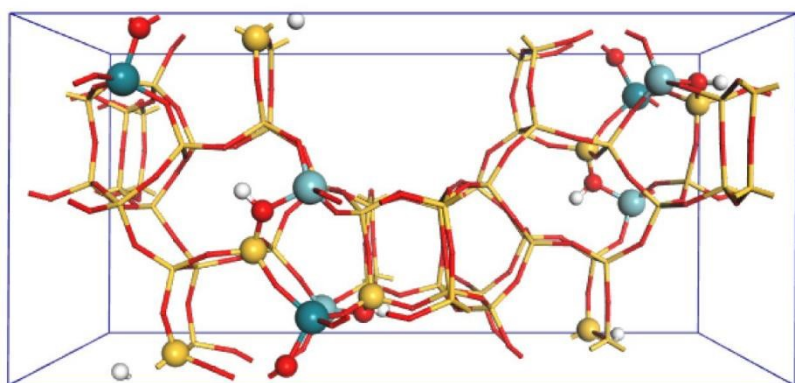
Table 7S

Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA(7).

T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)			
		323K	373K	423K	473K
T1T1T2T2T7T7T9	1	-268.0	-245.3	-221.8	-199.1
T1T2T2T7T7T7T9	1	-275.0	-252.0	-228.2	-205.2
T2T2T7T7T7T7T9	1	-295.8	-272.1	-247.5	-223.8
T1T1T1T7T7T7T7	2	-270.4	-246.4	-221.7	-197.8
T1T1T2T7T7T7T7	2	-258.0	-234.3	-209.8	-186.1
T1T1T2T7T7T7T9	4	-289.7	-266.3	-242.0	-218.6
T1T1T7T7T7T7T9	3	-330.5	-306.8	-282.3	-258.6
T1T2T2T7T7T7T9	1	-261.0	-237.4	-213.1	-189.4
T1T2T2T7T7T9T9	2	-278.7	-255.5	-231.5	-208.2
T1T2T7T7T7T7T9	5	-314.5	-290.8	-266.4	-242.7
T1T2T7T7T7T9T9	4	-320.3	-296.8	-272.4	-248.8
T1T7T7T7T7T9T9	11	-365.7	-342.0	-317.4	-293.5
AlSiAl- T2T2T2T7T7T7T9	1	-251.5	-227.6	-202.9	-179.0
T2T2T2T7T7T9T9	4	-269.2	-245.8	-221.5	-198.0
T2T2T7T7T7T7T9	1	-280.7	-256.7	-231.8	-207.7
T2T2T7T7T7T9T9	2	-289.8	-266.3	-241.9	-218.3
T2T2T7T7T9T9T9	4	-315.3	-291.8	-267.5	-243.9
T2T7T7T7T7T9T9	8	-352.6	-328.7	-304.0	-280.1
T2T7T7T7T9T9T9	1	-333.8	-310.1	-285.6	-261.8
T2T7T7T9T9T9T9	1	-315.4	-291.9	-267.6	-244.0
T7T7T7T7T9T9T9	5	-350.8	-325.7	-300.1	-274.7
T7T7T7T9T9T9T9	1	-331.0	-307.2	-282.7	-258.8



AlSiAl-T2T7T7T7T9T9 (a)



AlSiAl-T7T7T7T9T9T9 (b)

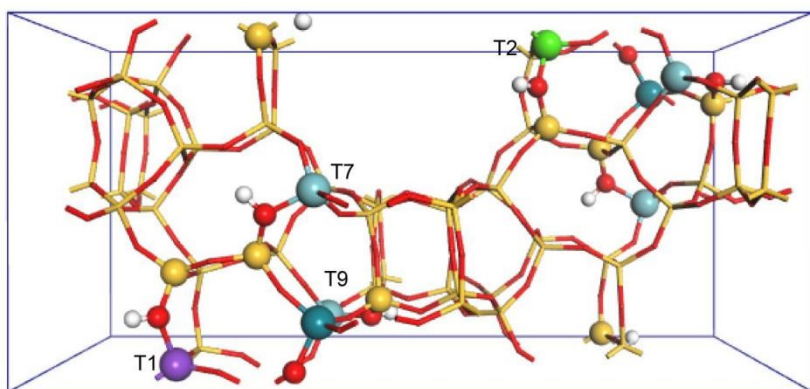
Fig. 7S. The unit cell of (a) AlSiAl-T2T7T7T7T9T9 and (b) AlSiAl-T7T7T7T9T9T9 in H-BEA(7). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

Table 8S shows the results of 19 structures in which T sites are occupied by 8 Al. The positions with the lowest substitution energy are listed in the table for the different structures of the same T sites.

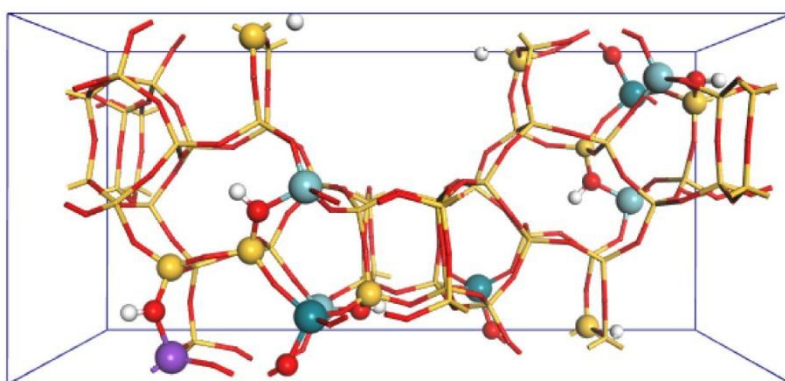
Table 8S

Substitution energy G_{Al-sub} at different synthesis temperatures of all possible structures of H-BEA (8).

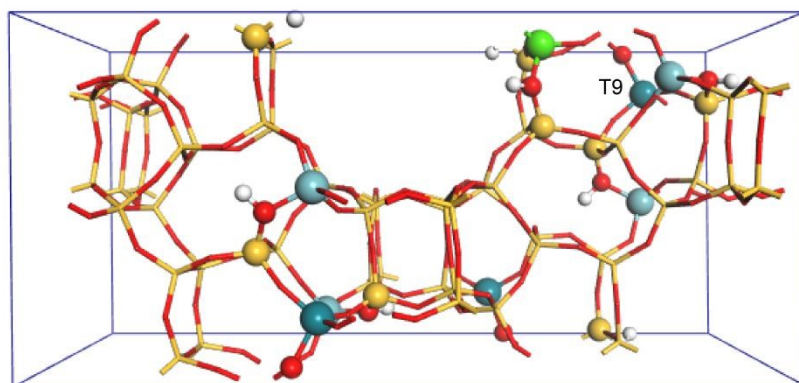
T sites occupied by Al	Number of distribution types	G_{Al-sub} (kJ/mol)			
		323K	373K	423K	473K
T1T1T1T7T7T7T7T9	2	-362.9	-336.2	-308.6	-281.9
T1T1T2T2T7T7T7T9	2	-308.1	-281.7	-254.3	-227.8
T1T1T2T2T7T7T9T9	1	-345.3	-318.9	-291.5	-265.1
T1T1T2T7T7T7T7T9	2	-354.6	-327.8	-300.1	-273.3
T1T1T2T7T7T7T9T9	1	-332.1	-304.6	-276.3	-248.8
T1T1T7T7T7T7T9T9	6	-408.8	-381.9	-354.1	-327.2
T1T2T2T7T7T7T7T9	2	-350.0	-323.2	-295.3	-268.4
T1T2T2T7T7T7T9T9	3	-342.3	-315.4	-287.6	-260.7
T1T2T7T7T7T7T9T9	3	-394.4	-367.5	-339.6	-312.6
AlSiAl- T1T2T7T7T7T9T9T9	1	-348.9	-322.1	-294.4	-267.5
T1T7T7T7T7T9T9T9	1	-390.2	-363.1	-335.1	-308.0
T2T2T2T7T7T9T9T9	3	-327.0	-300.3	-272.7	-245.9
T2T2T7T7T7T7T7T9	2	-326.0	-298.9	-270.9	-243.7
T2T2T7T7T7T7T9T9	6	-383.1	-356.1	-328.1	-301.0
T2T2T7T7T7T9T9T9	2	-347.2	-319.6	-291.1	-263.4
T2T2T7T7T9T9T9T9	1	-346.1	-318.3	-289.7	-261.8
T2T7T7T7T7T9T9T9	2	-391.8	-364.6	-336.0	-309.4
T2T7T7T7T9T9T9T9	1	-373.8	-346.8	-318.9	-291.9
T7T7T7T7T9T9T9T9	1	-382.4	-355.2	-327.1	-299.8



AlSiAl-T1T2T7T7T7T9T9 (a)



AlSiAl-T1T7T7T7T9T9T9 (b)



AlSiAl-T2T7T7T7T9T9T9 (c)

Fig. 8S. The unit cell of (a) AlSiAl-T1T2T7T7T7T9T9, (b) AlSiAl-T1T7T7T7T9T9T9, (c) AlSiAl-T2T7T7T7T9T9T9 in H-BEA(8). H, O and Si atoms are depicted as white, red and yellow spheres, respectively. The color of T site occupied by Al corresponds to that of Fig. 2.

Table 9SSubstitution energy G_{Al-sub} at different synthesis temperatures of H-BEA(n).

Number of Al atoms in H-BEA(n)	G_{Al-sub} (kJ/mol)				
	323K	373K	423K	473K	
Normal Structure	1	-66.1	-62.7	-59.2	-55.8
	2	-103.3	-95.5	-91.9	-84.8
	3	-144.3	-135.0	-124.6	-114.5
	4	-186.9	-173.1	-159.6	-146.7
	5	-226.8	-209.8	-192.2	-175.1
	6	-263.0	-243.1	-222.6	-202.7
	7	-295.8	-272.1	-247.5	-223.8
AlSiAl Structure	2	-97.2	-89.6	-86.2	-79.2
	3	-154.0	-143.6	-132.9	-122.5
	4	-186.3	-172.3	-160.9	-147.1
	5	-236.7	-219.5	-201.8	-184.6
	6	-329.4	-316.6	-295.2	-274.5
	7	-356.4	-332.1	-310.7	-286.8
	8	-396.3	-369.3	-346.9	-319.9

Table 10SAverage substitution energy \overline{G}_{Al-sub} at different synthesis temperatures of H-BEA(n).

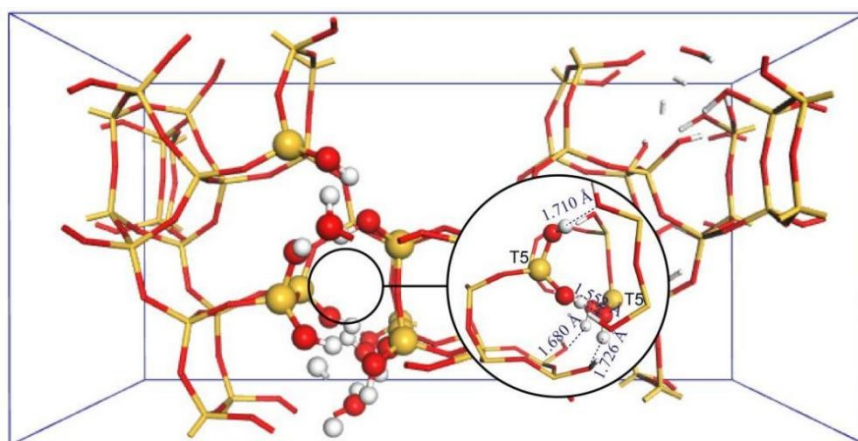
Number of Al atoms	\overline{G}_{Al-sub} (kJ/mol)				
	323K	373K	423K	473K	
Normal Structure	1	-66.1	-62.7	-59.2	-55.8
	2	-51.6	-47.8	-45.9	-42.4
	3	-48.1	-45.0	-41.5	-38.2
	4	-46.7	-43.3	-39.9	-36.7
	5	-45.4	-42.0	-38.4	-35.0
	6	-43.8	-40.5	-37.1	-33.8
	7	-42.3	-38.9	-35.4	-32.0
AlSiAl Structure	2	-48.6	-44.8	-43.1	-39.6
	3	-51.3	-47.9	-44.3	-40.8
	4	-46.6	-43.1	-40.2	-36.8
	5	-47.3	-43.9	-40.4	-36.9
	6	-54.9	-52.8	-49.2	-45.8
	7	-50.9	-47.4	-44.4	-41.0
	8	-49.5	-46.2	-43.4	-40.0

Table 11S shows the substitution energy of silanol nests with different silanol orientations and the most stable orientation after the dealuminization of Al atoms.

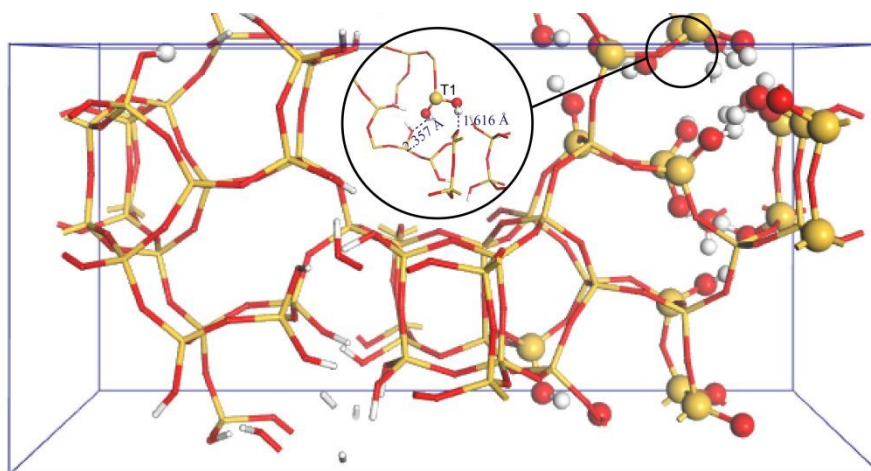
Table 11S

The substitution energies of RAl-BEA after silanol nests formation at different dealuminization sites. T1T2T3T9 represents that in silanol nest, the silanol of T1 site forms hydrogen bond with O atom of T2 site, the silanol of T2 site forms hydrogen bond with T3 site, the silanol of T3 site forms hydrogen bond with T9 site, and the silanol of T9 site forms hydrogen bond with T1 site.

Dealuminated T site	Silanol nests orientation	$G_{RAI-sub}$ (kJ/mol)			
		373K	473K	573K	673K
T1	T1T2T3T9	-311.5	-295.8	-278.5	-259.8
	T1T2T9T3	-316.0	-300.9	-283.9	-265.4
	T1T3T2T9	-309.8	-293.9	-276.5	-257.7
	T1T3T9T2	-301.9	-285.2	-267.3	-248.1
	T1T9T2T3	-298.9	-283.4	-266.3	-247.6
	T1T9T3T2	-297.2	-282.2	-265.3	-246.9
	T1T2T4T7	-308.7	-293.2	-276.0	-257.4
T2	T1T2T7T4	-292.4	-277.6	-260.8	-242.4
	T1T4T2T7	-299.5	-284.6	-267.9	-249.5
	T1T4T7T2	-299.4	-285.9	-270.0	-252.2
	T1T7T2T4	-297.6	-283.4	-267.0	-248.8
	T1T7T4T2	-294.7	-280.1	-263.4	-245.1
T7	T2T3T5T6	-301.0	-286.7	-268.4	-250.2
	T2T3T6T5	-317.8	-307.4	-296.1	-283.8
	T2T5T3T6	-294.3	-280.0	-263.5	-245.3
	T2T5T6T3	-314.6	-299.5	-282.6	-264.1
	T2T6T3T5	-299.5	-284.1	-267.0	-248.3
	T2T6T5T3	-297.5	-283.2	-266.7	-248.5
	T1XT1YT5XT5Y	-321.2	-311.2	-300.1	-288.0
T9	T1XT1YT5YT5X	-303.2	-293.1	-283.8	-271.7
	T1XT5XT1YT5Y	-312.1	-303.3	-293.0	-281.5
	T1XT1YT5YT5X	-319.1	-308.2	-296.6	-284.2
	T1XT5YT1YT5X	-312.4	-302.8	-291.1	-278.7
	T1XT5YT5XT1Y	-322.0	-312.0	-300.9	-288.9



RAI-AISiAl-T7T7T7T7T9T9 (a)



RAI-AISiAl-T1T1T7T7T7T7T9T9 (b)

Fig. 9S. The dealuminized cells of (a)AISiAl-T7T7T7T7T9T9 and (b)AISiAl-T1T1T7T7T7T7T9T9. H, O and Si atoms are depicted as white, red and yellow spheres and sticks, respectively.

References

- [1] La Iglesia A, Aznar A. A method of estimating the Gibbs energies of formation of zeolites. *Zeolites* 1986;6(1):26-9.
- [2] Bonelli B, Onida B, Fubini B, Arean CO, Garrone E. Vibrational and thermodynamic study of the adsorption of carbon dioxide on the zeolite Na⁻ ZSM-5. *Langmuir* 2000;16(11):4976-83.
- [3] Nguyen CM, Reyniers M-F, Marin GB. Adsorption thermodynamics of C1–C4 alcohols in H-FAU, H-MOR, H-ZSM-5, and H-ZSM-22. *J Catal* 2015;322:91-103.

CIF data

T7:

data_image0

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Si Si3 1.0 0.70799 0.79880 0.05478 1.0000
Si Si4 1.0 0.71324 0.54527 0.06182 1.0000
Si Si5 1.0 0.95291 0.80421 0.05316 1.0000
Si Si6 1.0 0.95821 0.54731 0.05654 1.0000
Si Si7 1.0 0.52982 0.85720 0.12685 1.0000

Si	Si8	1.0	0.66275	0.19887	0.54956	1.0000
Si	Si9	1.0	0.66632	0.45475	0.55907	1.0000
Si	Si10	1.0	0.27397	0.20635	0.56211	1.0000
Si	Si11	1.0	0.28518	0.46145	0.55652	1.0000
Si	Si12	1.0	0.02874	0.21290	0.55187	1.0000
Si	Si13	1.0	0.04213	0.47013	0.55176	1.0000
Si	Si14	1.0	0.20863	0.33890	0.30671	1.0000
Si	Si15	1.0	0.46152	0.34371	0.30504	1.0000
Si	Si16	1.0	0.20218	0.71219	0.30372	1.0000
Si	Si17	1.0	0.45864	0.71595	0.30742	1.0000
Si	Si18	1.0	0.19681	0.95371	0.30304	1.0000
Si	Si19	1.0	0.45511	0.95801	0.30726	1.0000
Si	Si20	1.0	0.13484	0.52796	0.37476	1.0000
Si	Si21	1.0	0.78999	0.66329	0.80894	1.0000
Si	Si22	1.0	0.53725	0.66077	0.80539	1.0000
Si	Si23	1.0	0.80141	0.28470	0.80947	1.0000
Si	Si24	1.0	0.54610	0.28407	0.80948	1.0000
Si	Si25	1.0	0.80175	0.03953	0.80489	1.0000
Si	Si26	1.0	0.54493	0.03992	0.80245	1.0000
Si	Si27	1.0	0.85539	0.46741	0.87869	1.0000
Si	Si28	1.0	0.67138	0.78469	0.94063	1.0000
Si	Si29	1.0	0.66596	0.52978	0.94747	1.0000
Si	Si30	1.0	0.29441	0.79262	0.94278	1.0000
Si	Si31	1.0	0.28771	0.54144	0.93928	1.0000
Si	Si32	1.0	0.05096	0.80110	0.94705	1.0000
Si	Si33	1.0	0.04398	0.54379	0.94736	1.0000
Si	Si34	1.0	0.47297	0.85188	0.87052	1.0000
Si	Si35	1.0	0.33348	0.20068	0.44843	1.0000
Si	Si36	1.0	0.32789	0.45428	0.44312	1.0000
Si	Si37	1.0	0.71239	0.21356	0.43520	1.0000
Si	Si38	1.0	0.70573	0.46539	0.44426	1.0000
Si	Si39	1.0	0.95925	0.21718	0.44027	1.0000
Si	Si40	1.0	0.95465	0.47048	0.44387	1.0000
Si	Si41	1.0	0.51905	0.14556	0.37598	1.0000

Si	Si42	1.0	0.79602	0.33933	0.69566	1.0000
Si	Si43	1.0	0.54445	0.34175	0.69528	1.0000
Si	Si44	1.0	0.79780	0.70931	0.69459	1.0000
Si	Si45	1.0	0.54386	0.70812	0.69229	1.0000
Si	Si46	1.0	0.80327	0.95171	0.69651	1.0000
Si	Si47	1.0	0.54459	0.95204	0.69371	1.0000
Si	Si48	1.0	0.86711	0.52392	0.62711	1.0000
Si	Si49	1.0	0.21240	0.66837	0.19099	1.0000
Si	Si50	1.0	0.46581	0.66726	0.19469	1.0000
Si	Si51	1.0	0.20366	0.28673	0.19216	1.0000
Si	Si52	1.0	0.45987	0.28629	0.19151	1.0000
Si	Si53	1.0	0.20357	0.04193	0.19470	1.0000
Si	Si54	1.0	0.46083	0.04263	0.19836	1.0000
Si	Si55	1.0	0.14892	0.47026	0.12243	1.0000
Si	Si56	1.0	0.13695	0.85818	0.12211	1.0000
Si	Si57	1.0	0.52606	0.47111	0.12575	1.0000
Si	Si58	1.0	0.84236	0.13741	0.62525	1.0000
Si	Si59	1.0	0.46814	0.52402	0.62705	1.0000
Si	Si60	1.0	0.15162	0.13694	0.37565	1.0000
Si	Si61	1.0	0.52609	0.52803	0.37476	1.0000
Si	Si62	1.0	0.86862	0.85471	0.87545	1.0000
Si	Si63	1.0	0.47442	0.46668	0.87644	1.0000
Al	Al1	1.0	0.46601	0.13766	0.62713	1.0000
O	O1	1.0	0.32691	0.65887	0.06946	1.0000
O	O2	1.0	0.34968	0.80708	0.99816	1.0000
O	O3	1.0	0.22138	0.83981	0.07623	1.0000
O	O4	1.0	0.43101	0.84008	0.08807	1.0000
O	O5	1.0	0.34315	0.51808	0.99377	1.0000
O	O6	1.0	0.23381	0.46979	0.07591	1.0000
O	O7	1.0	0.44630	0.48583	0.07787	1.0000
O	O8	1.0	0.70369	0.67310	0.06824	1.0000
O	O9	1.0	0.82985	0.84124	0.05672	1.0000
O	O10	1.0	0.64107	0.86503	0.09630	1.0000
O	O11	1.0	0.83663	0.50788	0.06596	1.0000

O	O12	1.0	0.64790	0.49050	0.10770	1.0000
O	O13	1.0	0.96428	0.67605	0.05778	1.0000
O	O14	1.0	0.01684	0.85955	0.09955	1.0000
O	O15	1.0	0.03115	0.49951	0.10170	1.0000
O	O16	1.0	0.67415	0.32465	0.56003	1.0000
O	O17	1.0	0.67757	0.16801	0.49076	1.0000
O	O18	1.0	0.74157	0.13236	0.58540	1.0000
O	O19	1.0	0.53678	0.15884	0.56348	1.0000
O	O20	1.0	0.66549	0.49442	0.50079	1.0000
O	O21	1.0	0.76964	0.50333	0.58744	1.0000
O	O22	1.0	0.55665	0.49239	0.58465	1.0000
O	O23	1.0	0.28060	0.33486	0.56682	1.0000
O	O24	1.0	0.14967	0.16887	0.55835	1.0000
O	O25	1.0	0.33546	0.15057	0.60751	1.0000
O	O26	1.0	0.16514	0.50782	0.55556	1.0000
O	O27	1.0	0.35118	0.52039	0.60083	1.0000
O	O28	1.0	0.02848	0.34168	0.55461	1.0000
O	O29	1.0	0.95193	0.16598	0.59567	1.0000
O	O30	1.0	0.98001	0.52469	0.59802	1.0000
O	O31	1.0	0.33481	0.37001	0.31070	1.0000
O	O32	1.0	0.17174	0.33104	0.24802	1.0000
O	O33	1.0	0.18806	0.22523	0.33423	1.0000
O	O34	1.0	0.14018	0.43160	0.33378	1.0000
O	O35	1.0	0.49479	0.33434	0.24623	1.0000
O	O36	1.0	0.48659	0.23169	0.33314	1.0000
O	O37	1.0	0.53032	0.44057	0.32935	1.0000
O	O38	1.0	0.33015	0.71355	0.31060	1.0000
O	O39	1.0	0.15572	0.83196	0.30833	1.0000
O	O40	1.0	0.15044	0.64197	0.34813	1.0000
O	O41	1.0	0.49988	0.83784	0.31329	1.0000
O	O42	1.0	0.50587	0.64647	0.35349	1.0000
O	O43	1.0	0.32586	0.95993	0.30731	1.0000
O	O44	1.0	0.14407	0.02177	0.34856	1.0000
O	O45	1.0	0.49829	0.02663	0.35501	1.0000

O	O46	1.0	0.66311	0.68683	0.81612	1.0000
O	O47	1.0	0.81995	0.65559	0.74950	1.0000
O	O48	1.0	0.85707	0.76077	0.83358	1.0000
O	O49	1.0	0.82120	0.55188	0.83528	1.0000
O	O50	1.0	0.51629	0.64814	0.74524	1.0000
O	O51	1.0	0.46744	0.75877	0.82771	1.0000
O	O52	1.0	0.50210	0.55065	0.83188	1.0000
O	O53	1.0	0.67396	0.29746	0.81784	1.0000
O	O54	1.0	0.83716	0.16174	0.81432	1.0000
O	O55	1.0	0.86435	0.35075	0.85302	1.0000
O	O56	1.0	0.51073	0.16095	0.81461	1.0000
O	O57	1.0	0.48566	0.34755	0.85425	1.0000
O	O58	1.0	0.67329	0.02562	0.80718	1.0000
O	O59	1.0	0.85542	0.96979	0.84939	1.0000
O	O60	1.0	0.48834	0.96658	0.84470	1.0000
O	O61	1.0	0.68167	0.65603	0.93582	1.0000
O	O62	1.0	0.65550	0.81858	0.99937	1.0000
O	O63	1.0	0.78066	0.83838	0.91995	1.0000
O	O64	1.0	0.56961	0.82691	0.90952	1.0000
O	O65	1.0	0.66260	0.50859	0.00791	1.0000
O	O66	1.0	0.76641	0.46616	0.92344	1.0000
O	O67	1.0	0.55457	0.48670	0.92402	1.0000
O	O68	1.0	0.29356	0.66776	0.92715	1.0000
O	O69	1.0	0.17420	0.83909	0.94355	1.0000
O	O70	1.0	0.36164	0.85814	0.90127	1.0000
O	O71	1.0	0.16472	0.50089	0.93941	1.0000
O	O72	1.0	0.35218	0.47855	0.89571	1.0000
O	O73	1.0	0.04179	0.67247	0.94542	1.0000
O	O74	1.0	0.98736	0.85161	0.89964	1.0000
O	O75	1.0	0.97113	0.49658	0.90213	1.0000
O	O76	1.0	0.31173	0.32589	0.43760	1.0000
O	O77	1.0	0.33853	0.17500	0.50897	1.0000
O	O78	1.0	0.23920	0.13229	0.42146	1.0000
O	O79	1.0	0.44992	0.16613	0.42731	1.0000

O	O80	1.0	0.34189	0.48522	0.50223	1.0000
O	O81	1.0	0.22371	0.51125	0.41907	1.0000
O	O82	1.0	0.43448	0.49249	0.41442	1.0000
O	O83	1.0	0.68583	0.33942	0.43361	1.0000
O	O84	1.0	0.83688	0.18940	0.42500	1.0000
O	O85	1.0	0.64429	0.15429	0.39135	1.0000
O	O86	1.0	0.82961	0.49527	0.43696	1.0000
O	O87	1.0	0.63998	0.53396	0.40339	1.0000
O	O88	1.0	0.97983	0.34433	0.43875	1.0000
O	O89	1.0	0.03505	0.16156	0.39879	1.0000
O	O90	1.0	0.01694	0.53228	0.39933	1.0000
O	O91	1.0	0.67146	0.37380	0.69111	1.0000
O	O92	1.0	0.83355	0.33031	0.75409	1.0000
O	O93	1.0	0.81589	0.22535	0.66810	1.0000
O	O94	1.0	0.86882	0.43032	0.66928	1.0000
O	O95	1.0	0.51228	0.32997	0.75455	1.0000
O	O96	1.0	0.52259	0.23547	0.66364	1.0000
O	O97	1.0	0.47484	0.44127	0.67377	1.0000
O	O98	1.0	0.67139	0.70631	0.68214	1.0000
O	O99	1.0	0.84438	0.82977	0.69181	1.0000
O	O100	1.0	0.85859	0.64034	0.65218	1.0000
O	O101	1.0	0.50252	0.82929	0.69415	1.0000
O	O102	1.0	0.48552	0.64496	0.64644	1.0000
O	O103	1.0	0.67475	0.95479	0.69349	1.0000
O	O104	1.0	0.85491	0.02109	0.65058	1.0000
O	O105	1.0	0.49817	0.01169	0.64532	1.0000
O	O106	1.0	0.33954	0.69630	0.18899	1.0000
O	O107	1.0	0.17229	0.66015	0.24920	1.0000
O	O108	1.0	0.14777	0.76313	0.16337	1.0000
O	O109	1.0	0.18891	0.55471	0.16494	1.0000
O	O110	1.0	0.49826	0.66497	0.25417	1.0000
O	O111	1.0	0.53521	0.75840	0.16645	1.0000
O	O112	1.0	0.49149	0.55156	0.17104	1.0000
O	O113	1.0	0.33171	0.29733	0.18443	1.0000

O	O114	1.0	0.16670	0.16383	0.18643	1.0000
O	O115	1.0	0.14257	0.35396	0.14874	1.0000
O	O116	1.0	0.49730	0.16373	0.18736	1.0000
O	O117	1.0	0.51958	0.35058	0.14694	1.0000
O	O118	1.0	0.33234	0.03124	0.19438	1.0000
O	O119	1.0	0.15545	0.97248	0.14865	1.0000
O	O120	1.0	0.51691	0.96835	0.15663	1.0000
O	O121	1.0	0.00113	0.84444	0.99969	1.0000
O	O122	1.0	0.99964	0.50407	0.00204	1.0000
O	O123	1.0	0.98296	0.17365	0.49706	1.0000
O	O124	1.0	0.99304	0.51289	0.49876	1.0000
O	O125	1.0	0.15827	0.00015	0.24871	1.0000
O	O126	1.0	0.49941	0.00878	0.25487	1.0000
O	O127	1.0	0.84481	0.00075	0.75000	1.0000
O	O128	1.0	0.50471	0.00776	0.74622	1.0000
H	H1	1.0	0.48470	0.15587	0.53526	1.0000

T7T7:

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O O3 1.0 0.22581 0.84419 0.08034 1.0000
O O4 1.0 0.43617 0.82989 0.08685 1.0000
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O O6 1.0 0.23453 0.46400 0.07800 1.0000

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O	O8	1.0	0.70074	0.67152	0.06449	1.0000
O	O9	1.0	0.83249	0.83707	0.05882	1.0000
O	O10	1.0	0.64313	0.86260	0.09683	1.0000
O	O11	1.0	0.83528	0.50689	0.06479	1.0000
O	O12	1.0	0.64706	0.48720	0.10470	1.0000
O	O13	1.0	0.96776	0.67220	0.05750	1.0000
O	O14	1.0	0.01980	0.85533	0.10029	1.0000
O	O15	1.0	0.02969	0.49125	0.09897	1.0000
O	O16	1.0	0.63755	0.32723	0.55368	1.0000
O	O17	1.0	0.68467	0.16670	0.49052	1.0000
O	O18	1.0	0.74031	0.15361	0.58781	1.0000
O	O19	1.0	0.53772	0.14152	0.56039	1.0000
O	O20	1.0	0.67564	0.50282	0.50134	1.0000
O	O21	1.0	0.76999	0.47126	0.59104	1.0000
O	O22	1.0	0.56129	0.51318	0.58302	1.0000
O	O23	1.0	0.28231	0.33022	0.56760	1.0000
O	O24	1.0	0.15402	0.15932	0.55569	1.0000
O	O25	1.0	0.33610	0.14428	0.60626	1.0000
O	O26	1.0	0.17071	0.50297	0.55190	1.0000
O	O27	1.0	0.35361	0.51650	0.60196	1.0000
O	O28	1.0	0.03836	0.33316	0.55254	1.0000
O	O29	1.0	0.95447	0.15542	0.59091	1.0000
O	O30	1.0	0.99538	0.50576	0.60608	1.0000
O	O31	1.0	0.33925	0.37525	0.31176	1.0000
O	O32	1.0	0.17390	0.33880	0.25061	1.0000
O	O33	1.0	0.19857	0.22233	0.33310	1.0000
O	O34	1.0	0.14447	0.42734	0.34010	1.0000
O	O35	1.0	0.49569	0.33767	0.24559	1.0000
O	O36	1.0	0.48800	0.23257	0.33192	1.0000
O	O37	1.0	0.53670	0.44114	0.32930	1.0000
O	O38	1.0	0.33403	0.71155	0.31238	1.0000
O	O39	1.0	0.16052	0.82968	0.30967	1.0000
O	O40	1.0	0.15446	0.63941	0.34931	1.0000

O	O41	1.0	0.50297	0.83709	0.31226	1.0000
O	O42	1.0	0.51143	0.64683	0.35409	1.0000
O	O43	1.0	0.32958	0.96015	0.30796	1.0000
O	O44	1.0	0.14769	0.02053	0.34951	1.0000
O	O45	1.0	0.50673	0.02759	0.35211	1.0000
O	O46	1.0	0.67338	0.68181	0.81541	1.0000
O	O47	1.0	0.82197	0.65387	0.74231	1.0000
O	O48	1.0	0.86668	0.76004	0.82712	1.0000
O	O49	1.0	0.83650	0.54773	0.82529	1.0000
O	O50	1.0	0.52152	0.64651	0.74755	1.0000
O	O51	1.0	0.48083	0.75961	0.83096	1.0000
O	O52	1.0	0.50930	0.55142	0.83482	1.0000
O	O53	1.0	0.66198	0.32046	0.81454	1.0000
O	O54	1.0	0.79846	0.15833	0.82649	1.0000
O	O55	1.0	0.84919	0.35043	0.85743	1.0000
O	O56	1.0	0.52179	0.16128	0.81780	1.0000
O	O57	1.0	0.46683	0.34799	0.84850	1.0000
O	O58	1.0	0.65820	0.00037	0.80942	1.0000
O	O59	1.0	0.84237	0.96369	0.85274	1.0000
O	O60	1.0	0.46451	0.96928	0.84195	1.0000
O	O61	1.0	0.63130	0.66027	0.93704	1.0000
O	O62	1.0	0.66245	0.82627	0.99854	1.0000
O	O63	1.0	0.77857	0.80723	0.91576	1.0000
O	O64	1.0	0.57246	0.85516	0.90998	1.0000
O	O65	1.0	0.66500	0.50535	0.00479	1.0000
O	O66	1.0	0.76398	0.50149	0.91722	1.0000
O	O67	1.0	0.55438	0.46483	0.92298	1.0000
O	O68	1.0	0.28534	0.66631	0.93112	1.0000
O	O69	1.0	0.17053	0.84090	0.94195	1.0000
O	O70	1.0	0.36057	0.85112	0.90194	1.0000
O	O71	1.0	0.16138	0.49589	0.93830	1.0000
O	O72	1.0	0.35059	0.48380	0.89522	1.0000
O	O73	1.0	0.04147	0.67070	0.94443	1.0000
O	O74	1.0	0.98214	0.84973	0.89996	1.0000

O	O75	1.0	0.97052	0.49566	0.89934	1.0000
O	O76	1.0	0.31749	0.32570	0.43660	1.0000
O	O77	1.0	0.34392	0.17385	0.50814	1.0000
O	O78	1.0	0.23762	0.13377	0.42272	1.0000
O	O79	1.0	0.44998	0.16205	0.42521	1.0000
O	O80	1.0	0.35352	0.47948	0.50390	1.0000
O	O81	1.0	0.23703	0.51635	0.42117	1.0000
O	O82	1.0	0.44523	0.49056	0.41583	1.0000
O	O83	1.0	0.69539	0.34264	0.43618	1.0000
O	O84	1.0	0.84016	0.18858	0.42317	1.0000
O	O85	1.0	0.64588	0.16047	0.39114	1.0000
O	O86	1.0	0.83666	0.50178	0.43582	1.0000
O	O87	1.0	0.64799	0.53537	0.40292	1.0000
O	O88	1.0	0.98011	0.34573	0.44042	1.0000
O	O89	1.0	0.03739	0.16871	0.39456	1.0000
O	O90	1.0	0.02970	0.53613	0.40708	1.0000
O	O91	1.0	0.67248	0.35917	0.69674	1.0000
O	O92	1.0	0.83478	0.30956	0.75825	1.0000
O	O93	1.0	0.84415	0.25705	0.66061	1.0000
O	O94	1.0	0.49932	0.31698	0.74995	1.0000
O	O95	1.0	0.52660	0.23055	0.65810	1.0000
O	O96	1.0	0.48681	0.43949	0.67056	1.0000
O	O97	1.0	0.66798	0.71692	0.68215	1.0000
O	O98	1.0	0.83896	0.84457	0.69483	1.0000
O	O99	1.0	0.85395	0.66176	0.64436	1.0000
O	O100	1.0	0.49811	0.83094	0.70074	1.0000
O	O101	1.0	0.47994	0.64733	0.65019	1.0000
O	O102	1.0	0.66735	0.96342	0.69531	1.0000
O	O103	1.0	0.84547	0.04222	0.65602	1.0000
O	O104	1.0	0.49201	0.00349	0.64415	1.0000
O	O105	1.0	0.34065	0.69115	0.18784	1.0000
O	O106	1.0	0.17732	0.65669	0.25051	1.0000
O	O107	1.0	0.15154	0.77015	0.16780	1.0000
O	O108	1.0	0.18007	0.55987	0.16319	1.0000

O	O109	1.0	0.49792	0.66110	0.25457	1.0000
O	O110	1.0	0.53506	0.76346	0.16936	1.0000
O	O111	1.0	0.49766	0.55415	0.16968	1.0000
O	O112	1.0	0.33035	0.30090	0.18554	1.0000
O	O113	1.0	0.16692	0.16645	0.19129	1.0000
O	O114	1.0	0.13957	0.35472	0.15171	1.0000
O	O115	1.0	0.49394	0.16513	0.18715	1.0000
O	O116	1.0	0.51630	0.35131	0.14577	1.0000
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O	O119	1.0	0.51360	0.97145	0.15286	1.0000
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O	O124	1.0	0.16074	0.99708	0.24986	1.0000
O	O125	1.0	0.49914	0.00496	0.25203	1.0000
O	O126	1.0	0.83296	0.01523	0.75422	1.0000
O	O127	1.0	0.49542	0.01917	0.74491	1.0000
O	O128	1.0	0.85733	0.45947	0.68935	1.0000
Al	Al1	1.0	0.46667	0.12977	0.62390	1.0000
Al	Al2	1.0	0.86929	0.53126	0.62605	1.0000
Si	Si1	1.0	0.33087	0.78545	0.05880	1.0000
Si	Si2	1.0	0.33375	0.53099	0.05442	1.0000
Si	Si3	1.0	0.70975	0.79884	0.05429	1.0000
Si	Si4	1.0	0.71247	0.54322	0.05927	1.0000
Si	Si5	1.0	0.95507	0.80076	0.05394	1.0000
Si	Si6	1.0	0.95725	0.54329	0.05502	1.0000
Si	Si7	1.0	0.53099	0.85642	0.12661	1.0000
Si	Si8	1.0	0.65642	0.20143	0.54788	1.0000
Si	Si9	1.0	0.66394	0.45578	0.55843	1.0000
Si	Si10	1.0	0.27632	0.20165	0.56098	1.0000
Si	Si11	1.0	0.28984	0.45713	0.55664	1.0000
Si	Si12	1.0	0.03422	0.20497	0.54856	1.0000

Si	Si13	1.0	0.04739	0.46312	0.55516	1.0000
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Si	Si19	1.0	0.45849	0.95739	0.30579	1.0000
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Si	Si21	1.0	0.79839	0.66186	0.80304	1.0000
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Si	Si23	1.0	0.78540	0.28354	0.81424	1.0000
Si	Si24	1.0	0.53722	0.28657	0.80663	1.0000
Si	Si25	1.0	0.78308	0.03428	0.81025	1.0000
Si	Si26	1.0	0.53495	0.03768	0.80262	1.0000
Si	Si27	1.0	0.85396	0.47440	0.87546	1.0000
Si	Si28	1.0	0.66131	0.78713	0.93993	1.0000
Si	Si29	1.0	0.65399	0.53343	0.94528	1.0000
Si	Si30	1.0	0.28956	0.79243	0.94396	1.0000
Si	Si31	1.0	0.28344	0.53893	0.94003	1.0000
Si	Si32	1.0	0.04845	0.79999	0.94668	1.0000
Si	Si33	1.0	0.04191	0.54147	0.94565	1.0000
Si	Si34	1.0	0.47120	0.85712	0.87140	1.0000
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Si	Si36	1.0	0.33816	0.45369	0.44429	1.0000
Si	Si37	1.0	0.71733	0.21565	0.43522	1.0000
Si	Si38	1.0	0.71393	0.47022	0.44499	1.0000
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Si	Si40	1.0	0.95856	0.47255	0.44793	1.0000
Si	Si41	1.0	0.52227	0.14672	0.37457	1.0000
Si	Si42	1.0	0.54401	0.33390	0.69265	1.0000
Si	Si43	1.0	0.79607	0.72201	0.68943	1.0000
Si	Si44	1.0	0.54202	0.71086	0.69487	1.0000
Si	Si45	1.0	0.79512	0.96593	0.69969	1.0000
Si	Si46	1.0	0.53775	0.95431	0.69503	1.0000

Si	Si47	1.0	0.21285	0.66898	0.19184	1.0000
Si	Si48	1.0	0.46724	0.66727	0.19503	1.0000
Si	Si49	1.0	0.20317	0.29026	0.19515	1.0000
Si	Si50	1.0	0.45819	0.28843	0.19138	1.0000
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Si	Si53	1.0	0.14585	0.46831	0.12277	1.0000
Si	Si54	1.0	0.13785	0.86096	0.12462	1.0000
Si	Si55	1.0	0.52614	0.47170	0.12433	1.0000
Si	Si56	1.0	0.84643	0.15170	0.62384	1.0000
Si	Si57	1.0	0.47159	0.52790	0.62643	1.0000
Si	Si58	1.0	0.15488	0.13791	0.37506	1.0000
Si	Si59	1.0	0.53381	0.52824	0.37521	1.0000
Si	Si60	1.0	0.86562	0.84537	0.87393	1.0000
Si	Si61	1.0	0.47065	0.46354	0.87574	1.0000
Si	Si62	1.0	0.79801	0.34005	0.70147	1.0000

T7T9:

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O O6 1.0 0.23224 0.47148 0.07216 1.0000

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O	O8	1.0	0.70069	0.67283	0.06782	1.0000
O	O9	1.0	0.83054	0.83846	0.05813	1.0000
O	O10	1.0	0.64078	0.86558	0.09634	1.0000
O	O11	1.0	0.83507	0.50814	0.06542	1.0000
O	O12	1.0	0.64717	0.49007	0.10760	1.0000
O	O13	1.0	0.96676	0.67376	0.05842	1.0000
O	O14	1.0	0.01740	0.85712	0.10075	1.0000
O	O15	1.0	0.02953	0.49235	0.09957	1.0000
O	O16	1.0	0.67180	0.32623	0.56021	1.0000
O	O17	1.0	0.66981	0.16986	0.49073	1.0000
O	O18	1.0	0.74245	0.13441	0.58413	1.0000
O	O19	1.0	0.53500	0.16008	0.56516	1.0000
O	O20	1.0	0.66830	0.49649	0.50090	1.0000
O	O21	1.0	0.76963	0.50353	0.58801	1.0000
O	O22	1.0	0.55650	0.49597	0.58389	1.0000
O	O23	1.0	0.27850	0.33726	0.56718	1.0000
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O	O25	1.0	0.33471	0.15567	0.61039	1.0000
O	O26	1.0	0.16454	0.51065	0.55425	1.0000
O	O27	1.0	0.35045	0.52282	0.60041	1.0000
O	O28	1.0	0.03026	0.34219	0.55495	1.0000
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O	O31	1.0	0.33708	0.37613	0.30847	1.0000
O	O32	1.0	0.17443	0.34031	0.24558	1.0000
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O	O34	1.0	0.14115	0.42516	0.33474	1.0000
O	O35	1.0	0.49894	0.33226	0.24645	1.0000
O	O36	1.0	0.48274	0.23182	0.33362	1.0000
O	O37	1.0	0.53416	0.43938	0.32925	1.0000
O	O38	1.0	0.32810	0.71195	0.30776	1.0000
O	O39	1.0	0.15179	0.82418	0.30424	1.0000
O	O40	1.0	0.14995	0.63659	0.34676	1.0000

O	O41	1.0	0.49425	0.83781	0.31624	1.0000
O	O42	1.0	0.50015	0.64359	0.35366	1.0000
O	O43	1.0	0.32016	0.96042	0.30980	1.0000
O	O44	1.0	0.49205	0.02832	0.35743	1.0000
O	O45	1.0	0.66382	0.68920	0.81692	1.0000
O	O46	1.0	0.81884	0.65682	0.74951	1.0000
O	O47	1.0	0.85916	0.76009	0.83404	1.0000
O	O48	1.0	0.82050	0.55180	0.83490	1.0000
O	O49	1.0	0.51837	0.64787	0.74560	1.0000
O	O50	1.0	0.46776	0.76030	0.82754	1.0000
O	O51	1.0	0.50314	0.55197	0.83211	1.0000
O	O52	1.0	0.67395	0.29905	0.81814	1.0000
O	O53	1.0	0.83625	0.16221	0.81443	1.0000
O	O54	1.0	0.86458	0.35108	0.85306	1.0000
O	O55	1.0	0.51110	0.16225	0.81368	1.0000
O	O56	1.0	0.48498	0.34809	0.85412	1.0000
O	O57	1.0	0.67307	0.02551	0.80697	1.0000
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O	O60	1.0	0.68181	0.65681	0.93676	1.0000
O	O61	1.0	0.65730	0.82099	0.99943	1.0000
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O	O63	1.0	0.56699	0.82634	0.91053	1.0000
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O	O65	1.0	0.76857	0.46803	0.92370	1.0000
O	O66	1.0	0.55581	0.48637	0.92355	1.0000
O	O67	1.0	0.29191	0.66912	0.92717	1.0000
O	O68	1.0	0.17372	0.84098	0.94427	1.0000
O	O69	1.0	0.36025	0.85936	0.90088	1.0000
O	O70	1.0	0.16591	0.50112	0.94066	1.0000
O	O71	1.0	0.35254	0.48035	0.89535	1.0000
O	O72	1.0	0.04290	0.67316	0.94533	1.0000
O	O73	1.0	0.98593	0.85347	0.90095	1.0000
O	O74	1.0	0.97312	0.49798	0.90074	1.0000

O	O75	1.0	0.30716	0.32330	0.44010	1.0000
O	O76	1.0	0.34374	0.17609	0.51201	1.0000
O	O77	1.0	0.24774	0.12404	0.42400	1.0000
O	O78	1.0	0.45492	0.17285	0.42990	1.0000
O	O79	1.0	0.34283	0.48627	0.50220	1.0000
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O	O82	1.0	0.68313	0.34113	0.43336	1.0000
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O	O91	1.0	0.83321	0.33060	0.75405	1.0000
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O	O93	1.0	0.86998	0.43023	0.66932	1.0000
O	O94	1.0	0.51283	0.33421	0.75483	1.0000
O	O95	1.0	0.52609	0.23327	0.66594	1.0000
O	O96	1.0	0.47409	0.43942	0.67216	1.0000
O	O97	1.0	0.67127	0.70635	0.68155	1.0000
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O	O99	1.0	0.85933	0.64058	0.65249	1.0000
O	O100	1.0	0.50202	0.82886	0.69473	1.0000
O	O101	1.0	0.48443	0.64496	0.64713	1.0000
O	O102	1.0	0.67338	0.95540	0.69353	1.0000
O	O103	1.0	0.85276	0.02163	0.64987	1.0000
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O	O105	1.0	0.34085	0.69185	0.18930	1.0000
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O	O107	1.0	0.15269	0.76880	0.16567	1.0000
O	O108	1.0	0.18713	0.55799	0.16003	1.0000

O	O109	1.0	0.50109	0.66862	0.25420	1.0000
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O	O111	1.0	0.49296	0.54673	0.17289	1.0000
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O	O121	1.0	0.99629	0.50370	0.00044	1.0000
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O	O127	1.0	0.50336	0.00701	0.74669	1.0000
O	O128	1.0	0.13222	0.00858	0.34639	1.0000
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Al	Al2	1.0	0.15439	0.14236	0.37700	1.0000
Si	Si1	1.0	0.33369	0.78669	0.05774	1.0000
Si	Si2	1.0	0.33914	0.53372	0.05353	1.0000
Si	Si3	1.0	0.70785	0.79885	0.05494	1.0000
Si	Si4	1.0	0.71155	0.54493	0.06151	1.0000
Si	Si5	1.0	0.95373	0.80205	0.05407	1.0000
Si	Si6	1.0	0.95703	0.54500	0.05548	1.0000
Si	Si7	1.0	0.52997	0.85534	0.12702	1.0000
Si	Si8	1.0	0.65988	0.20024	0.54975	1.0000
Si	Si9	1.0	0.66634	0.45645	0.55907	1.0000
Si	Si10	1.0	0.27440	0.20829	0.56368	1.0000
Si	Si11	1.0	0.28445	0.46351	0.55616	1.0000
Si	Si12	1.0	0.02928	0.21310	0.55237	1.0000

Si	Si13	1.0	0.04191	0.47073	0.55143	1.0000
Si	Si14	1.0	0.21208	0.33719	0.30473	1.0000
Si	Si15	1.0	0.46261	0.34426	0.30483	1.0000
Si	Si16	1.0	0.20072	0.70347	0.30140	1.0000
Si	Si17	1.0	0.45692	0.71500	0.30756	1.0000
Si	Si18	1.0	0.45106	0.95859	0.30995	1.0000
Si	Si19	1.0	0.13584	0.52276	0.37478	1.0000
Si	Si20	1.0	0.79028	0.66414	0.80899	1.0000
Si	Si21	1.0	0.53828	0.66216	0.80564	1.0000
Si	Si22	1.0	0.80118	0.28546	0.80945	1.0000
Si	Si23	1.0	0.54626	0.28569	0.80925	1.0000
Si	Si24	1.0	0.80142	0.03996	0.80435	1.0000
Si	Si25	1.0	0.54475	0.04050	0.80245	1.0000
Si	Si26	1.0	0.85632	0.46818	0.87838	1.0000
Si	Si27	1.0	0.67064	0.78566	0.94073	1.0000
Si	Si28	1.0	0.66657	0.52991	0.94739	1.0000
Si	Si29	1.0	0.29383	0.79412	0.94274	1.0000
Si	Si30	1.0	0.28870	0.54254	0.93926	1.0000
Si	Si31	1.0	0.05075	0.80199	0.94769	1.0000
Si	Si32	1.0	0.04457	0.54425	0.94673	1.0000
Si	Si33	1.0	0.47227	0.85291	0.87064	1.0000
Si	Si34	1.0	0.33519	0.19798	0.45081	1.0000
Si	Si35	1.0	0.32801	0.45119	0.44364	1.0000
Si	Si36	1.0	0.70834	0.21469	0.43569	1.0000
Si	Si37	1.0	0.70561	0.46676	0.44407	1.0000
Si	Si38	1.0	0.95659	0.21397	0.44098	1.0000
Si	Si39	1.0	0.95384	0.46817	0.44367	1.0000
Si	Si40	1.0	0.51701	0.14822	0.37734	1.0000
Si	Si41	1.0	0.79583	0.34017	0.69560	1.0000
Si	Si42	1.0	0.54533	0.34278	0.69548	1.0000
Si	Si43	1.0	0.79748	0.70987	0.69438	1.0000
Si	Si44	1.0	0.54411	0.70794	0.69250	1.0000
Si	Si45	1.0	0.80195	0.95274	0.69604	1.0000
Si	Si46	1.0	0.54323	0.95194	0.69405	1.0000

Si	Si47	1.0	0.86777	0.52412	0.62723	1.0000
Si	Si48	1.0	0.21328	0.66672	0.18960	1.0000
Si	Si49	1.0	0.46744	0.66415	0.19481	1.0000
Si	Si50	1.0	0.20698	0.28875	0.19158	1.0000
Si	Si51	1.0	0.46365	0.28347	0.19210	1.0000
Si	Si52	1.0	0.20421	0.04367	0.19312	1.0000
Si	Si53	1.0	0.46120	0.04052	0.19988	1.0000
Si	Si54	1.0	0.14929	0.46899	0.11929	1.0000
Si	Si55	1.0	0.13842	0.85904	0.12208	1.0000
Si	Si56	1.0	0.52649	0.46831	0.12648	1.0000
Si	Si57	1.0	0.84178	0.13875	0.62487	1.0000
Si	Si58	1.0	0.46758	0.52480	0.62646	1.0000
Si	Si59	1.0	0.52555	0.52568	0.37504	1.0000
Si	Si60	1.0	0.86841	0.85535	0.87537	1.0000
Si	Si61	1.0	0.47479	0.46743	0.87623	1.0000
Si	Si62	1.0	0.19540	0.94433	0.29871	1.0000

AlSiAl-T7T9:

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O	O1	1.0	0.32599	0.65896	0.06896	1.0000
O	O2	1.0	0.34973	0.80891	0.99851	1.0000
O	O3	1.0	0.22095	0.84055	0.07599	1.0000
O	O4	1.0	0.43069	0.83988	0.08854	1.0000
O	O5	1.0	0.34387	0.51839	0.99324	1.0000
O	O6	1.0	0.23317	0.46932	0.07502	1.0000

O	O7	1.0	0.44639	0.48605	0.07728	1.0000
O	O8	1.0	0.70655	0.67587	0.07003	1.0000
O	O9	1.0	0.82943	0.84558	0.05630	1.0000
O	O10	1.0	0.64021	0.86785	0.09601	1.0000
O	O11	1.0	0.83616	0.50821	0.06541	1.0000
O	O12	1.0	0.64778	0.49292	0.10871	1.0000
O	O13	1.0	0.96202	0.67804	0.05727	1.0000
O	O14	1.0	0.01687	0.86189	0.09899	1.0000
O	O15	1.0	0.03133	0.50280	0.10221	1.0000
O	O16	1.0	0.67691	0.32130	0.55836	1.0000
O	O17	1.0	0.67278	0.16739	0.48818	1.0000
O	O18	1.0	0.73596	0.12513	0.58338	1.0000
O	O19	1.0	0.53360	0.16084	0.56156	1.0000
O	O20	1.0	0.66369	0.49386	0.50102	1.0000
O	O21	1.0	0.76911	0.50127	0.58744	1.0000
O	O22	1.0	0.55694	0.48693	0.58507	1.0000
O	O23	1.0	0.28526	0.33496	0.56625	1.0000
O	O24	1.0	0.15581	0.16726	0.55376	1.0000
O	O25	1.0	0.33702	0.14895	0.60653	1.0000
O	O26	1.0	0.16622	0.50715	0.55731	1.0000
O	O27	1.0	0.35278	0.52192	0.60079	1.0000
O	O28	1.0	0.03222	0.33877	0.55349	1.0000
O	O29	1.0	0.96386	0.15812	0.59533	1.0000
O	O30	1.0	0.97957	0.52022	0.59797	1.0000
O	O31	1.0	0.33559	0.37304	0.31081	1.0000
O	O32	1.0	0.17299	0.33243	0.24795	1.0000
O	O33	1.0	0.19180	0.22491	0.33376	1.0000
O	O34	1.0	0.14001	0.43087	0.33420	1.0000
O	O35	1.0	0.49375	0.34089	0.24518	1.0000
O	O36	1.0	0.48579	0.22998	0.32948	1.0000
O	O37	1.0	0.53262	0.43908	0.33020	1.0000
O	O38	1.0	0.32939	0.71222	0.31082	1.0000
O	O39	1.0	0.15575	0.83238	0.30765	1.0000
O	O40	1.0	0.14759	0.64218	0.34695	1.0000

O	O41	1.0	0.49929	0.83714	0.31374	1.0000
O	O42	1.0	0.50564	0.64538	0.35332	1.0000
O	O43	1.0	0.32604	0.96024	0.30705	1.0000
O	O44	1.0	0.14471	0.02216	0.34876	1.0000
O	O45	1.0	0.49872	0.02676	0.35501	1.0000
O	O46	1.0	0.66254	0.69038	0.81406	1.0000
O	O47	1.0	0.82373	0.64431	0.75189	1.0000
O	O48	1.0	0.85560	0.76419	0.83209	1.0000
O	O49	1.0	0.81579	0.55466	0.84061	1.0000
O	O50	1.0	0.51101	0.64958	0.74596	1.0000
O	O51	1.0	0.46503	0.75298	0.83079	1.0000
O	O52	1.0	0.50891	0.54653	0.83192	1.0000
O	O53	1.0	0.67122	0.29423	0.81930	1.0000
O	O54	1.0	0.83768	0.16385	0.81326	1.0000
O	O55	1.0	0.85948	0.35073	0.85609	1.0000
O	O56	1.0	0.50756	0.15886	0.81407	1.0000
O	O57	1.0	0.48193	0.34486	0.85431	1.0000
O	O58	1.0	0.67319	0.02648	0.80786	1.0000
O	O59	1.0	0.85383	0.97252	0.85192	1.0000
O	O60	1.0	0.48608	0.96240	0.84133	1.0000
O	O61	1.0	0.67417	0.65534	0.93454	1.0000
O	O62	1.0	0.65515	0.81708	0.99949	1.0000
O	O63	1.0	0.78188	0.83402	0.92046	1.0000
O	O64	1.0	0.57104	0.83278	0.90946	1.0000
O	O65	1.0	0.65780	0.51365	0.00956	1.0000
O	O66	1.0	0.76746	0.46663	0.92812	1.0000
O	O67	1.0	0.55482	0.48076	0.92463	1.0000
O	O68	1.0	0.29244	0.66974	0.92748	1.0000
O	O69	1.0	0.17389	0.84152	0.94375	1.0000
O	O70	1.0	0.36193	0.86085	0.90205	1.0000
O	O71	1.0	0.16553	0.50076	0.93919	1.0000
O	O72	1.0	0.35302	0.48219	0.89482	1.0000
O	O73	1.0	0.04310	0.67286	0.94588	1.0000
O	O74	1.0	0.98768	0.85062	0.89908	1.0000

O	O75	1.0	0.97098	0.49591	0.90338	1.0000
O	O76	1.0	0.30842	0.32803	0.43805	1.0000
O	O77	1.0	0.34573	0.17640	0.50794	1.0000
O	O78	1.0	0.23947	0.13309	0.42178	1.0000
O	O79	1.0	0.45012	0.17204	0.42459	1.0000
O	O80	1.0	0.34101	0.48851	0.50210	1.0000
O	O81	1.0	0.22507	0.51531	0.41831	1.0000
O	O82	1.0	0.43535	0.49160	0.41467	1.0000
O	O83	1.0	0.69448	0.34106	0.43294	1.0000
O	O84	1.0	0.83698	0.18326	0.42454	1.0000
O	O85	1.0	0.64463	0.15901	0.38867	1.0000
O	O86	1.0	0.83015	0.50432	0.43913	1.0000
O	O87	1.0	0.64055	0.53500	0.40394	1.0000
O	O88	1.0	0.97188	0.34487	0.43870	1.0000
O	O89	1.0	0.03611	0.16593	0.39741	1.0000
O	O90	1.0	0.01720	0.53199	0.39959	1.0000
O	O91	1.0	0.67068	0.37529	0.69233	1.0000
O	O92	1.0	0.83041	0.34046	0.75715	1.0000
O	O93	1.0	0.81153	0.21715	0.67609	1.0000
O	O94	1.0	0.86860	0.42209	0.66834	1.0000
O	O95	1.0	0.51129	0.32881	0.75471	1.0000
O	O96	1.0	0.52251	0.23492	0.66361	1.0000
O	O97	1.0	0.47354	0.44089	0.67445	1.0000
O	O98	1.0	0.67345	0.70092	0.68612	1.0000
O	O99	1.0	0.84737	0.82043	0.69655	1.0000
O	O100	1.0	0.85954	0.63343	0.65368	1.0000
O	O101	1.0	0.50790	0.82906	0.69284	1.0000
O	O102	1.0	0.49013	0.64359	0.64619	1.0000
O	O103	1.0	0.68007	0.95506	0.69056	1.0000
O	O104	1.0	0.50224	0.01142	0.64334	1.0000
O	O105	1.0	0.33973	0.70036	0.18874	1.0000
O	O106	1.0	0.17252	0.66043	0.24839	1.0000
O	O107	1.0	0.14633	0.76275	0.16255	1.0000
O	O108	1.0	0.19280	0.55525	0.16409	1.0000

O	O109	1.0	0.49739	0.66481	0.25408	1.0000
O	O110	1.0	0.53652	0.75962	0.16672	1.0000
O	O111	1.0	0.48893	0.55283	0.17043	1.0000
O	O112	1.0	0.33141	0.29727	0.18370	1.0000
O	O113	1.0	0.16549	0.16483	0.18633	1.0000
O	O114	1.0	0.14202	0.35508	0.14864	1.0000
O	O115	1.0	0.49861	0.16549	0.18899	1.0000
O	O116	1.0	0.51899	0.35102	0.14625	1.0000
O	O117	1.0	0.33259	0.03382	0.19491	1.0000
O	O118	1.0	0.15664	0.97281	0.14887	1.0000
O	O119	1.0	0.51616	0.97010	0.15660	1.0000
O	O120	1.0	0.99999	0.84618	0.99916	1.0000
O	O121	1.0	0.00165	0.50471	0.00284	1.0000
O	O122	1.0	0.98533	0.17189	0.49568	1.0000
O	O123	1.0	0.99721	0.51255	0.49887	1.0000
O	O124	1.0	0.15814	0.00165	0.24884	1.0000
O	O125	1.0	0.50014	0.00729	0.25492	1.0000
O	O126	1.0	0.84555	0.99644	0.75246	1.0000
O	O127	1.0	0.51046	0.00852	0.74409	1.0000
O	O128	1.0	0.86716	0.00505	0.65245	1.0000
Al	Al1	1.0	0.46873	0.13811	0.62530	1.0000
Al	Al2	1.0	0.84273	0.14093	0.62443	1.0000
Si	Si1	1.0	0.33227	0.78675	0.05815	1.0000
Si	Si2	1.0	0.33708	0.53324	0.05378	1.0000
Si	Si3	1.0	0.70816	0.80110	0.05510	1.0000
Si	Si4	1.0	0.71302	0.54769	0.06291	1.0000
Si	Si5	1.0	0.95206	0.80674	0.05278	1.0000
Si	Si6	1.0	0.95788	0.54877	0.05675	1.0000
Si	Si7	1.0	0.52976	0.85847	0.12707	1.0000
Si	Si8	1.0	0.66159	0.19459	0.54778	1.0000
Si	Si9	1.0	0.66657	0.45093	0.55876	1.0000
Si	Si10	1.0	0.27825	0.20614	0.56065	1.0000
Si	Si11	1.0	0.28673	0.46216	0.55659	1.0000
Si	Si12	1.0	0.03295	0.20897	0.55073	1.0000

Si	Si13	1.0	0.04398	0.46730	0.55184	1.0000
Si	Si14	1.0	0.20991	0.33970	0.30669	1.0000
Si	Si15	1.0	0.46188	0.34540	0.30421	1.0000
Si	Si16	1.0	0.20155	0.71210	0.30315	1.0000
Si	Si17	1.0	0.45790	0.71510	0.30754	1.0000
Si	Si18	1.0	0.19696	0.95449	0.30299	1.0000
Si	Si19	1.0	0.45525	0.95775	0.30737	1.0000
Si	Si20	1.0	0.13441	0.52867	0.37457	1.0000
Si	Si21	1.0	0.78922	0.66250	0.81036	1.0000
Si	Si22	1.0	0.53677	0.65931	0.80584	1.0000
Si	Si23	1.0	0.79905	0.28728	0.81074	1.0000
Si	Si24	1.0	0.54365	0.28241	0.80955	1.0000
Si	Si25	1.0	0.80137	0.04115	0.80670	1.0000
Si	Si26	1.0	0.54477	0.03898	0.80134	1.0000
Si	Si27	1.0	0.85325	0.46742	0.88212	1.0000
Si	Si28	1.0	0.67010	0.78445	0.94066	1.0000
Si	Si29	1.0	0.66320	0.52941	0.94892	1.0000
Si	Si30	1.0	0.29411	0.79487	0.94323	1.0000
Si	Si31	1.0	0.28814	0.54278	0.93898	1.0000
Si	Si32	1.0	0.05109	0.80190	0.94706	1.0000
Si	Si33	1.0	0.04513	0.54382	0.94804	1.0000
Si	Si34	1.0	0.47225	0.85145	0.87081	1.0000
Si	Si35	1.0	0.33455	0.20283	0.44759	1.0000
Si	Si36	1.0	0.32753	0.45651	0.44310	1.0000
Si	Si37	1.0	0.71338	0.21336	0.43390	1.0000
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Si	Si42	1.0	0.79435	0.33548	0.69787	1.0000
Si	Si43	1.0	0.54440	0.34123	0.69551	1.0000
Si	Si44	1.0	0.79980	0.69843	0.69743	1.0000
Si	Si45	1.0	0.54494	0.70602	0.69306	1.0000
Si	Si46	1.0	0.54828	0.95234	0.69163	1.0000

Si	Si47	1.0	0.86711	0.51702	0.62717	1.0000
Si	Si48	1.0	0.21311	0.66958	0.19045	1.0000
Si	Si49	1.0	0.46553	0.66884	0.19462	1.0000
Si	Si50	1.0	0.20345	0.28777	0.19202	1.0000
Si	Si51	1.0	0.45962	0.28815	0.19134	1.0000
Si	Si52	1.0	0.20370	0.04315	0.19496	1.0000
Si	Si53	1.0	0.46122	0.04388	0.19895	1.0000
Si	Si54	1.0	0.14944	0.47119	0.12203	1.0000
Si	Si55	1.0	0.13678	0.85903	0.12185	1.0000
Si	Si56	1.0	0.52534	0.47216	0.12556	1.0000
Si	Si57	1.0	0.46962	0.52213	0.62710	1.0000
Si	Si58	1.0	0.15275	0.13818	0.37551	1.0000
Si	Si59	1.0	0.52698	0.52747	0.37523	1.0000
Si	Si60	1.0	0.86820	0.85482	0.87583	1.0000
Si	Si61	1.0	0.47508	0.46465	0.87653	1.0000
Si	Si62	1.0	0.80452	0.94115	0.70101	1.0000

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H	H3	1.0	0.10393	0.81953	0.34567	1.0000
O	O1	1.0	0.32749	0.65578	0.06728	1.0000
O	O2	1.0	0.34626	0.80971	0.99802	1.0000
O	O3	1.0	0.22158	0.83520	0.07699	1.0000
O	O4	1.0	0.43225	0.83703	0.08669	1.0000
O	O5	1.0	0.33603	0.50840	0.99393	1.0000

O	O6	1.0	0.23393	0.46724	0.07909	1.0000
O	O7	1.0	0.44570	0.48176	0.07581	1.0000
O	O8	1.0	0.69647	0.67165	0.06257	1.0000
O	O9	1.0	0.83130	0.83522	0.05837	1.0000
O	O10	1.0	0.64112	0.86366	0.09467	1.0000
O	O11	1.0	0.83558	0.51050	0.06530	1.0000
O	O12	1.0	0.64697	0.48747	0.10412	1.0000
O	O13	1.0	0.97078	0.67379	0.05813	1.0000
O	O14	1.0	0.01856	0.85996	0.09878	1.0000
O	O15	1.0	0.02951	0.49259	0.10024	1.0000
O	O16	1.0	0.63441	0.32978	0.55499	1.0000
O	O17	1.0	0.68149	0.17132	0.49141	1.0000
O	O18	1.0	0.73895	0.15631	0.58838	1.0000
O	O19	1.0	0.53595	0.14286	0.56136	1.0000
O	O20	1.0	0.67087	0.50680	0.50276	1.0000
O	O21	1.0	0.77198	0.47144	0.59028	1.0000
O	O22	1.0	0.56367	0.51612	0.58623	1.0000
O	O23	1.0	0.28151	0.32845	0.56967	1.0000
O	O24	1.0	0.15292	0.15996	0.55477	1.0000
O	O25	1.0	0.33360	0.14050	0.60662	1.0000
O	O26	1.0	0.17310	0.50370	0.55297	1.0000
O	O27	1.0	0.35506	0.51500	0.60282	1.0000
O	O28	1.0	0.03903	0.33569	0.55105	1.0000
O	O29	1.0	0.95336	0.15852	0.58986	1.0000
O	O30	1.0	0.99587	0.50612	0.60581	1.0000
O	O31	1.0	0.33495	0.37759	0.31211	1.0000
O	O32	1.0	0.17136	0.33225	0.25126	1.0000
O	O33	1.0	0.20298	0.21592	0.33386	1.0000
O	O34	1.0	0.13815	0.41707	0.34100	1.0000
O	O35	1.0	0.49449	0.33819	0.24824	1.0000
O	O36	1.0	0.47722	0.22945	0.33384	1.0000
O	O37	1.0	0.53308	0.43633	0.33345	1.0000
O	O38	1.0	0.33872	0.71958	0.30975	1.0000
O	O39	1.0	0.16913	0.62562	0.34994	1.0000

O	O40	1.0	0.51420	0.83633	0.30953	1.0000
O	O41	1.0	0.51405	0.64615	0.35099	1.0000
O	O42	1.0	0.34109	0.95960	0.31084	1.0000
O	O43	1.0	0.14011	0.01962	0.35543	1.0000
O	O44	1.0	0.52588	0.02644	0.34893	1.0000
O	O45	1.0	0.67492	0.67868	0.81726	1.0000
O	O46	1.0	0.81938	0.65440	0.74197	1.0000
O	O47	1.0	0.86803	0.75983	0.82614	1.0000
O	O48	1.0	0.84056	0.54724	0.82449	1.0000
O	O49	1.0	0.52717	0.64513	0.74779	1.0000
O	O50	1.0	0.48126	0.75634	0.83068	1.0000
O	O51	1.0	0.50918	0.54837	0.83458	1.0000
O	O52	1.0	0.66206	0.32070	0.81477	1.0000
O	O53	1.0	0.79730	0.15751	0.82614	1.0000
O	O54	1.0	0.84971	0.34956	0.85696	1.0000
O	O55	1.0	0.52413	0.15938	0.81895	1.0000
O	O56	1.0	0.46708	0.34537	0.84967	1.0000
O	O57	1.0	0.65876	0.99789	0.80878	1.0000
O	O58	1.0	0.84315	0.96299	0.85207	1.0000
O	O59	1.0	0.46396	0.96618	0.84043	1.0000
O	O60	1.0	0.63080	0.65958	0.93751	1.0000
O	O61	1.0	0.66325	0.82813	0.99693	1.0000
O	O62	1.0	0.77921	0.80504	0.91456	1.0000
O	O63	1.0	0.57300	0.85372	0.90857	1.0000
O	O64	1.0	0.66779	0.50285	0.00412	1.0000
O	O65	1.0	0.76100	0.50091	0.91507	1.0000
O	O66	1.0	0.55214	0.46466	0.92375	1.0000
O	O67	1.0	0.28439	0.66436	0.93100	1.0000
O	O68	1.0	0.17101	0.83954	0.94235	1.0000
O	O69	1.0	0.36042	0.84848	0.90089	1.0000
O	O70	1.0	0.15996	0.49435	0.93811	1.0000
O	O71	1.0	0.34923	0.48189	0.89507	1.0000
O	O72	1.0	0.04093	0.66988	0.94396	1.0000
O	O73	1.0	0.98337	0.84884	0.89893	1.0000

O	O74	1.0	0.96850	0.49385	0.90071	1.0000
O	O75	1.0	0.33982	0.32157	0.43510	1.0000
O	O76	1.0	0.34606	0.17422	0.50916	1.0000
O	O77	1.0	0.22833	0.14195	0.42727	1.0000
O	O78	1.0	0.44281	0.14028	0.42396	1.0000
O	O79	1.0	0.35497	0.47359	0.50505	1.0000
O	O80	1.0	0.22834	0.49741	0.42499	1.0000
O	O81	1.0	0.43746	0.50615	0.41618	1.0000
O	O82	1.0	0.70456	0.34894	0.43864	1.0000
O	O83	1.0	0.83679	0.18636	0.42362	1.0000
O	O84	1.0	0.64016	0.17335	0.39269	1.0000
O	O85	1.0	0.83453	0.51858	0.43908	1.0000
O	O86	1.0	0.64452	0.53715	0.40430	1.0000
O	O87	1.0	0.96509	0.35162	0.44185	1.0000
O	O88	1.0	0.03462	0.18256	0.39349	1.0000
O	O89	1.0	0.02704	0.53697	0.40536	1.0000
O	O90	1.0	0.67129	0.35642	0.69664	1.0000
O	O91	1.0	0.83429	0.30906	0.75802	1.0000
O	O92	1.0	0.84509	0.25822	0.66056	1.0000
O	O93	1.0	0.49871	0.31481	0.75109	1.0000
O	O94	1.0	0.52168	0.23115	0.65872	1.0000
O	O95	1.0	0.48626	0.44053	0.67283	1.0000
O	O96	1.0	0.66812	0.71896	0.68034	1.0000
O	O97	1.0	0.83961	0.84537	0.69454	1.0000
O	O98	1.0	0.85489	0.66207	0.64445	1.0000
O	O99	1.0	0.49952	0.83148	0.70270	1.0000
O	O100	1.0	0.47737	0.64855	0.65185	1.0000
O	O101	1.0	0.66831	0.96446	0.69474	1.0000
O	O102	1.0	0.84640	0.04354	0.65551	1.0000
O	O103	1.0	0.49199	0.00254	0.64427	1.0000
O	O104	1.0	0.33878	0.69541	0.18748	1.0000
O	O105	1.0	0.17633	0.66417	0.25041	1.0000
O	O106	1.0	0.14760	0.77093	0.16609	1.0000
O	O107	1.0	0.17911	0.56083	0.16489	1.0000

O	O108	1.0	0.49815	0.66003	0.25201	1.0000
O	O109	1.0	0.53247	0.76938	0.16838	1.0000
O	O110	1.0	0.49453	0.55975	0.16593	1.0000
O	O111	1.0	0.33071	0.30332	0.18708	1.0000
O	O112	1.0	0.16935	0.16399	0.18964	1.0000
O	O113	1.0	0.14016	0.35571	0.15285	1.0000
O	O114	1.0	0.49554	0.16827	0.18849	1.0000
O	O115	1.0	0.51810	0.35481	0.14873	1.0000
O	O116	1.0	0.33384	0.03109	0.19239	1.0000
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O	O118	1.0	0.51684	0.97796	0.15055	1.0000
O	O119	1.0	0.99824	0.84186	0.99872	1.0000
O	O120	1.0	0.99586	0.50178	0.00076	1.0000
O	O121	1.0	0.98921	0.17092	0.49221	1.0000
O	O122	1.0	0.99171	0.51535	0.50475	1.0000
O	O123	1.0	0.15994	0.98724	0.24566	1.0000
O	O124	1.0	0.50565	0.00326	0.24986	1.0000
O	O125	1.0	0.83352	0.01584	0.75374	1.0000
O	O126	1.0	0.49691	0.02188	0.74441	1.0000
O	O127	1.0	0.85518	0.46014	0.68931	1.0000
O	O128	1.0	0.15742	0.82036	0.31898	1.0000
Al	Al1	1.0	0.46448	0.12894	0.62455	1.0000
Al	Al2	1.0	0.86990	0.53169	0.62604	1.0000
Al	Al3	1.0	0.20546	0.96113	0.30549	1.0000
Si	Si1	1.0	0.33224	0.78423	0.05762	1.0000
Si	Si2	1.0	0.33535	0.52895	0.05423	1.0000
Si	Si3	1.0	0.70812	0.79909	0.05285	1.0000
Si	Si4	1.0	0.71219	0.54364	0.05858	1.0000
Si	Si5	1.0	0.95458	0.80187	0.05327	1.0000
Si	Si6	1.0	0.95831	0.54501	0.05586	1.0000
Si	Si7	1.0	0.52974	0.86189	0.12517	1.0000
Si	Si8	1.0	0.65405	0.20416	0.54895	1.0000
Si	Si9	1.0	0.66318	0.45783	0.55967	1.0000
Si	Si10	1.0	0.27574	0.20020	0.56144	1.0000

Si	Si11	1.0	0.29094	0.45500	0.55803	1.0000
Si	Si12	1.0	0.03385	0.20743	0.54747	1.0000
Si	Si13	1.0	0.04911	0.46539	0.55492	1.0000
Si	Si14	1.0	0.21179	0.33439	0.30947	1.0000
Si	Si15	1.0	0.46015	0.34450	0.30707	1.0000
Si	Si16	1.0	0.46810	0.71639	0.30531	1.0000
Si	Si17	1.0	0.46757	0.95730	0.30458	1.0000
Si	Si18	1.0	0.14201	0.51615	0.38044	1.0000
Si	Si19	1.0	0.79946	0.66107	0.80294	1.0000
Si	Si20	1.0	0.54771	0.65750	0.80778	1.0000
Si	Si21	1.0	0.78524	0.28297	0.81407	1.0000
Si	Si22	1.0	0.53754	0.28496	0.80764	1.0000
Si	Si23	1.0	0.78334	0.03355	0.80974	1.0000
Si	Si24	1.0	0.53583	0.03654	0.80235	1.0000
Si	Si25	1.0	0.85378	0.47351	0.87495	1.0000
Si	Si26	1.0	0.66175	0.78635	0.93892	1.0000
Si	Si27	1.0	0.65328	0.53250	0.94498	1.0000
Si	Si28	1.0	0.28989	0.79049	0.94346	1.0000
Si	Si29	1.0	0.28221	0.53691	0.93988	1.0000
Si	Si30	1.0	0.04835	0.79918	0.94611	1.0000
Si	Si31	1.0	0.04106	0.54069	0.94618	1.0000
Si	Si32	1.0	0.47116	0.85455	0.87042	1.0000
Si	Si33	1.0	0.33776	0.19474	0.44811	1.0000
Si	Si34	1.0	0.34017	0.44952	0.44547	1.0000
Si	Si35	1.0	0.71610	0.22074	0.43646	1.0000
Si	Si36	1.0	0.71352	0.47715	0.44691	1.0000
Si	Si37	1.0	0.95747	0.22291	0.43802	1.0000
Si	Si38	1.0	0.95492	0.47959	0.44867	1.0000
Si	Si39	1.0	0.52066	0.14289	0.37450	1.0000
Si	Si40	1.0	0.54211	0.33301	0.69369	1.0000
Si	Si41	1.0	0.79605	0.72298	0.68892	1.0000
Si	Si42	1.0	0.54316	0.71167	0.69538	1.0000
Si	Si43	1.0	0.79608	0.96686	0.69925	1.0000
Si	Si44	1.0	0.53869	0.95485	0.69525	1.0000

Si	Si45	1.0	0.21134	0.67266	0.19089	1.0000
Si	Si46	1.0	0.46584	0.67102	0.19284	1.0000
Si	Si47	1.0	0.20330	0.28771	0.19537	1.0000
Si	Si48	1.0	0.45849	0.29053	0.19354	1.0000
Si	Si49	1.0	0.20463	0.03975	0.19461	1.0000
Si	Si50	1.0	0.46154	0.04448	0.19580	1.0000
Si	Si51	1.0	0.14574	0.46954	0.12404	1.0000
Si	Si52	1.0	0.13784	0.86151	0.12204	1.0000
Si	Si53	1.0	0.52589	0.47190	0.12368	1.0000
Si	Si54	1.0	0.84631	0.15361	0.62353	1.0000
Si	Si55	1.0	0.47156	0.52875	0.62849	1.0000
Si	Si56	1.0	0.15059	0.13821	0.37744	1.0000
Si	Si57	1.0	0.53124	0.53014	0.37591	1.0000
Si	Si58	1.0	0.86667	0.84441	0.87306	1.0000
Si	Si59	1.0	0.46974	0.46163	0.87609	1.0000
Si	Si60	1.0	0.79718	0.33976	0.70139	1.0000
Si	Si61	1.0	0.21367	0.70042	0.30597	1.0000

T2T7T7:

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H	H3	1.0	0.56320	0.83230	0.34753	1.0000
O	O1	1.0	0.29862	0.65762	0.06227	1.0000
O	O2	1.0	0.34495	0.81695	0.99844	1.0000
O	O3	1.0	0.23279	0.85399	0.08065	1.0000
O	O4	1.0	0.44051	0.80752	0.08590	1.0000
O	O5	1.0	0.33969	0.50399	0.99485	1.0000

O	O6	1.0	0.23371	0.45994	0.07879	1.0000
O	O7	1.0	0.44205	0.50508	0.08071	1.0000
O	O8	1.0	0.69887	0.67150	0.06382	1.0000
O	O9	1.0	0.83239	0.83689	0.05936	1.0000
O	O10	1.0	0.64214	0.86235	0.09685	1.0000
O	O11	1.0	0.83392	0.50728	0.06494	1.0000
O	O12	1.0	0.64485	0.48668	0.10423	1.0000
O	O13	1.0	0.96728	0.67206	0.05687	1.0000
O	O14	1.0	0.02344	0.85501	0.09800	1.0000
O	O15	1.0	0.02844	0.49172	0.09922	1.0000
O	O16	1.0	0.63782	0.33133	0.55260	1.0000
O	O17	1.0	0.68854	0.17037	0.49087	1.0000
O	O18	1.0	0.73898	0.15805	0.58902	1.0000
O	O19	1.0	0.53841	0.14486	0.55972	1.0000
O	O20	1.0	0.67911	0.50812	0.50066	1.0000
O	O21	1.0	0.77278	0.47261	0.59041	1.0000
O	O22	1.0	0.56400	0.51741	0.58237	1.0000
O	O23	1.0	0.28400	0.32886	0.56799	1.0000
O	O24	1.0	0.15358	0.15877	0.55814	1.0000
O	O25	1.0	0.33716	0.14296	0.60697	1.0000
O	O26	1.0	0.17214	0.50232	0.55167	1.0000
O	O27	1.0	0.35550	0.51664	0.60103	1.0000
O	O28	1.0	0.03899	0.33376	0.55386	1.0000
O	O29	1.0	0.95296	0.15578	0.59111	1.0000
O	O30	1.0	0.99872	0.50528	0.60860	1.0000
O	O31	1.0	0.34209	0.37676	0.31145	1.0000
O	O32	1.0	0.17396	0.34120	0.25198	1.0000
O	O33	1.0	0.20576	0.21869	0.33233	1.0000
O	O34	1.0	0.14706	0.42177	0.34316	1.0000
O	O35	1.0	0.49551	0.33159	0.24431	1.0000
O	O36	1.0	0.48611	0.22866	0.33172	1.0000
O	O37	1.0	0.54220	0.43543	0.32738	1.0000
O	O38	1.0	0.32938	0.72181	0.31081	1.0000
O	O39	1.0	0.14835	0.82887	0.31044	1.0000

O	O40	1.0	0.15484	0.63481	0.34719	1.0000
O	O41	1.0	0.49526	0.63260	0.35720	1.0000
O	O42	1.0	0.31806	0.95868	0.31008	1.0000
O	O43	1.0	0.13387	0.02180	0.34863	1.0000
O	O44	1.0	0.51425	0.02721	0.35720	1.0000
O	O45	1.0	0.67450	0.67837	0.81534	1.0000
O	O46	1.0	0.82199	0.65352	0.74153	1.0000
O	O47	1.0	0.86594	0.76144	0.82578	1.0000
O	O48	1.0	0.84105	0.54822	0.82481	1.0000
O	O49	1.0	0.52381	0.64556	0.74671	1.0000
O	O50	1.0	0.48289	0.75874	0.82992	1.0000
O	O51	1.0	0.50865	0.55002	0.83390	1.0000
O	O52	1.0	0.65984	0.31921	0.81347	1.0000
O	O53	1.0	0.79780	0.15860	0.82663	1.0000
O	O54	1.0	0.84516	0.35077	0.85816	1.0000
O	O55	1.0	0.51760	0.16097	0.81716	1.0000
O	O56	1.0	0.46527	0.34743	0.84829	1.0000
O	O57	1.0	0.65648	0.00204	0.80869	1.0000
O	O58	1.0	0.83931	0.96359	0.85353	1.0000
O	O59	1.0	0.46258	0.96777	0.84080	1.0000
O	O60	1.0	0.62780	0.66055	0.93768	1.0000
O	O61	1.0	0.66346	0.82768	0.99808	1.0000
O	O62	1.0	0.77844	0.80370	0.91524	1.0000
O	O63	1.0	0.57246	0.85545	0.90924	1.0000
O	O64	1.0	0.66452	0.50427	0.00441	1.0000
O	O65	1.0	0.76457	0.50628	0.91667	1.0000
O	O66	1.0	0.55561	0.46363	0.92215	1.0000
O	O67	1.0	0.28650	0.66442	0.93444	1.0000
O	O68	1.0	0.17031	0.83914	0.94142	1.0000
O	O69	1.0	0.36006	0.84666	0.90037	1.0000
O	O70	1.0	0.16192	0.49423	0.93922	1.0000
O	O71	1.0	0.35099	0.48414	0.89562	1.0000
O	O72	1.0	0.04069	0.66904	0.94330	1.0000
O	O73	1.0	0.98232	0.84827	0.89847	1.0000

O	O74	1.0	0.97136	0.49213	0.89968	1.0000
O	O75	1.0	0.30421	0.32152	0.43842	1.0000
O	O76	1.0	0.34094	0.16986	0.50845	1.0000
O	O77	1.0	0.24303	0.12428	0.42061	1.0000
O	O78	1.0	0.45329	0.17044	0.42724	1.0000
O	O79	1.0	0.35508	0.47625	0.50343	1.0000
O	O80	1.0	0.25333	0.52113	0.41715	1.0000
O	O81	1.0	0.45617	0.46427	0.41766	1.0000
O	O82	1.0	0.71166	0.34783	0.43768	1.0000
O	O83	1.0	0.84435	0.18439	0.42308	1.0000
O	O84	1.0	0.64826	0.17197	0.39151	1.0000
O	O85	1.0	0.84172	0.51712	0.43541	1.0000
O	O86	1.0	0.65074	0.53490	0.40121	1.0000
O	O87	1.0	0.97079	0.34971	0.44316	1.0000
O	O88	1.0	0.04488	0.18105	0.39585	1.0000
O	O89	1.0	0.04213	0.53560	0.41197	1.0000
O	O90	1.0	0.67286	0.35891	0.69725	1.0000
O	O91	1.0	0.83564	0.31121	0.75891	1.0000
O	O92	1.0	0.84625	0.25930	0.66129	1.0000
O	O93	1.0	0.49714	0.31764	0.74930	1.0000
O	O94	1.0	0.52742	0.23144	0.65770	1.0000
O	O95	1.0	0.48901	0.44075	0.66967	1.0000
O	O96	1.0	0.66854	0.71947	0.68115	1.0000
O	O97	1.0	0.84079	0.84532	0.69489	1.0000
O	O98	1.0	0.85461	0.66340	0.64360	1.0000
O	O99	1.0	0.49717	0.83123	0.70066	1.0000
O	O100	1.0	0.48002	0.64874	0.64964	1.0000
O	O101	1.0	0.66781	0.96200	0.69665	1.0000
O	O102	1.0	0.84401	0.04426	0.65683	1.0000
O	O103	1.0	0.49636	0.00364	0.64301	1.0000
O	O104	1.0	0.34294	0.68821	0.18808	1.0000
O	O105	1.0	0.17595	0.65988	0.24911	1.0000
O	O106	1.0	0.15621	0.77372	0.16616	1.0000
O	O107	1.0	0.17996	0.56252	0.16214	1.0000

O	O108	1.0	0.49764	0.66378	0.25686	1.0000
O	O109	1.0	0.53705	0.76634	0.17198	1.0000
O	O110	1.0	0.50538	0.55460	0.17339	1.0000
O	O111	1.0	0.32696	0.29759	0.18603	1.0000
O	O112	1.0	0.15880	0.16795	0.19377	1.0000
O	O113	1.0	0.13618	0.35688	0.15376	1.0000
O	O114	1.0	0.49158	0.16197	0.18372	1.0000
O	O115	1.0	0.50951	0.35310	0.14467	1.0000
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O	O118	1.0	0.49703	0.96903	0.14649	1.0000
O	O119	1.0	0.99803	0.84099	0.99833	1.0000
O	O120	1.0	0.99396	0.50029	0.99978	1.0000
O	O121	1.0	0.99320	0.16913	0.49373	1.0000
O	O122	1.0	0.98437	0.51168	0.50820	1.0000
O	O123	1.0	0.15130	0.99381	0.24922	1.0000
O	O124	1.0	0.49998	0.99424	0.24674	1.0000
O	O125	1.0	0.83363	0.01460	0.75499	1.0000
O	O126	1.0	0.49366	0.02016	0.74386	1.0000
O	O127	1.0	0.85638	0.46182	0.68983	1.0000
O	O128	1.0	0.50682	0.82764	0.32215	1.0000
Al	Al1	1.0	0.46863	0.13024	0.62353	1.0000
Al	Al2	1.0	0.87095	0.53233	0.62640	1.0000
Al	Al3	1.0	0.45357	0.96572	0.30637	1.0000
Si	Si1	1.0	0.32932	0.78429	0.05731	1.0000
Si	Si2	1.0	0.32898	0.53188	0.05451	1.0000
Si	Si3	1.0	0.70921	0.79915	0.05414	1.0000
Si	Si4	1.0	0.71080	0.54310	0.05892	1.0000
Si	Si5	1.0	0.95508	0.80058	0.05300	1.0000
Si	Si6	1.0	0.95622	0.54325	0.05497	1.0000
Si	Si7	1.0	0.52853	0.85265	0.12570	1.0000
Si	Si8	1.0	0.65733	0.20539	0.54779	1.0000
Si	Si9	1.0	0.66641	0.45936	0.55767	1.0000
Si	Si10	1.0	0.27649	0.20008	0.56178	1.0000

Si	Si11	1.0	0.29131	0.45563	0.55647	1.0000
Si	Si12	1.0	0.03462	0.20561	0.54962	1.0000
Si	Si13	1.0	0.04849	0.46349	0.55700	1.0000
Si	Si14	1.0	0.21690	0.33905	0.30991	1.0000
Si	Si15	1.0	0.46641	0.34157	0.30365	1.0000
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Si	Si18	1.0	0.15021	0.52637	0.37973	1.0000
Si	Si19	1.0	0.79978	0.66135	0.80244	1.0000
Si	Si20	1.0	0.54690	0.65855	0.80661	1.0000
Si	Si21	1.0	0.78387	0.28385	0.81436	1.0000
Si	Si22	1.0	0.53466	0.28618	0.80602	1.0000
Si	Si23	1.0	0.78178	0.03469	0.81055	1.0000
Si	Si24	1.0	0.53259	0.03781	0.80174	1.0000
Si	Si25	1.0	0.85440	0.47482	0.87544	1.0000
Si	Si26	1.0	0.66060	0.78686	0.93977	1.0000
Si	Si27	1.0	0.65348	0.53392	0.94502	1.0000
Si	Si28	1.0	0.29000	0.79166	0.94396	1.0000
Si	Si29	1.0	0.28439	0.53650	0.94135	1.0000
Si	Si30	1.0	0.04785	0.79836	0.94552	1.0000
Si	Si31	1.0	0.04201	0.53981	0.94578	1.0000
Si	Si32	1.0	0.47135	0.85564	0.87037	1.0000
Si	Si33	1.0	0.33455	0.19641	0.44788	1.0000
Si	Si34	1.0	0.34131	0.44628	0.44428	1.0000
Si	Si35	1.0	0.72332	0.21943	0.43568	1.0000
Si	Si36	1.0	0.72085	0.47625	0.44473	1.0000
Si	Si37	1.0	0.96422	0.22115	0.43914	1.0000
Si	Si38	1.0	0.96038	0.47769	0.45025	1.0000
Si	Si39	1.0	0.52489	0.14778	0.37643	1.0000
Si	Si40	1.0	0.54425	0.33444	0.69235	1.0000
Si	Si41	1.0	0.79682	0.72328	0.68881	1.0000
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Si	Si43	1.0	0.79570	0.96620	0.70044	1.0000
Si	Si44	1.0	0.53811	0.95430	0.69474	1.0000

Si	Si45	1.0	0.21390	0.67101	0.19067	1.0000
Si	Si46	1.0	0.46976	0.66819	0.19636	1.0000
Si	Si47	1.0	0.19975	0.29024	0.19659	1.0000
Si	Si48	1.0	0.45533	0.28459	0.18995	1.0000
Si	Si49	1.0	0.19636	0.04462	0.19699	1.0000
Si	Si50	1.0	0.45420	0.03900	0.19416	1.0000
Si	Si51	1.0	0.14442	0.46856	0.12332	1.0000
Si	Si52	1.0	0.14029	0.86566	0.12339	1.0000
Si	Si53	1.0	0.52466	0.47490	0.12568	1.0000
Si	Si54	1.0	0.84571	0.15397	0.62467	1.0000
Si	Si55	1.0	0.47335	0.52956	0.62567	1.0000
Si	Si56	1.0	0.15664	0.13670	0.37446	1.0000
Si	Si57	1.0	0.53536	0.51510	0.37575	1.0000
Si	Si58	1.0	0.86471	0.84448	0.87339	1.0000
Si	Si59	1.0	0.47054	0.46282	0.87544	1.0000
Si	Si60	1.0	0.79882	0.34166	0.70209	1.0000
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T2T7T9:

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O	O7	1.0	0.44820	0.51214	0.08128	1.0000
O	O8	1.0	0.70789	0.66937	0.06646	1.0000
O	O9	1.0	0.83528	0.83712	0.05606	1.0000
O	O10	1.0	0.64827	0.86060	0.09640	1.0000
O	O11	1.0	0.83884	0.50304	0.06546	1.0000
O	O12	1.0	0.64990	0.48767	0.10730	1.0000
O	O13	1.0	0.96737	0.67107	0.05616	1.0000
O	O14	1.0	0.02359	0.85262	0.09787	1.0000
O	O15	1.0	0.03461	0.49194	0.09752	1.0000
O	O16	1.0	0.67057	0.32666	0.56133	1.0000
O	O17	1.0	0.66748	0.17185	0.49136	1.0000
O	O18	1.0	0.74277	0.13552	0.58421	1.0000
O	O19	1.0	0.53467	0.16020	0.56600	1.0000
O	O20	1.0	0.66395	0.49296	0.49987	1.0000
O	O21	1.0	0.77122	0.50436	0.58561	1.0000
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O	O25	1.0	0.33475	0.15525	0.61077	1.0000
O	O26	1.0	0.16552	0.51029	0.55443	1.0000
O	O27	1.0	0.35159	0.52375	0.59958	1.0000
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O	O31	1.0	0.33651	0.37324	0.30867	1.0000
O	O32	1.0	0.17279	0.34249	0.24696	1.0000
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O	O34	1.0	0.14154	0.42053	0.33707	1.0000
O	O35	1.0	0.49526	0.33038	0.24532	1.0000
O	O36	1.0	0.48621	0.23129	0.33259	1.0000
O	O37	1.0	0.53251	0.44039	0.32717	1.0000
O	O38	1.0	0.32616	0.71024	0.30902	1.0000
O	O39	1.0	0.15015	0.82353	0.30611	1.0000

O	O40	1.0	0.14549	0.63277	0.34470	1.0000
O	O41	1.0	0.48982	0.83877	0.32190	1.0000
O	O42	1.0	0.49700	0.64160	0.35532	1.0000
O	O43	1.0	0.31754	0.96032	0.31093	1.0000
O	O44	1.0	0.48485	0.02984	0.36123	1.0000
O	O45	1.0	0.66528	0.68710	0.81673	1.0000
O	O46	1.0	0.81876	0.65502	0.74853	1.0000
O	O47	1.0	0.85868	0.76239	0.83166	1.0000
O	O48	1.0	0.82452	0.55330	0.83487	1.0000
O	O49	1.0	0.51925	0.64617	0.74583	1.0000
O	O50	1.0	0.47074	0.76165	0.82653	1.0000
O	O51	1.0	0.50325	0.55312	0.83330	1.0000
O	O52	1.0	0.67378	0.29464	0.81785	1.0000
O	O53	1.0	0.84011	0.16293	0.81225	1.0000
O	O54	1.0	0.86339	0.35062	0.85213	1.0000
O	O55	1.0	0.50777	0.16218	0.81261	1.0000
O	O56	1.0	0.48578	0.34793	0.85371	1.0000
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O	O58	1.0	0.85283	0.97116	0.84827	1.0000
O	O59	1.0	0.49525	0.96835	0.84627	1.0000
O	O60	1.0	0.68179	0.65426	0.93699	1.0000
O	O61	1.0	0.66017	0.81853	0.99911	1.0000
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O	O63	1.0	0.56520	0.82227	0.91141	1.0000
O	O64	1.0	0.66516	0.50308	0.00759	1.0000
O	O65	1.0	0.77232	0.46808	0.92342	1.0000
O	O66	1.0	0.55940	0.48192	0.92356	1.0000
O	O67	1.0	0.29729	0.66956	0.92743	1.0000
O	O68	1.0	0.17281	0.83835	0.93912	1.0000
O	O69	1.0	0.36063	0.85993	0.89871	1.0000
O	O70	1.0	0.16849	0.50289	0.94053	1.0000
O	O71	1.0	0.35544	0.47916	0.89690	1.0000
O	O72	1.0	0.04051	0.67124	0.94183	1.0000
O	O73	1.0	0.98390	0.85379	0.89913	1.0000

O	O74	1.0	0.97706	0.49258	0.89929	1.0000
O	O75	1.0	0.29879	0.32407	0.44107	1.0000
O	O76	1.0	0.34386	0.17732	0.51242	1.0000
O	O77	1.0	0.24955	0.12286	0.42457	1.0000
O	O78	1.0	0.45423	0.18297	0.42987	1.0000
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O	O81	1.0	0.43557	0.47709	0.41346	1.0000
O	O82	1.0	0.69294	0.33976	0.43243	1.0000
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O	O85	1.0	0.82857	0.50328	0.43687	1.0000
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O	O87	1.0	0.96619	0.34155	0.44028	1.0000
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O	O89	1.0	0.01833	0.52630	0.39996	1.0000
O	O90	1.0	0.67095	0.37657	0.68977	1.0000
O	O91	1.0	0.83103	0.33344	0.75334	1.0000
O	O92	1.0	0.81332	0.22517	0.66841	1.0000
O	O93	1.0	0.86872	0.42973	0.66764	1.0000
O	O94	1.0	0.51390	0.33587	0.75472	1.0000
O	O95	1.0	0.52524	0.23153	0.66699	1.0000
O	O96	1.0	0.47308	0.43770	0.67128	1.0000
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O	O98	1.0	0.84271	0.82971	0.69084	1.0000
O	O99	1.0	0.85793	0.64019	0.65140	1.0000
O	O100	1.0	0.50193	0.82749	0.69497	1.0000
O	O101	1.0	0.48347	0.64424	0.64768	1.0000
O	O102	1.0	0.67291	0.95431	0.69410	1.0000
O	O103	1.0	0.85143	0.02131	0.64968	1.0000
O	O104	1.0	0.49531	0.01024	0.64630	1.0000
O	O105	1.0	0.34457	0.68756	0.18888	1.0000
O	O106	1.0	0.17202	0.65522	0.24628	1.0000
O	O107	1.0	0.15962	0.76987	0.16346	1.0000

O	O108	1.0	0.18681	0.55858	0.16055	1.0000
O	O109	1.0	0.50146	0.67561	0.25664	1.0000
O	O110	1.0	0.53837	0.75898	0.16667	1.0000
O	O111	1.0	0.50580	0.55225	0.17657	1.0000
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O	O121	1.0	0.98180	0.17344	0.49949	1.0000
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O	O125	1.0	0.84516	0.00011	0.74888	1.0000
O	O126	1.0	0.50219	0.00447	0.74703	1.0000
O	O127	1.0	0.13126	0.00641	0.34953	1.0000
O	O128	1.0	0.50604	0.16850	0.18174	1.0000
Al	Al1	1.0	0.46533	0.13780	0.62934	1.0000
Al	Al2	1.0	0.15491	0.14089	0.37816	1.0000
Al	Al3	1.0	0.45587	0.03241	0.20011	1.0000
Si	Si1	1.0	0.33228	0.79243	0.05630	1.0000
Si	Si2	1.0	0.33627	0.54187	0.05397	1.0000
Si	Si3	1.0	0.71297	0.79589	0.05410	1.0000
Si	Si4	1.0	0.71603	0.54157	0.06099	1.0000
Si	Si5	1.0	0.95780	0.79941	0.05190	1.0000
Si	Si6	1.0	0.95968	0.54260	0.05401	1.0000
Si	Si7	1.0	0.53413	0.85501	0.12496	1.0000
Si	Si8	1.0	0.65916	0.20108	0.55036	1.0000
Si	Si9	1.0	0.66590	0.45663	0.55856	1.0000
Si	Si10	1.0	0.27499	0.20884	0.56417	1.0000

Si	Si11	1.0	0.28534	0.46370	0.55587	1.0000
Si	Si12	1.0	0.02984	0.21345	0.55325	1.0000
Si	Si13	1.0	0.04291	0.47068	0.55168	1.0000
Si	Si14	1.0	0.21129	0.33461	0.30586	1.0000
Si	Si15	1.0	0.46173	0.34315	0.30463	1.0000
Si	Si16	1.0	0.19915	0.70377	0.30143	1.0000
Si	Si17	1.0	0.45474	0.71708	0.31036	1.0000
Si	Si18	1.0	0.44917	0.96021	0.31241	1.0000
Si	Si19	1.0	0.13517	0.52128	0.37491	1.0000
Si	Si20	1.0	0.79161	0.66387	0.80803	1.0000
Si	Si21	1.0	0.53952	0.66182	0.80567	1.0000
Si	Si22	1.0	0.80106	0.28507	0.80842	1.0000
Si	Si23	1.0	0.54586	0.28500	0.80885	1.0000
Si	Si24	1.0	0.80220	0.04134	0.80309	1.0000
Si	Si25	1.0	0.54505	0.04144	0.80190	1.0000
Si	Si26	1.0	0.85873	0.46726	0.87758	1.0000
Si	Si27	1.0	0.67058	0.78288	0.94052	1.0000
Si	Si28	1.0	0.66936	0.52721	0.94730	1.0000
Si	Si29	1.0	0.29394	0.79549	0.94082	1.0000
Si	Si30	1.0	0.29155	0.54333	0.93986	1.0000
Si	Si31	1.0	0.05038	0.79985	0.94456	1.0000
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Si	Si33	1.0	0.47431	0.85247	0.87021	1.0000
Si	Si34	1.0	0.33372	0.20020	0.45133	1.0000
Si	Si35	1.0	0.32645	0.45088	0.44340	1.0000
Si	Si36	1.0	0.70959	0.21225	0.43614	1.0000
Si	Si37	1.0	0.70638	0.46609	0.44364	1.0000
Si	Si38	1.0	0.95456	0.21266	0.44208	1.0000
Si	Si39	1.0	0.95135	0.46881	0.44434	1.0000
Si	Si40	1.0	0.51559	0.14964	0.37828	1.0000
Si	Si41	1.0	0.79479	0.34041	0.69470	1.0000
Si	Si42	1.0	0.54484	0.34220	0.69514	1.0000
Si	Si43	1.0	0.79700	0.70885	0.69353	1.0000
Si	Si44	1.0	0.54396	0.70684	0.69266	1.0000

Si	Si45	1.0	0.80145	0.95152	0.69579	1.0000
Si	Si46	1.0	0.54284	0.95059	0.69441	1.0000
Si	Si47	1.0	0.86753	0.52442	0.62588	1.0000
Si	Si48	1.0	0.21622	0.66783	0.18899	1.0000
Si	Si49	1.0	0.47196	0.66929	0.19705	1.0000
Si	Si50	1.0	0.19900	0.28679	0.19343	1.0000
Si	Si51	1.0	0.19419	0.04588	0.19596	1.0000
Si	Si52	1.0	0.15183	0.46884	0.11999	1.0000
Si	Si53	1.0	0.14114	0.86439	0.12235	1.0000
Si	Si54	1.0	0.52809	0.48056	0.12687	1.0000
Si	Si55	1.0	0.84155	0.13895	0.62513	1.0000
Si	Si56	1.0	0.46784	0.52490	0.62624	1.0000
Si	Si57	1.0	0.52416	0.52278	0.37458	1.0000
Si	Si58	1.0	0.86640	0.85557	0.87382	1.0000
Si	Si59	1.0	0.47670	0.46628	0.87670	1.0000
Si	Si60	1.0	0.19282	0.94435	0.30073	1.0000
Si	Si61	1.0	0.45556	0.29262	0.19056	1.0000

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H	H3	1.0	0.51775	0.84244	0.03618	1.0000
O	O1	1.0	0.32318	0.67339	0.05996	1.0000
O	O2	1.0	0.33496	0.82709	0.98898	1.0000
O	O3	1.0	0.25775	0.86735	0.08152	1.0000
O	O4	1.0	0.32717	0.49759	0.00394	1.0000
O	O5	1.0	0.25453	0.48719	0.09707	1.0000

O	O6	1.0	0.45996	0.51907	0.07956	1.0000
O	O7	1.0	0.72007	0.65747	0.06110	1.0000
O	O8	1.0	0.85001	0.82493	0.05567	1.0000
O	O9	1.0	0.66638	0.83783	0.10693	1.0000
O	O10	1.0	0.84347	0.48831	0.06372	1.0000
O	O11	1.0	0.65538	0.47503	0.10326	1.0000
O	O12	1.0	0.97695	0.65588	0.05686	1.0000
O	O13	1.0	0.04744	0.83650	0.09392	1.0000
O	O14	1.0	0.04329	0.46918	0.08907	1.0000
O	O15	1.0	0.63325	0.33084	0.55284	1.0000
O	O16	1.0	0.68494	0.17259	0.49047	1.0000
O	O17	1.0	0.73966	0.15989	0.58800	1.0000
O	O18	1.0	0.53701	0.14239	0.56014	1.0000
O	O19	1.0	0.67997	0.50587	0.50027	1.0000
O	O20	1.0	0.76707	0.47174	0.59135	1.0000
O	O21	1.0	0.55910	0.51796	0.58032	1.0000
O	O22	1.0	0.28071	0.33180	0.57011	1.0000
O	O23	1.0	0.15194	0.16380	0.55463	1.0000
O	O24	1.0	0.33428	0.14428	0.60620	1.0000
O	O25	1.0	0.16793	0.50168	0.54982	1.0000
O	O26	1.0	0.35053	0.52085	0.60080	1.0000
O	O27	1.0	0.03213	0.33533	0.55615	1.0000
O	O28	1.0	0.95428	0.15460	0.59383	1.0000
O	O29	1.0	0.99380	0.51282	0.60599	1.0000
O	O30	1.0	0.33896	0.38155	0.31116	1.0000
O	O31	1.0	0.16908	0.33402	0.25364	1.0000
O	O32	1.0	0.20048	0.23023	0.33864	1.0000
O	O33	1.0	0.14405	0.43429	0.34006	1.0000
O	O34	1.0	0.49662	0.34650	0.24483	1.0000
O	O35	1.0	0.48910	0.24094	0.33200	1.0000
O	O36	1.0	0.53747	0.44862	0.32840	1.0000
O	O37	1.0	0.33032	0.71869	0.30702	1.0000
O	O38	1.0	0.15781	0.83673	0.31410	1.0000
O	O39	1.0	0.15762	0.64487	0.35130	1.0000

O	O40	1.0	0.50144	0.84151	0.31323	1.0000
O	O41	1.0	0.50258	0.65076	0.35417	1.0000
O	O42	1.0	0.32917	0.96582	0.30816	1.0000
O	O43	1.0	0.14665	0.02823	0.34866	1.0000
O	O44	1.0	0.50879	0.03452	0.34841	1.0000
O	O45	1.0	0.67336	0.62905	0.81105	1.0000
O	O46	1.0	0.82983	0.65813	0.74150	1.0000
O	O47	1.0	0.83383	0.76405	0.82847	1.0000
O	O48	1.0	0.86422	0.55226	0.82355	1.0000
O	O49	1.0	0.50881	0.64840	0.74863	1.0000
O	O50	1.0	0.53051	0.77723	0.82823	1.0000
O	O51	1.0	0.47903	0.57410	0.84131	1.0000
O	O52	1.0	0.65469	0.28842	0.80857	1.0000
O	O53	1.0	0.82057	0.16114	0.82601	1.0000
O	O54	1.0	0.82254	0.35720	0.85828	1.0000
O	O55	1.0	0.48457	0.16410	0.81644	1.0000
O	O56	1.0	0.47149	0.36194	0.84295	1.0000
O	O57	1.0	0.65329	0.03415	0.81087	1.0000
O	O58	1.0	0.82695	0.96419	0.85689	1.0000
O	O59	1.0	0.47068	0.97231	0.84995	1.0000
O	O60	1.0	0.62943	0.66001	0.94322	1.0000
O	O61	1.0	0.65792	0.82185	0.00781	1.0000
O	O62	1.0	0.77210	0.81160	0.92270	1.0000
O	O63	1.0	0.56213	0.85332	0.92129	1.0000
O	O64	1.0	0.67473	0.49383	0.00221	1.0000
O	O65	1.0	0.78192	0.52637	0.91619	1.0000
O	O66	1.0	0.57723	0.46538	0.91458	1.0000
O	O67	1.0	0.29186	0.65199	0.93883	1.0000
O	O68	1.0	0.16964	0.82187	0.92569	1.0000
O	O69	1.0	0.36407	0.81651	0.88899	1.0000
O	O70	1.0	0.16640	0.48330	0.93816	1.0000
O	O71	1.0	0.36393	0.46598	0.90763	1.0000
O	O72	1.0	0.03926	0.65439	0.93231	1.0000
O	O73	1.0	0.97217	0.83931	0.89653	1.0000

O	O74	1.0	0.98090	0.46761	0.89502	1.0000
O	O75	1.0	0.31759	0.32603	0.43514	1.0000
O	O76	1.0	0.34547	0.17954	0.50870	1.0000
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O	O78	1.0	0.44745	0.16086	0.42367	1.0000
O	O79	1.0	0.35400	0.47536	0.50395	1.0000
O	O80	1.0	0.23902	0.51760	0.42150	1.0000
O	O81	1.0	0.44807	0.49045	0.41642	1.0000
O	O82	1.0	0.67970	0.34730	0.43449	1.0000
O	O83	1.0	0.83814	0.20673	0.42286	1.0000
O	O84	1.0	0.64548	0.16260	0.39098	1.0000
O	O85	1.0	0.83681	0.49044	0.43240	1.0000
O	O86	1.0	0.64849	0.54405	0.40200	1.0000
O	O87	1.0	0.99375	0.34845	0.44090	1.0000
O	O88	1.0	0.03402	0.16672	0.39686	1.0000
O	O89	1.0	0.03094	0.54165	0.40863	1.0000
O	O90	1.0	0.67079	0.36327	0.69691	1.0000
O	O91	1.0	0.83420	0.31866	0.75884	1.0000
O	O92	1.0	0.84336	0.26111	0.66153	1.0000
O	O93	1.0	0.49176	0.31689	0.74629	1.0000
O	O94	1.0	0.52858	0.23414	0.65528	1.0000
O	O95	1.0	0.48603	0.44155	0.66796	1.0000
O	O96	1.0	0.66457	0.71822	0.68798	1.0000
O	O97	1.0	0.83594	0.84744	0.69292	1.0000
O	O98	1.0	0.84527	0.66534	0.64243	1.0000
O	O99	1.0	0.49035	0.83016	0.69924	1.0000
O	O100	1.0	0.48024	0.64833	0.64945	1.0000
O	O101	1.0	0.66152	0.96121	0.70076	1.0000
O	O102	1.0	0.83597	0.04809	0.65928	1.0000
O	O103	1.0	0.49010	0.00876	0.64782	1.0000
O	O104	1.0	0.32926	0.62475	0.19437	1.0000
O	O105	1.0	0.16042	0.67148	0.25175	1.0000
O	O106	1.0	0.18861	0.77237	0.16461	1.0000
O	O107	1.0	0.13121	0.56932	0.16726	1.0000

O	O108	1.0	0.49911	0.66941	0.25384	1.0000
O	O109	1.0	0.47494	0.76233	0.16322	1.0000
O	O110	1.0	0.52545	0.55731	0.17348	1.0000
O	O111	1.0	0.32725	0.29568	0.18983	1.0000
O	O112	1.0	0.15824	0.16604	0.19130	1.0000
O	O113	1.0	0.13987	0.35802	0.15574	1.0000
O	O114	1.0	0.49806	0.17193	0.18912	1.0000
O	O115	1.0	0.50366	0.35789	0.14387	1.0000
O	O116	1.0	0.32953	0.04138	0.19120	1.0000
O	O117	1.0	0.14827	0.97683	0.14923	1.0000
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O	O119	1.0	0.01776	0.81818	0.99511	1.0000
O	O120	1.0	0.99120	0.49336	0.99353	1.0000
O	O121	1.0	0.98108	0.17249	0.49550	1.0000
O	O122	1.0	0.97932	0.50866	0.50575	1.0000
O	O123	1.0	0.16062	0.99571	0.24907	1.0000
O	O124	1.0	0.49756	0.00298	0.24870	1.0000
O	O125	1.0	0.83058	0.00768	0.75747	1.0000
O	O126	1.0	0.48574	0.00912	0.74961	1.0000
O	O127	1.0	0.85671	0.46383	0.68856	1.0000
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Al	Al1	1.0	0.46576	0.13173	0.62381	1.0000
Al	Al2	1.0	0.86583	0.53571	0.62509	1.0000
Al	Al3	1.0	0.53748	0.85814	0.12766	1.0000
Si	Si1	1.0	0.34060	0.54427	0.06055	1.0000
Si	Si2	1.0	0.72568	0.78627	0.05986	1.0000
Si	Si3	1.0	0.72211	0.52922	0.05747	1.0000
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Si	Si5	1.0	0.96345	0.52820	0.05094	1.0000
Si	Si6	1.0	0.65485	0.20582	0.54777	1.0000
Si	Si7	1.0	0.66244	0.45848	0.55715	1.0000
Si	Si8	1.0	0.27520	0.20436	0.56127	1.0000
Si	Si9	1.0	0.28767	0.45729	0.55644	1.0000
Si	Si10	1.0	0.03045	0.20784	0.55028	1.0000

Si	Si11	1.0	0.04340	0.46486	0.55557	1.0000
Si	Si12	1.0	0.21338	0.34509	0.31115	1.0000
Si	Si13	1.0	0.46546	0.35370	0.30425	1.0000
Si	Si14	1.0	0.20169	0.71765	0.30585	1.0000
Si	Si15	1.0	0.45917	0.72000	0.30687	1.0000
Si	Si16	1.0	0.20003	0.95710	0.30469	1.0000
Si	Si17	1.0	0.45851	0.96129	0.30383	1.0000
Si	Si18	1.0	0.14435	0.53280	0.38003	1.0000
Si	Si19	1.0	0.79948	0.65348	0.80158	1.0000
Si	Si20	1.0	0.54687	0.65721	0.80701	1.0000
Si	Si21	1.0	0.78260	0.28067	0.81302	1.0000
Si	Si22	1.0	0.52582	0.28300	0.80304	1.0000
Si	Si23	1.0	0.78236	0.04075	0.81229	1.0000
Si	Si24	1.0	0.52438	0.04441	0.80563	1.0000
Si	Si25	1.0	0.86042	0.47575	0.87353	1.0000
Si	Si26	1.0	0.65686	0.78633	0.94808	1.0000
Si	Si27	1.0	0.66634	0.53579	0.94421	1.0000
Si	Si28	1.0	0.28942	0.77951	0.93541	1.0000
Si	Si29	1.0	0.28743	0.52492	0.94710	1.0000
Si	Si30	1.0	0.04831	0.78258	0.93791	1.0000
Si	Si31	1.0	0.04528	0.52642	0.94021	1.0000
Si	Si32	1.0	0.48269	0.85376	0.87207	1.0000
Si	Si33	1.0	0.33558	0.20092	0.44761	1.0000
Si	Si34	1.0	0.33945	0.45287	0.44403	1.0000
Si	Si35	1.0	0.71291	0.22314	0.43463	1.0000
Si	Si36	1.0	0.71130	0.47211	0.44304	1.0000
Si	Si37	1.0	0.96178	0.22335	0.43947	1.0000
Si	Si38	1.0	0.95983	0.47220	0.44769	1.0000
Si	Si39	1.0	0.52185	0.15086	0.37302	1.0000
Si	Si40	1.0	0.54255	0.33629	0.69024	1.0000
Si	Si41	1.0	0.79402	0.72476	0.68939	1.0000
Si	Si42	1.0	0.53632	0.71130	0.69573	1.0000
Si	Si43	1.0	0.79001	0.96623	0.70202	1.0000
Si	Si44	1.0	0.53144	0.95317	0.69812	1.0000

Si	Si45	1.0	0.20439	0.66014	0.19431	1.0000
Si	Si46	1.0	0.45725	0.65638	0.19569	1.0000
Si	Si47	1.0	0.19953	0.28757	0.19812	1.0000
Si	Si48	1.0	0.45644	0.29244	0.19208	1.0000
Si	Si49	1.0	0.20097	0.04507	0.19541	1.0000
Si	Si50	1.0	0.45982	0.04824	0.19342	1.0000
Si	Si51	1.0	0.14279	0.47172	0.12764	1.0000
Si	Si52	1.0	0.15922	0.86180	0.12280	1.0000
Si	Si53	1.0	0.53504	0.47727	0.12595	1.0000
Si	Si54	1.0	0.84365	0.15533	0.62552	1.0000
Si	Si55	1.0	0.46995	0.53107	0.62440	1.0000
Si	Si56	1.0	0.15337	0.14091	0.37739	1.0000
Si	Si57	1.0	0.53294	0.53382	0.37468	1.0000
Si	Si58	1.0	0.85057	0.84467	0.87591	1.0000
Si	Si59	1.0	0.47467	0.46796	0.87652	1.0000
Si	Si60	1.0	0.79702	0.34521	0.70144	1.0000
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O	O7	1.0	0.44298	0.48609	0.07900	1.0000
O	O8	1.0	0.69878	0.67247	0.06421	1.0000
O	O9	1.0	0.83204	0.83716	0.05916	1.0000
O	O10	1.0	0.64232	0.86423	0.09638	1.0000
O	O11	1.0	0.83342	0.50738	0.06407	1.0000
O	O12	1.0	0.64605	0.48899	0.10510	1.0000
O	O13	1.0	0.96734	0.67166	0.05761	1.0000
O	O14	1.0	0.01935	0.85376	0.10125	1.0000
O	O15	1.0	0.02793	0.48840	0.09788	1.0000
O	O16	1.0	0.63711	0.32807	0.55372	1.0000
O	O17	1.0	0.67959	0.16601	0.49070	1.0000
O	O18	1.0	0.74084	0.15454	0.58735	1.0000
O	O19	1.0	0.53568	0.14327	0.56144	1.0000
O	O20	1.0	0.68127	0.50346	0.50194	1.0000
O	O21	1.0	0.76821	0.47156	0.59308	1.0000
O	O22	1.0	0.56028	0.51469	0.58183	1.0000
O	O23	1.0	0.28074	0.33271	0.56776	1.0000
O	O24	1.0	0.15423	0.16059	0.55565	1.0000
O	O25	1.0	0.33517	0.14891	0.60848	1.0000
O	O26	1.0	0.16900	0.50533	0.55083	1.0000
O	O27	1.0	0.35262	0.51984	0.60091	1.0000
O	O28	1.0	0.03779	0.33409	0.55323	1.0000
O	O29	1.0	0.95598	0.15718	0.59309	1.0000
O	O30	1.0	0.99453	0.50821	0.60523	1.0000
O	O31	1.0	0.34089	0.37864	0.31083	1.0000
O	O32	1.0	0.17826	0.34597	0.24767	1.0000
O	O33	1.0	0.20331	0.21668	0.32619	1.0000
O	O34	1.0	0.14445	0.42029	0.33952	1.0000
O	O35	1.0	0.49766	0.33649	0.24593	1.0000
O	O36	1.0	0.48658	0.23194	0.33224	1.0000
O	O37	1.0	0.53993	0.44006	0.32944	1.0000
O	O38	1.0	0.33084	0.70932	0.31002	1.0000
O	O39	1.0	0.15498	0.82099	0.30395	1.0000

O	O40	1.0	0.15106	0.63301	0.34647	1.0000
O	O41	1.0	0.49750	0.83630	0.31567	1.0000
O	O42	1.0	0.50474	0.64335	0.35504	1.0000
O	O43	1.0	0.32332	0.95798	0.31015	1.0000
O	O44	1.0	0.49758	0.02835	0.35555	1.0000
O	O45	1.0	0.67331	0.68584	0.81579	1.0000
O	O46	1.0	0.82174	0.65525	0.74294	1.0000
O	O47	1.0	0.86824	0.76043	0.82794	1.0000
O	O48	1.0	0.83396	0.54881	0.82601	1.0000
O	O49	1.0	0.52266	0.64699	0.74753	1.0000
O	O50	1.0	0.47872	0.75892	0.83126	1.0000
O	O51	1.0	0.51173	0.55131	0.83437	1.0000
O	O52	1.0	0.66127	0.32197	0.81481	1.0000
O	O53	1.0	0.79764	0.15953	0.82695	1.0000
O	O54	1.0	0.84877	0.35156	0.85798	1.0000
O	O55	1.0	0.52102	0.16244	0.81725	1.0000
O	O56	1.0	0.46553	0.34850	0.84834	1.0000
O	O57	1.0	0.65750	0.00128	0.80946	1.0000
O	O58	1.0	0.84175	0.96453	0.85308	1.0000
O	O59	1.0	0.46375	0.96961	0.84125	1.0000
O	O60	1.0	0.63133	0.66053	0.93722	1.0000
O	O61	1.0	0.66235	0.82758	0.99819	1.0000
O	O62	1.0	0.77910	0.80748	0.91606	1.0000
O	O63	1.0	0.57275	0.85545	0.90939	1.0000
O	O64	1.0	0.66171	0.50511	0.00507	1.0000
O	O65	1.0	0.76519	0.50200	0.91857	1.0000
O	O66	1.0	0.55475	0.46459	0.92250	1.0000
O	O67	1.0	0.28479	0.66891	0.93107	1.0000
O	O68	1.0	0.17121	0.84389	0.94352	1.0000
O	O69	1.0	0.36063	0.85368	0.90220	1.0000
O	O70	1.0	0.16286	0.49749	0.93930	1.0000
O	O71	1.0	0.35074	0.48698	0.89422	1.0000
O	O72	1.0	0.04306	0.67241	0.94504	1.0000
O	O73	1.0	0.98261	0.85183	0.90086	1.0000

O	O74	1.0	0.97150	0.49817	0.89887	1.0000
O	O75	1.0	0.31112	0.32270	0.43828	1.0000
O	O76	1.0	0.34753	0.17488	0.51052	1.0000
O	O77	1.0	0.24939	0.12282	0.42342	1.0000
O	O78	1.0	0.45728	0.17108	0.42841	1.0000
O	O79	1.0	0.35158	0.48068	0.50313	1.0000
O	O80	1.0	0.23973	0.51588	0.41859	1.0000
O	O81	1.0	0.44674	0.48172	0.41608	1.0000
O	O82	1.0	0.68419	0.34252	0.43619	1.0000
O	O83	1.0	0.83592	0.19408	0.42540	1.0000
O	O84	1.0	0.64657	0.15803	0.39023	1.0000
O	O85	1.0	0.83660	0.49182	0.43354	1.0000
O	O86	1.0	0.64717	0.53841	0.40404	1.0000
O	O87	1.0	0.98672	0.34172	0.44054	1.0000
O	O88	1.0	0.02913	0.15644	0.39644	1.0000
O	O89	1.0	0.03048	0.53220	0.40640	1.0000
O	O90	1.0	0.67237	0.36357	0.69762	1.0000
O	O91	1.0	0.83443	0.31082	0.75877	1.0000
O	O92	1.0	0.84223	0.25851	0.66111	1.0000
O	O93	1.0	0.49857	0.32007	0.74992	1.0000
O	O94	1.0	0.52988	0.22955	0.65956	1.0000
O	O95	1.0	0.48565	0.43874	0.66897	1.0000
O	O96	1.0	0.66824	0.71864	0.68215	1.0000
O	O97	1.0	0.83930	0.84597	0.69566	1.0000
O	O98	1.0	0.85461	0.66304	0.64515	1.0000
O	O99	1.0	0.49755	0.83124	0.70095	1.0000
O	O100	1.0	0.48054	0.64757	0.65013	1.0000
O	O101	1.0	0.66671	0.96405	0.69547	1.0000
O	O102	1.0	0.84449	0.04348	0.65653	1.0000
O	O103	1.0	0.49065	0.00354	0.64401	1.0000
O	O104	1.0	0.34314	0.69050	0.18811	1.0000
O	O105	1.0	0.17698	0.64692	0.24739	1.0000
O	O106	1.0	0.15552	0.77267	0.16835	1.0000
O	O107	1.0	0.18362	0.56232	0.15776	1.0000

O	O108	1.0	0.50031	0.66410	0.25518	1.0000
O	O109	1.0	0.53891	0.75700	0.16769	1.0000
O	O110	1.0	0.49735	0.54904	0.17185	1.0000
O	O111	1.0	0.33417	0.29744	0.18398	1.0000
O	O112	1.0	0.16738	0.16819	0.19106	1.0000
O	O113	1.0	0.14525	0.35488	0.14873	1.0000
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O	O115	1.0	0.52118	0.34788	0.14623	1.0000
O	O116	1.0	0.33132	0.03052	0.19298	1.0000
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O	O119	1.0	0.00080	0.84294	0.00091	1.0000
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O	O125	1.0	0.83228	0.01669	0.75469	1.0000
O	O126	1.0	0.49443	0.02016	0.74454	1.0000
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O	O128	1.0	0.13587	0.00509	0.34728	1.0000
Al	Al1	1.0	0.46641	0.13121	0.62483	1.0000
Al	Al2	1.0	0.86938	0.53241	0.62663	1.0000
Al	Al3	1.0	0.15713	0.14143	0.37597	1.0000
Si	Si1	1.0	0.33216	0.78597	0.05874	1.0000
Si	Si2	1.0	0.33543	0.53111	0.05323	1.0000
Si	Si3	1.0	0.70893	0.79984	0.05403	1.0000
Si	Si4	1.0	0.71040	0.54396	0.05916	1.0000
Si	Si5	1.0	0.95462	0.80039	0.05437	1.0000
Si	Si6	1.0	0.95572	0.54269	0.05426	1.0000
Si	Si7	1.0	0.53212	0.85479	0.12745	1.0000
Si	Si8	1.0	0.65445	0.20173	0.54815	1.0000
Si	Si9	1.0	0.66424	0.45644	0.55875	1.0000
Si	Si10	1.0	0.27637	0.20370	0.56199	1.0000

Si	Si11	1.0	0.28823	0.45930	0.55592	1.0000
Si	Si12	1.0	0.03353	0.20559	0.54951	1.0000
Si	Si13	1.0	0.04598	0.46416	0.55454	1.0000
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Si	Si15	1.0	0.46571	0.34621	0.30504	1.0000
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Si	Si18	1.0	0.45387	0.95693	0.30896	1.0000
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Si	Si22	1.0	0.78482	0.28492	0.81457	1.0000
Si	Si23	1.0	0.53645	0.28803	0.80642	1.0000
Si	Si24	1.0	0.78241	0.03547	0.81054	1.0000
Si	Si25	1.0	0.53420	0.03866	0.80219	1.0000
Si	Si26	1.0	0.85375	0.47564	0.87602	1.0000
Si	Si27	1.0	0.66145	0.78756	0.93970	1.0000
Si	Si28	1.0	0.65372	0.53343	0.94545	1.0000
Si	Si29	1.0	0.29029	0.79493	0.94434	1.0000
Si	Si30	1.0	0.28503	0.54126	0.93964	1.0000
Si	Si31	1.0	0.04919	0.80190	0.94755	1.0000
Si	Si32	1.0	0.04278	0.54297	0.94559	1.0000
Si	Si33	1.0	0.47062	0.85781	0.87107	1.0000
Si	Si34	1.0	0.33824	0.19709	0.44938	1.0000
Si	Si35	1.0	0.33710	0.45012	0.44396	1.0000
Si	Si36	1.0	0.71234	0.21630	0.43579	1.0000
Si	Si37	1.0	0.71275	0.46857	0.44499	1.0000
Si	Si38	1.0	0.96062	0.21410	0.43915	1.0000
Si	Si39	1.0	0.95944	0.46744	0.44707	1.0000
Si	Si40	1.0	0.52094	0.14866	0.37617	1.0000
Si	Si41	1.0	0.54435	0.33538	0.69276	1.0000
Si	Si42	1.0	0.79635	0.72340	0.68993	1.0000
Si	Si43	1.0	0.54235	0.71142	0.69481	1.0000
Si	Si44	1.0	0.79457	0.96719	0.70014	1.0000

Si	Si45	1.0	0.53698	0.95478	0.69491	1.0000
Si	Si46	1.0	0.21529	0.66735	0.18962	1.0000
Si	Si47	1.0	0.46952	0.66465	0.19547	1.0000
Si	Si48	1.0	0.20660	0.29209	0.19359	1.0000
Si	Si49	1.0	0.46184	0.28606	0.19184	1.0000
Si	Si50	1.0	0.20346	0.04519	0.19438	1.0000
Si	Si51	1.0	0.45974	0.04077	0.19863	1.0000
Si	Si52	1.0	0.14681	0.46794	0.11926	1.0000
Si	Si53	1.0	0.13887	0.86100	0.12402	1.0000
Si	Si54	1.0	0.52630	0.46923	0.12536	1.0000
Si	Si55	1.0	0.84600	0.15314	0.62431	1.0000
Si	Si56	1.0	0.47101	0.52887	0.62545	1.0000
Si	Si57	1.0	0.53331	0.52543	0.37599	1.0000
Si	Si58	1.0	0.86611	0.84641	0.87444	1.0000
Si	Si59	1.0	0.47084	0.46442	0.87521	1.0000
Si	Si60	1.0	0.79782	0.34213	0.70197	1.0000
Si	Si61	1.0	0.19855	0.94177	0.29934	1.0000

AlSiAl-T7T7T9

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O O3 1.0 0.22449 0.84709 0.07975 1.0000
O O4 1.0 0.43470 0.82622 0.08890 1.0000
O O5 1.0 0.34100 0.51092 0.99301 1.0000

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O	O8	1.0	0.70329	0.67471	0.06452	1.0000
O	O9	1.0	0.83039	0.84397	0.05764	1.0000
O	O10	1.0	0.64117	0.86500	0.09693	1.0000
O	O11	1.0	0.83244	0.50578	0.06266	1.0000
O	O12	1.0	0.64576	0.49272	0.10630	1.0000
O	O13	1.0	0.96024	0.67470	0.05669	1.0000
O	O14	1.0	0.01803	0.85678	0.10042	1.0000
O	O15	1.0	0.02728	0.49750	0.10065	1.0000
O	O16	1.0	0.63958	0.32489	0.54965	1.0000
O	O17	1.0	0.68273	0.16526	0.48618	1.0000
O	O18	1.0	0.73567	0.14719	0.58480	1.0000
O	O19	1.0	0.53517	0.14208	0.55631	1.0000
O	O20	1.0	0.68244	0.50534	0.50230	1.0000
O	O21	1.0	0.76902	0.46616	0.59343	1.0000
O	O22	1.0	0.56118	0.50689	0.58263	1.0000
O	O23	1.0	0.28504	0.32819	0.56574	1.0000
O	O24	1.0	0.16130	0.15408	0.54876	1.0000
O	O25	1.0	0.33856	0.14153	0.60386	1.0000
O	O26	1.0	0.17023	0.50090	0.55439	1.0000
O	O27	1.0	0.35457	0.51226	0.60363	1.0000
O	O28	1.0	0.04326	0.32645	0.55222	1.0000
O	O29	1.0	0.96843	0.14275	0.58967	1.0000
O	O30	1.0	0.99633	0.49373	0.60970	1.0000
O	O31	1.0	0.34090	0.38098	0.31300	1.0000
O	O32	1.0	0.17708	0.34503	0.25050	1.0000
O	O33	1.0	0.20224	0.22291	0.33114	1.0000
O	O34	1.0	0.14506	0.42661	0.34212	1.0000
O	O35	1.0	0.49304	0.34985	0.24400	1.0000
O	O36	1.0	0.48798	0.23250	0.32593	1.0000
O	O37	1.0	0.54086	0.44150	0.33069	1.0000
O	O38	1.0	0.33103	0.71022	0.31369	1.0000
O	O39	1.0	0.15868	0.83027	0.30847	1.0000

O	O40	1.0	0.14724	0.63951	0.34755	1.0000
O	O41	1.0	0.50063	0.83677	0.31452	1.0000
O	O42	1.0	0.50721	0.64551	0.35634	1.0000
O	O43	1.0	0.32856	0.96053	0.30764	1.0000
O	O44	1.0	0.14680	0.02170	0.34866	1.0000
O	O45	1.0	0.50640	0.03022	0.35158	1.0000
O	O46	1.0	0.67032	0.68005	0.81533	1.0000
O	O47	1.0	0.82150	0.64326	0.74480	1.0000
O	O48	1.0	0.86454	0.75619	0.82797	1.0000
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O	O50	1.0	0.51702	0.64929	0.74738	1.0000
O	O51	1.0	0.47389	0.74284	0.83611	1.0000
O	O52	1.0	0.51345	0.53742	0.83036	1.0000
O	O53	1.0	0.65602	0.31274	0.81731	1.0000
O	O54	1.0	0.79823	0.15629	0.82854	1.0000
O	O55	1.0	0.83953	0.34750	0.86423	1.0000
O	O56	1.0	0.51547	0.15293	0.81890	1.0000
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O	O62	1.0	0.65845	0.82767	0.99829	1.0000
O	O63	1.0	0.77800	0.80425	0.91690	1.0000
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O	O65	1.0	0.65422	0.50788	0.00665	1.0000
O	O66	1.0	0.76508	0.50585	0.92304	1.0000
O	O67	1.0	0.55514	0.46197	0.92143	1.0000
O	O68	1.0	0.28684	0.66910	0.93153	1.0000
O	O69	1.0	0.17088	0.84295	0.94259	1.0000
O	O70	1.0	0.36119	0.85584	0.90262	1.0000
O	O71	1.0	0.16315	0.49716	0.93774	1.0000
O	O72	1.0	0.35192	0.48784	0.89363	1.0000
O	O73	1.0	0.04273	0.67092	0.94539	1.0000

O	O74	1.0	0.98196	0.84802	0.90003	1.0000
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O	O76	1.0	0.31208	0.33033	0.43737	1.0000
O	O77	1.0	0.35201	0.17504	0.50563	1.0000
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O	O89	1.0	0.03936	0.17378	0.39220	1.0000
O	O90	1.0	0.04037	0.53729	0.41302	1.0000
O	O91	1.0	0.67205	0.35506	0.70179	1.0000
O	O92	1.0	0.83411	0.31522	0.76436	1.0000
O	O93	1.0	0.84444	0.24919	0.66820	1.0000
O	O94	1.0	0.49540	0.30856	0.75045	1.0000
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O	O99	1.0	0.85747	0.65531	0.64661	1.0000
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O	O101	1.0	0.48345	0.64528	0.64909	1.0000
O	O102	1.0	0.67458	0.96317	0.69089	1.0000
O	O103	1.0	0.49946	0.00264	0.63942	1.0000
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O	O107	1.0	0.18682	0.56308	0.16107	1.0000

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O	O109	1.0	0.53763	0.76745	0.17169	1.0000
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O	O111	1.0	0.32950	0.29979	0.18403	1.0000
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O	O121	1.0	0.99054	0.16429	0.49067	1.0000
O	O122	1.0	0.98404	0.50535	0.50914	1.0000
O	O123	1.0	0.16008	0.99799	0.24904	1.0000
O	O124	1.0	0.49805	0.00110	0.25153	1.0000
O	O125	1.0	0.83465	0.01527	0.75490	1.0000
O	O126	1.0	0.50269	0.02271	0.74011	1.0000
O	O127	1.0	0.85659	0.45609	0.69253	1.0000
O	O128	1.0	0.86233	0.02063	0.65530	1.0000
Al	Al1	1.0	0.47070	0.12988	0.62024	1.0000
Al	Al2	1.0	0.87045	0.52238	0.62885	1.0000
Al	Al3	1.0	0.84990	0.15387	0.62111	1.0000
Si	Si1	1.0	0.32928	0.78673	0.05898	1.0000
Si	Si2	1.0	0.33145	0.53180	0.05344	1.0000
Si	Si3	1.0	0.70808	0.80236	0.05409	1.0000
Si	Si4	1.0	0.70996	0.54563	0.05974	1.0000
Si	Si5	1.0	0.95212	0.80394	0.05367	1.0000
Si	Si6	1.0	0.95490	0.54515	0.05529	1.0000
Si	Si7	1.0	0.53027	0.85821	0.12778	1.0000
Si	Si8	1.0	0.65645	0.19766	0.54447	1.0000
Si	Si9	1.0	0.66588	0.45229	0.55809	1.0000
Si	Si10	1.0	0.28096	0.19953	0.55800	1.0000

Si	Si11	1.0	0.29007	0.45619	0.55719	1.0000
Si	Si12	1.0	0.03946	0.19739	0.54635	1.0000
Si	Si13	1.0	0.04813	0.45609	0.55772	1.0000
Si	Si14	1.0	0.21584	0.34383	0.30942	1.0000
Si	Si15	1.0	0.46575	0.35126	0.30381	1.0000
Si	Si16	1.0	0.20380	0.70963	0.30458	1.0000
Si	Si17	1.0	0.45914	0.71363	0.31004	1.0000
Si	Si18	1.0	0.19966	0.95286	0.30340	1.0000
Si	Si19	1.0	0.45751	0.95719	0.30603	1.0000
Si	Si20	1.0	0.14704	0.53068	0.37994	1.0000
Si	Si21	1.0	0.79550	0.65632	0.80528	1.0000
Si	Si22	1.0	0.54330	0.65290	0.80733	1.0000
Si	Si23	1.0	0.78114	0.28251	0.81829	1.0000
Si	Si24	1.0	0.53156	0.27897	0.80761	1.0000
Si	Si25	1.0	0.78280	0.03312	0.81130	1.0000
Si	Si26	1.0	0.53444	0.03238	0.79951	1.0000
Si	Si27	1.0	0.85054	0.47271	0.88019	1.0000
Si	Si28	1.0	0.65881	0.78724	0.93973	1.0000
Si	Si29	1.0	0.64962	0.53418	0.94674	1.0000
Si	Si30	1.0	0.29050	0.79567	0.94451	1.0000
Si	Si31	1.0	0.28539	0.54098	0.93931	1.0000
Si	Si32	1.0	0.04902	0.80057	0.94726	1.0000
Si	Si33	1.0	0.04371	0.54133	0.94678	1.0000
Si	Si34	1.0	0.46964	0.85123	0.87033	1.0000
Si	Si35	1.0	0.33789	0.20437	0.44562	1.0000
Si	Si36	1.0	0.34188	0.45732	0.44472	1.0000
Si	Si37	1.0	0.71887	0.21845	0.43248	1.0000
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Si	Si39	1.0	0.96286	0.21829	0.43659	1.0000
Si	Si40	1.0	0.96180	0.47339	0.45049	1.0000
Si	Si41	1.0	0.52313	0.15222	0.37096	1.0000
Si	Si42	1.0	0.54439	0.33036	0.69400	1.0000
Si	Si43	1.0	0.79793	0.71182	0.69213	1.0000
Si	Si44	1.0	0.54320	0.70946	0.69435	1.0000

Si	Si45	1.0	0.54317	0.95491	0.69076	1.0000
Si	Si46	1.0	0.21447	0.67249	0.19115	1.0000
Si	Si47	1.0	0.46774	0.67098	0.19652	1.0000
Si	Si48	1.0	0.20246	0.29361	0.19502	1.0000
Si	Si49	1.0	0.45766	0.29180	0.19117	1.0000
Si	Si50	1.0	0.20115	0.04744	0.19598	1.0000
Si	Si51	1.0	0.45818	0.04560	0.19700	1.0000
Si	Si52	1.0	0.14551	0.47130	0.12185	1.0000
Si	Si53	1.0	0.13693	0.86380	0.12424	1.0000
Si	Si54	1.0	0.52426	0.47509	0.12496	1.0000
Si	Si55	1.0	0.47395	0.52363	0.62687	1.0000
Si	Si56	1.0	0.15639	0.14017	0.37354	1.0000
Si	Si57	1.0	0.53768	0.52826	0.37711	1.0000
Si	Si58	1.0	0.86449	0.84217	0.87482	1.0000
Si	Si59	1.0	0.47015	0.45833	0.87441	1.0000
Si	Si60	1.0	0.79840	0.33597	0.70593	1.0000
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O	O8	1.0	0.70068	0.67394	0.06269	1.0000
O	O9	1.0	0.83452	0.83842	0.05815	1.0000
O	O10	1.0	0.64474	0.86260	0.09756	1.0000
O	O11	1.0	0.83303	0.50790	0.06508	1.0000
O	O12	1.0	0.64419	0.49079	0.10481	1.0000
O	O13	1.0	0.96667	0.67199	0.05716	1.0000
O	O14	1.0	0.02590	0.85545	0.09635	1.0000
O	O15	1.0	0.02640	0.49445	0.10233	1.0000
O	O16	1.0	0.63372	0.33625	0.55039	1.0000
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O	O20	1.0	0.68487	0.51072	0.49874	1.0000
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O	O27	1.0	0.35592	0.51772	0.59848	1.0000
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O	O31	1.0	0.34202	0.37577	0.31076	1.0000
O	O32	1.0	0.17409	0.33683	0.25165	1.0000
O	O33	1.0	0.20595	0.21855	0.33332	1.0000
O	O34	1.0	0.14680	0.42182	0.34159	1.0000
O	O35	1.0	0.49568	0.32803	0.24418	1.0000
O	O36	1.0	0.48590	0.22914	0.33234	1.0000
O	O37	1.0	0.54223	0.43576	0.32583	1.0000
O	O38	1.0	0.32935	0.72260	0.31088	1.0000

O	O39	1.0	0.14837	0.82923	0.31105	1.0000
O	O40	1.0	0.15471	0.63422	0.34680	1.0000
O	O41	1.0	0.49374	0.63085	0.35739	1.0000
O	O42	1.0	0.31884	0.95840	0.31007	1.0000
O	O43	1.0	0.13423	0.02152	0.34857	1.0000
O	O44	1.0	0.51543	0.02745	0.35670	1.0000
O	O45	1.0	0.67515	0.66663	0.81426	1.0000
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O	O47	1.0	0.85704	0.77194	0.82409	1.0000
O	O48	1.0	0.85333	0.55844	0.82672	1.0000
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O	O50	1.0	0.49151	0.76457	0.82782	1.0000
O	O51	1.0	0.49935	0.55555	0.83427	1.0000
O	O52	1.0	0.65525	0.28559	0.81191	1.0000
O	O53	1.0	0.82709	0.36389	0.86041	1.0000
O	O54	1.0	0.47842	0.16420	0.80952	1.0000
O	O55	1.0	0.47188	0.35028	0.84856	1.0000
O	O56	1.0	0.64807	0.03932	0.80844	1.0000
O	O57	1.0	0.83495	0.96613	0.86190	1.0000
O	O58	1.0	0.46074	0.97003	0.84093	1.0000
O	O59	1.0	0.61773	0.66617	0.94065	1.0000
O	O60	1.0	0.66309	0.83320	0.99848	1.0000
O	O61	1.0	0.78066	0.79404	0.91739	1.0000
O	O62	1.0	0.57820	0.86085	0.90771	1.0000
O	O63	1.0	0.66298	0.50666	0.00480	1.0000
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O	O67	1.0	0.17294	0.83351	0.93967	1.0000
O	O68	1.0	0.36575	0.84068	0.90016	1.0000
O	O69	1.0	0.16338	0.48973	0.94077	1.0000
O	O70	1.0	0.35229	0.47717	0.89794	1.0000
O	O71	1.0	0.04315	0.66386	0.94422	1.0000
O	O72	1.0	0.98361	0.83948	0.89727	1.0000

O	O73	1.0	0.97092	0.48503	0.90312	1.0000
O	O74	1.0	0.30508	0.31894	0.43751	1.0000
O	O75	1.0	0.34133	0.16965	0.50876	1.0000
O	O76	1.0	0.24258	0.12227	0.42122	1.0000
O	O77	1.0	0.45312	0.16736	0.42730	1.0000
O	O78	1.0	0.35575	0.47358	0.50184	1.0000
O	O79	1.0	0.25817	0.51844	0.41444	1.0000
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O	O87	1.0	0.04426	0.17843	0.39611	1.0000
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O	O107	1.0	0.49850	0.66516	0.25742	1.0000
O	O108	1.0	0.53814	0.76535	0.17182	1.0000
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O	O115	1.0	0.32535	0.03353	0.19418	1.0000
O	O116	1.0	0.14541	0.97947	0.14946	1.0000
O	O117	1.0	0.49746	0.96753	0.14653	1.0000
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Al	Al3	1.0	0.45466	0.96517	0.30631	1.0000
Al	Al4	1.0	0.78337	0.03230	0.81053	1.0000
Si	Si1	1.0	0.33108	0.78377	0.05720	1.0000
Si	Si2	1.0	0.32783	0.53280	0.05589	1.0000
Si	Si3	1.0	0.71062	0.80164	0.05384	1.0000
Si	Si4	1.0	0.71032	0.54571	0.05910	1.0000
Si	Si5	1.0	0.95676	0.80011	0.05200	1.0000
Si	Si6	1.0	0.95618	0.54363	0.05669	1.0000
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Si	Si9	1.0	0.66712	0.46274	0.55559	1.0000
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Si	Si26	1.0	0.29316	0.78694	0.94311	1.0000
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Si	Si38	1.0	0.54507	0.33698	0.69136	1.0000
Si	Si39	1.0	0.79816	0.72303	0.68783	1.0000
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Si	Si41	1.0	0.79683	0.96555	0.70009	1.0000
Si	Si42	1.0	0.53858	0.95181	0.69429	1.0000

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Si	Si45	1.0	0.19997	0.28780	0.19609	1.0000
Si	Si46	1.0	0.45596	0.28302	0.18954	1.0000
Si	Si47	1.0	0.19699	0.04297	0.19693	1.0000
Si	Si48	1.0	0.45527	0.03802	0.19397	1.0000
Si	Si49	1.0	0.14353	0.46836	0.12478	1.0000
Si	Si50	1.0	0.14207	0.86440	0.12268	1.0000
Si	Si51	1.0	0.52461	0.47600	0.12697	1.0000
Si	Si52	1.0	0.84483	0.15475	0.62491	1.0000
Si	Si53	1.0	0.47455	0.53122	0.62243	1.0000
Si	Si54	1.0	0.15660	0.13542	0.37491	1.0000
Si	Si55	1.0	0.53636	0.51359	0.37470	1.0000
Si	Si56	1.0	0.86252	0.84549	0.87531	1.0000
Si	Si57	1.0	0.47155	0.46469	0.87558	1.0000
Si	Si58	1.0	0.79997	0.34261	0.70194	1.0000
Si	Si59	1.0	0.45470	0.70412	0.31130	1.0000
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H H3 1.0 0.52152 0.84307 0.03330 1.0000
H H4 1.0 0.10696 0.82440 0.35239 1.0000
O O1 1.0 0.32897 0.67252 0.05766 1.0000
O O2 1.0 0.33378 0.82652 0.98670 1.0000
O O3 1.0 0.26100 0.86522 0.08003 1.0000
O O4 1.0 0.31658 0.49100 0.00627 1.0000

O	O5	1.0	0.25456	0.49377	0.10100	1.0000
O	O6	1.0	0.45951	0.51376	0.07758	1.0000
O	O7	1.0	0.72165	0.65739	0.06197	1.0000
O	O8	1.0	0.85152	0.82526	0.05431	1.0000
O	O9	1.0	0.66702	0.83939	0.10566	1.0000
O	O10	1.0	0.84494	0.48795	0.06379	1.0000
O	O11	1.0	0.65518	0.47378	0.10320	1.0000
O	O12	1.0	0.97749	0.65595	0.05341	1.0000
O	O13	1.0	0.05005	0.83634	0.09010	1.0000
O	O14	1.0	0.04306	0.47484	0.09258	1.0000
O	O15	1.0	0.62768	0.33495	0.55426	1.0000
O	O16	1.0	0.67814	0.17839	0.49150	1.0000
O	O17	1.0	0.73567	0.16360	0.58856	1.0000
O	O18	1.0	0.53305	0.14445	0.56154	1.0000
O	O19	1.0	0.66929	0.51237	0.50116	1.0000
O	O20	1.0	0.77045	0.47192	0.58846	1.0000
O	O21	1.0	0.56328	0.52357	0.58480	1.0000
O	O22	1.0	0.28240	0.33091	0.57036	1.0000
O	O23	1.0	0.15001	0.16659	0.55487	1.0000
O	O24	1.0	0.33048	0.14266	0.60763	1.0000
O	O25	1.0	0.17217	0.50423	0.55132	1.0000
O	O26	1.0	0.35307	0.52028	0.60130	1.0000
O	O27	1.0	0.03259	0.34081	0.55408	1.0000
O	O28	1.0	0.95058	0.15992	0.59152	1.0000
O	O29	1.0	0.99404	0.51787	0.60424	1.0000
O	O30	1.0	0.33257	0.38442	0.30958	1.0000
O	O31	1.0	0.16360	0.32657	0.25357	1.0000
O	O32	1.0	0.20677	0.22210	0.33816	1.0000
O	O33	1.0	0.13609	0.42188	0.34057	1.0000
O	O34	1.0	0.49425	0.34439	0.24628	1.0000
O	O35	1.0	0.47410	0.23874	0.33401	1.0000
O	O36	1.0	0.53181	0.44417	0.33069	1.0000
O	O37	1.0	0.33762	0.73062	0.30367	1.0000
O	O38	1.0	0.18067	0.62776	0.35158	1.0000

O	O39	1.0	0.51434	0.84421	0.31191	1.0000
O	O40	1.0	0.50679	0.65128	0.34975	1.0000
O	O41	1.0	0.34173	0.96925	0.31338	1.0000
O	O42	1.0	0.13809	0.02538	0.35660	1.0000
O	O43	1.0	0.53061	0.03753	0.34453	1.0000
O	O44	1.0	0.67463	0.61961	0.81019	1.0000
O	O45	1.0	0.83030	0.65588	0.74072	1.0000
O	O46	1.0	0.82687	0.76565	0.82615	1.0000
O	O47	1.0	0.86977	0.55573	0.82480	1.0000
O	O48	1.0	0.50743	0.64743	0.75070	1.0000
O	O49	1.0	0.53966	0.77390	0.82989	1.0000
O	O50	1.0	0.47935	0.57255	0.84361	1.0000
O	O51	1.0	0.65488	0.28738	0.80774	1.0000
O	O52	1.0	0.82197	0.16231	0.82478	1.0000
O	O53	1.0	0.82034	0.35898	0.85723	1.0000
O	O54	1.0	0.48586	0.16226	0.81857	1.0000
O	O55	1.0	0.47329	0.36049	0.84428	1.0000
O	O56	1.0	0.65502	0.03292	0.81172	1.0000
O	O57	1.0	0.83219	0.96481	0.85532	1.0000
O	O58	1.0	0.47105	0.96763	0.84915	1.0000
O	O59	1.0	0.63038	0.65957	0.94276	1.0000
O	O60	1.0	0.65996	0.82082	0.00713	1.0000
O	O61	1.0	0.77232	0.81285	0.92126	1.0000
O	O62	1.0	0.56162	0.85310	0.92217	1.0000
O	O63	1.0	0.67669	0.49456	0.00271	1.0000
O	O64	1.0	0.78341	0.52708	0.91640	1.0000
O	O65	1.0	0.58005	0.46303	0.91559	1.0000
O	O66	1.0	0.29351	0.64676	0.94043	1.0000
O	O67	1.0	0.17028	0.81441	0.92270	1.0000
O	O68	1.0	0.36665	0.80781	0.88744	1.0000
O	O69	1.0	0.16686	0.47853	0.93551	1.0000
O	O70	1.0	0.36765	0.46058	0.91103	1.0000
O	O71	1.0	0.03773	0.64868	0.93326	1.0000
O	O72	1.0	0.97268	0.83077	0.89279	1.0000

O	O73	1.0	0.97936	0.46157	0.89671	1.0000
O	O74	1.0	0.34224	0.32096	0.43537	1.0000
O	O75	1.0	0.34637	0.17531	0.51009	1.0000
O	O76	1.0	0.22437	0.14303	0.43061	1.0000
O	O77	1.0	0.43895	0.13829	0.42227	1.0000
O	O78	1.0	0.35662	0.47366	0.50439	1.0000
O	O79	1.0	0.22595	0.49278	0.42596	1.0000
O	O80	1.0	0.43591	0.50678	0.41457	1.0000
O	O81	1.0	0.70224	0.35600	0.43774	1.0000
O	O82	1.0	0.83406	0.19374	0.42378	1.0000
O	O83	1.0	0.63681	0.18179	0.39275	1.0000
O	O84	1.0	0.83370	0.52464	0.43711	1.0000
O	O85	1.0	0.64262	0.54380	0.40224	1.0000
O	O86	1.0	0.96486	0.35790	0.44061	1.0000
O	O87	1.0	0.03270	0.18633	0.39486	1.0000
O	O88	1.0	0.02802	0.54430	0.40448	1.0000
O	O89	1.0	0.66921	0.36239	0.69665	1.0000
O	O90	1.0	0.83415	0.32180	0.75805	1.0000
O	O91	1.0	0.84252	0.26187	0.66136	1.0000
O	O92	1.0	0.49044	0.31493	0.74754	1.0000
O	O93	1.0	0.52442	0.23440	0.65625	1.0000
O	O94	1.0	0.48372	0.44202	0.67028	1.0000
O	O95	1.0	0.66300	0.71788	0.68948	1.0000
O	O96	1.0	0.83503	0.84762	0.69285	1.0000
O	O97	1.0	0.84171	0.66644	0.64155	1.0000
O	O98	1.0	0.49012	0.83104	0.70203	1.0000
O	O99	1.0	0.47628	0.64987	0.65218	1.0000
O	O100	1.0	0.66162	0.96240	0.69989	1.0000
O	O101	1.0	0.83616	0.04857	0.65758	1.0000
O	O102	1.0	0.48813	0.00798	0.64842	1.0000
O	O103	1.0	0.32927	0.62766	0.19613	1.0000
O	O104	1.0	0.16220	0.68032	0.25277	1.0000
O	O105	1.0	0.18490	0.76658	0.16125	1.0000
O	O106	1.0	0.13130	0.56292	0.17371	1.0000

O	O107	1.0	0.50402	0.67555	0.25016	1.0000
O	O108	1.0	0.47064	0.76524	0.15926	1.0000
O	O109	1.0	0.52333	0.56100	0.17063	1.0000
O	O110	1.0	0.32546	0.29416	0.19135	1.0000
O	O111	1.0	0.15782	0.16020	0.19083	1.0000
O	O112	1.0	0.13955	0.35399	0.15554	1.0000
O	O113	1.0	0.49744	0.17223	0.18893	1.0000
O	O114	1.0	0.50194	0.35924	0.14536	1.0000
O	O115	1.0	0.32997	0.03949	0.18980	1.0000
O	O116	1.0	0.15046	0.97385	0.14699	1.0000
O	O117	1.0	0.51261	0.98696	0.14539	1.0000
O	O118	1.0	0.01634	0.81896	0.99154	1.0000
O	O119	1.0	0.99828	0.48613	0.99566	1.0000
O	O120	1.0	0.98424	0.17927	0.49363	1.0000
O	O121	1.0	0.98970	0.51878	0.50373	1.0000
O	O122	1.0	0.16140	0.98363	0.24712	1.0000
O	O123	1.0	0.50075	0.00065	0.24615	1.0000
O	O124	1.0	0.83038	0.01012	0.75600	1.0000
O	O125	1.0	0.48803	0.01258	0.74984	1.0000
O	O126	1.0	0.85497	0.46532	0.68684	1.0000
O	O127	1.0	0.46752	0.84223	0.06099	1.0000
O	O128	1.0	0.15897	0.82587	0.32486	1.0000
Al	Al1	1.0	0.46221	0.13152	0.62504	1.0000
Al	Al2	1.0	0.86561	0.53775	0.62354	1.0000
Al	Al3	1.0	0.53707	0.86176	0.12477	1.0000
Al	Al4	1.0	0.20570	0.96541	0.30781	1.0000
Si	Si1	1.0	0.33952	0.54283	0.06095	1.0000
Si	Si2	1.0	0.72721	0.78641	0.05937	1.0000
Si	Si3	1.0	0.72365	0.52903	0.05792	1.0000
Si	Si4	1.0	0.97327	0.78424	0.04764	1.0000
Si	Si5	1.0	0.96568	0.52751	0.05144	1.0000
Si	Si6	1.0	0.64982	0.20986	0.54903	1.0000
Si	Si7	1.0	0.66066	0.46201	0.55802	1.0000
Si	Si8	1.0	0.27425	0.20322	0.56200	1.0000

Si	Si9	1.0	0.29053	0.45691	0.55722	1.0000
Si	Si10	1.0	0.02991	0.21302	0.54886	1.0000
Si	Si11	1.0	0.04649	0.47029	0.55446	1.0000
Si	Si12	1.0	0.21000	0.33759	0.31040	1.0000
Si	Si13	1.0	0.45855	0.35180	0.30512	1.0000
Si	Si14	1.0	0.46799	0.72563	0.30363	1.0000
Si	Si15	1.0	0.46781	0.96416	0.30330	1.0000
Si	Si16	1.0	0.14364	0.51881	0.38050	1.0000
Si	Si17	1.0	0.79975	0.65156	0.80094	1.0000
Si	Si18	1.0	0.54918	0.65336	0.80842	1.0000
Si	Si19	1.0	0.78269	0.28180	0.81214	1.0000
Si	Si20	1.0	0.52589	0.28158	0.80409	1.0000
Si	Si21	1.0	0.78425	0.04143	0.81143	1.0000
Si	Si22	1.0	0.52611	0.04344	0.80628	1.0000
Si	Si23	1.0	0.86112	0.47578	0.87378	1.0000
Si	Si24	1.0	0.65794	0.78615	0.94758	1.0000
Si	Si25	1.0	0.66797	0.53549	0.94463	1.0000
Si	Si26	1.0	0.29010	0.77403	0.93410	1.0000
Si	Si27	1.0	0.28650	0.51937	0.94824	1.0000
Si	Si28	1.0	0.04808	0.77744	0.93551	1.0000
Si	Si29	1.0	0.04589	0.52045	0.94088	1.0000
Si	Si30	1.0	0.48517	0.84971	0.87211	1.0000
Si	Si31	1.0	0.33699	0.19441	0.44861	1.0000
Si	Si32	1.0	0.34036	0.44839	0.44504	1.0000
Si	Si33	1.0	0.71296	0.22822	0.43624	1.0000
Si	Si34	1.0	0.71169	0.48379	0.44503	1.0000
Si	Si35	1.0	0.95502	0.22944	0.43852	1.0000
Si	Si36	1.0	0.95403	0.48530	0.44732	1.0000
Si	Si37	1.0	0.51874	0.14928	0.37298	1.0000
Si	Si38	1.0	0.54043	0.33566	0.69133	1.0000
Si	Si39	1.0	0.79261	0.72469	0.68928	1.0000
Si	Si40	1.0	0.53465	0.71176	0.69795	1.0000
Si	Si41	1.0	0.79008	0.96720	0.70104	1.0000
Si	Si42	1.0	0.53153	0.95420	0.69879	1.0000

Si	Si43	1.0	0.20422	0.66043	0.19489	1.0000
Si	Si44	1.0	0.45706	0.66036	0.19319	1.0000
Si	Si45	1.0	0.19743	0.28179	0.19810	1.0000
Si	Si46	1.0	0.45469	0.29173	0.19318	1.0000
Si	Si47	1.0	0.20077	0.03835	0.19512	1.0000
Si	Si48	1.0	0.45983	0.04763	0.19196	1.0000
Si	Si49	1.0	0.14253	0.47154	0.13081	1.0000
Si	Si50	1.0	0.16041	0.86000	0.12025	1.0000
Si	Si51	1.0	0.53395	0.47691	0.12508	1.0000
Si	Si52	1.0	0.84154	0.15777	0.62456	1.0000
Si	Si53	1.0	0.46987	0.53276	0.62695	1.0000
Si	Si54	1.0	0.14944	0.14199	0.37973	1.0000
Si	Si55	1.0	0.52883	0.53546	0.37382	1.0000
Si	Si56	1.0	0.85066	0.84352	0.87381	1.0000
Si	Si57	1.0	0.47656	0.46520	0.87848	1.0000
Si	Si58	1.0	0.79581	0.34634	0.70071	1.0000
Si	Si59	1.0	0.34281	0.79851	0.04639	1.0000
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T2T2T7T7:

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H	H2	1.0	0.85694	0.51818	0.71456	1.0000
H	H3	1.0	0.52152	0.84307	0.03330	1.0000
H	H4	1.0	0.10696	0.82440	0.35239	1.0000
O	O1	1.0	0.32897	0.67252	0.05766	1.0000
O	O2	1.0	0.33378	0.82652	0.98670	1.0000
O	O3	1.0	0.26100	0.86522	0.08003	1.0000
O	O4	1.0	0.31658	0.49100	0.00627	1.0000

O	O5	1.0	0.25456	0.49377	0.10100	1.0000
O	O6	1.0	0.45951	0.51376	0.07758	1.0000
O	O7	1.0	0.72165	0.65739	0.06197	1.0000
O	O8	1.0	0.85152	0.82526	0.05431	1.0000
O	O9	1.0	0.66702	0.83939	0.10566	1.0000
O	O10	1.0	0.84494	0.48795	0.06379	1.0000
O	O11	1.0	0.65518	0.47378	0.10320	1.0000
O	O12	1.0	0.97749	0.65595	0.05341	1.0000
O	O13	1.0	0.05005	0.83634	0.09010	1.0000
O	O14	1.0	0.04306	0.47484	0.09258	1.0000
O	O15	1.0	0.62768	0.33495	0.55426	1.0000
O	O16	1.0	0.67814	0.17839	0.49150	1.0000
O	O17	1.0	0.73567	0.16360	0.58856	1.0000
O	O18	1.0	0.53305	0.14445	0.56154	1.0000
O	O19	1.0	0.66929	0.51237	0.50116	1.0000
O	O20	1.0	0.77045	0.47192	0.58846	1.0000
O	O21	1.0	0.56328	0.52357	0.58480	1.0000
O	O22	1.0	0.28240	0.33091	0.57036	1.0000
O	O23	1.0	0.15001	0.16659	0.55487	1.0000
O	O24	1.0	0.33048	0.14266	0.60763	1.0000
O	O25	1.0	0.17217	0.50423	0.55132	1.0000
O	O26	1.0	0.35307	0.52028	0.60130	1.0000
O	O27	1.0	0.03259	0.34081	0.55408	1.0000
O	O28	1.0	0.95058	0.15992	0.59152	1.0000
O	O29	1.0	0.99404	0.51787	0.60424	1.0000
O	O30	1.0	0.33257	0.38442	0.30958	1.0000
O	O31	1.0	0.16360	0.32657	0.25357	1.0000
O	O32	1.0	0.20677	0.22210	0.33816	1.0000
O	O33	1.0	0.13609	0.42188	0.34057	1.0000
O	O34	1.0	0.49425	0.34439	0.24628	1.0000
O	O35	1.0	0.47410	0.23874	0.33401	1.0000
O	O36	1.0	0.53181	0.44417	0.33069	1.0000
O	O37	1.0	0.33762	0.73062	0.30367	1.0000
O	O38	1.0	0.18067	0.62776	0.35158	1.0000

O	O39	1.0	0.51434	0.84421	0.31191	1.0000
O	O40	1.0	0.50679	0.65128	0.34975	1.0000
O	O41	1.0	0.34173	0.96925	0.31338	1.0000
O	O42	1.0	0.13809	0.02538	0.35660	1.0000
O	O43	1.0	0.53061	0.03753	0.34453	1.0000
O	O44	1.0	0.67463	0.61961	0.81019	1.0000
O	O45	1.0	0.83030	0.65588	0.74072	1.0000
O	O46	1.0	0.82687	0.76565	0.82615	1.0000
O	O47	1.0	0.86977	0.55573	0.82480	1.0000
O	O48	1.0	0.50743	0.64743	0.75070	1.0000
O	O49	1.0	0.53966	0.77390	0.82989	1.0000
O	O50	1.0	0.47935	0.57255	0.84361	1.0000
O	O51	1.0	0.65488	0.28738	0.80774	1.0000
O	O52	1.0	0.82197	0.16231	0.82478	1.0000
O	O53	1.0	0.82034	0.35898	0.85723	1.0000
O	O54	1.0	0.48586	0.16226	0.81857	1.0000
O	O55	1.0	0.47329	0.36049	0.84428	1.0000
O	O56	1.0	0.65502	0.03292	0.81172	1.0000
O	O57	1.0	0.83219	0.96481	0.85532	1.0000
O	O58	1.0	0.47105	0.96763	0.84915	1.0000
O	O59	1.0	0.63038	0.65957	0.94276	1.0000
O	O60	1.0	0.65996	0.82082	0.00713	1.0000
O	O61	1.0	0.77232	0.81285	0.92126	1.0000
O	O62	1.0	0.56162	0.85310	0.92217	1.0000
O	O63	1.0	0.67669	0.49456	0.00271	1.0000
O	O64	1.0	0.78341	0.52708	0.91640	1.0000
O	O65	1.0	0.58005	0.46303	0.91559	1.0000
O	O66	1.0	0.29351	0.64676	0.94043	1.0000
O	O67	1.0	0.17028	0.81441	0.92270	1.0000
O	O68	1.0	0.36665	0.80781	0.88744	1.0000
O	O69	1.0	0.16686	0.47853	0.93551	1.0000
O	O70	1.0	0.36765	0.46058	0.91103	1.0000
O	O71	1.0	0.03773	0.64868	0.93326	1.0000
O	O72	1.0	0.97268	0.83077	0.89279	1.0000

O	O73	1.0	0.97936	0.46157	0.89671	1.0000
O	O74	1.0	0.34224	0.32096	0.43537	1.0000
O	O75	1.0	0.34637	0.17531	0.51009	1.0000
O	O76	1.0	0.22437	0.14303	0.43061	1.0000
O	O77	1.0	0.43895	0.13829	0.42227	1.0000
O	O78	1.0	0.35662	0.47366	0.50439	1.0000
O	O79	1.0	0.22595	0.49278	0.42596	1.0000
O	O80	1.0	0.43591	0.50678	0.41457	1.0000
O	O81	1.0	0.70224	0.35600	0.43774	1.0000
O	O82	1.0	0.83406	0.19374	0.42378	1.0000
O	O83	1.0	0.63681	0.18179	0.39275	1.0000
O	O84	1.0	0.83370	0.52464	0.43711	1.0000
O	O85	1.0	0.64262	0.54380	0.40224	1.0000
O	O86	1.0	0.96486	0.35790	0.44061	1.0000
O	O87	1.0	0.03270	0.18633	0.39486	1.0000
O	O88	1.0	0.02802	0.54430	0.40448	1.0000
O	O89	1.0	0.66921	0.36239	0.69665	1.0000
O	O90	1.0	0.83415	0.32180	0.75805	1.0000
O	O91	1.0	0.84252	0.26187	0.66136	1.0000
O	O92	1.0	0.49044	0.31493	0.74754	1.0000
O	O93	1.0	0.52442	0.23440	0.65625	1.0000
O	O94	1.0	0.48372	0.44202	0.67028	1.0000
O	O95	1.0	0.66300	0.71788	0.68948	1.0000
O	O96	1.0	0.83503	0.84762	0.69285	1.0000
O	O97	1.0	0.84171	0.66644	0.64155	1.0000
O	O98	1.0	0.49012	0.83104	0.70203	1.0000
O	O99	1.0	0.47628	0.64987	0.65218	1.0000
O	O100	1.0	0.66162	0.96240	0.69989	1.0000
O	O101	1.0	0.83616	0.04857	0.65758	1.0000
O	O102	1.0	0.48813	0.00798	0.64842	1.0000
O	O103	1.0	0.32927	0.62766	0.19613	1.0000
O	O104	1.0	0.16220	0.68032	0.25277	1.0000
O	O105	1.0	0.18490	0.76658	0.16125	1.0000
O	O106	1.0	0.13130	0.56292	0.17371	1.0000

O	O107	1.0	0.50402	0.67555	0.25016	1.0000
O	O108	1.0	0.47064	0.76524	0.15926	1.0000
O	O109	1.0	0.52333	0.56100	0.17063	1.0000
O	O110	1.0	0.32546	0.29416	0.19135	1.0000
O	O111	1.0	0.15782	0.16020	0.19083	1.0000
O	O112	1.0	0.13955	0.35399	0.15554	1.0000
O	O113	1.0	0.49744	0.17223	0.18893	1.0000
O	O114	1.0	0.50194	0.35924	0.14536	1.0000
O	O115	1.0	0.32997	0.03949	0.18980	1.0000
O	O116	1.0	0.15046	0.97385	0.14699	1.0000
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O	O118	1.0	0.01634	0.81896	0.99154	1.0000
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O	O121	1.0	0.98970	0.51878	0.50373	1.0000
O	O122	1.0	0.16140	0.98363	0.24712	1.0000
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O	O124	1.0	0.83038	0.01012	0.75600	1.0000
O	O125	1.0	0.48803	0.01258	0.74984	1.0000
O	O126	1.0	0.85497	0.46532	0.68684	1.0000
O	O127	1.0	0.46752	0.84223	0.06099	1.0000
O	O128	1.0	0.15897	0.82587	0.32486	1.0000
Al	Al1	1.0	0.46221	0.13152	0.62504	1.0000
Al	Al2	1.0	0.86561	0.53775	0.62354	1.0000
Al	Al3	1.0	0.53707	0.86176	0.12477	1.0000
Al	Al4	1.0	0.20570	0.96541	0.30781	1.0000
Si	Si1	1.0	0.33952	0.54283	0.06095	1.0000
Si	Si2	1.0	0.72721	0.78641	0.05937	1.0000
Si	Si3	1.0	0.72365	0.52903	0.05792	1.0000
Si	Si4	1.0	0.97327	0.78424	0.04764	1.0000
Si	Si5	1.0	0.96568	0.52751	0.05144	1.0000
Si	Si6	1.0	0.64982	0.20986	0.54903	1.0000
Si	Si7	1.0	0.66066	0.46201	0.55802	1.0000
Si	Si8	1.0	0.27425	0.20322	0.56200	1.0000

Si	Si9	1.0	0.29053	0.45691	0.55722	1.0000
Si	Si10	1.0	0.02991	0.21302	0.54886	1.0000
Si	Si11	1.0	0.04649	0.47029	0.55446	1.0000
Si	Si12	1.0	0.21000	0.33759	0.31040	1.0000
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Si	Si14	1.0	0.46799	0.72563	0.30363	1.0000
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Si	Si21	1.0	0.78425	0.04143	0.81143	1.0000
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Si	Si23	1.0	0.86112	0.47578	0.87378	1.0000
Si	Si24	1.0	0.65794	0.78615	0.94758	1.0000
Si	Si25	1.0	0.66797	0.53549	0.94463	1.0000
Si	Si26	1.0	0.29010	0.77403	0.93410	1.0000
Si	Si27	1.0	0.28650	0.51937	0.94824	1.0000
Si	Si28	1.0	0.04808	0.77744	0.93551	1.0000
Si	Si29	1.0	0.04589	0.52045	0.94088	1.0000
Si	Si30	1.0	0.48517	0.84971	0.87211	1.0000
Si	Si31	1.0	0.33699	0.19441	0.44861	1.0000
Si	Si32	1.0	0.34036	0.44839	0.44504	1.0000
Si	Si33	1.0	0.71296	0.22822	0.43624	1.0000
Si	Si34	1.0	0.71169	0.48379	0.44503	1.0000
Si	Si35	1.0	0.95502	0.22944	0.43852	1.0000
Si	Si36	1.0	0.95403	0.48530	0.44732	1.0000
Si	Si37	1.0	0.51874	0.14928	0.37298	1.0000
Si	Si38	1.0	0.54043	0.33566	0.69133	1.0000
Si	Si39	1.0	0.79261	0.72469	0.68928	1.0000
Si	Si40	1.0	0.53465	0.71176	0.69795	1.0000
Si	Si41	1.0	0.79008	0.96720	0.70104	1.0000
Si	Si42	1.0	0.53153	0.95420	0.69879	1.0000

Si	Si43	1.0	0.20422	0.66043	0.19489	1.0000
Si	Si44	1.0	0.45706	0.66036	0.19319	1.0000
Si	Si45	1.0	0.19743	0.28179	0.19810	1.0000
Si	Si46	1.0	0.45469	0.29173	0.19318	1.0000
Si	Si47	1.0	0.20077	0.03835	0.19512	1.0000
Si	Si48	1.0	0.45983	0.04763	0.19196	1.0000
Si	Si49	1.0	0.14253	0.47154	0.13081	1.0000
Si	Si50	1.0	0.16041	0.86000	0.12025	1.0000
Si	Si51	1.0	0.53395	0.47691	0.12508	1.0000
Si	Si52	1.0	0.84154	0.15777	0.62456	1.0000
Si	Si53	1.0	0.46987	0.53276	0.62695	1.0000
Si	Si54	1.0	0.14944	0.14199	0.37973	1.0000
Si	Si55	1.0	0.52883	0.53546	0.37382	1.0000
Si	Si56	1.0	0.85066	0.84352	0.87381	1.0000
Si	Si57	1.0	0.47656	0.46520	0.87848	1.0000
Si	Si58	1.0	0.79581	0.34634	0.70071	1.0000
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T2T7T7T9:

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O	O8	1.0	0.85152	0.82526	0.05431	1.0000
O	O9	1.0	0.66702	0.83939	0.10566	1.0000
O	O10	1.0	0.84494	0.48795	0.06379	1.0000
O	O11	1.0	0.65518	0.47378	0.10320	1.0000
O	O12	1.0	0.97749	0.65595	0.05341	1.0000
O	O13	1.0	0.05005	0.83634	0.09010	1.0000
O	O14	1.0	0.04306	0.47484	0.09258	1.0000
O	O15	1.0	0.62768	0.33495	0.55426	1.0000
O	O16	1.0	0.67814	0.17839	0.49150	1.0000
O	O17	1.0	0.73567	0.16360	0.58856	1.0000
O	O18	1.0	0.53305	0.14445	0.56154	1.0000
O	O19	1.0	0.66929	0.51237	0.50116	1.0000
O	O20	1.0	0.77045	0.47192	0.58846	1.0000
O	O21	1.0	0.56328	0.52357	0.58480	1.0000
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O	O24	1.0	0.33048	0.14266	0.60763	1.0000
O	O25	1.0	0.17217	0.50423	0.55132	1.0000
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O	O33	1.0	0.13609	0.42188	0.34057	1.0000
O	O34	1.0	0.49425	0.34439	0.24628	1.0000
O	O35	1.0	0.47410	0.23874	0.33401	1.0000
O	O36	1.0	0.53181	0.44417	0.33069	1.0000
O	O37	1.0	0.33762	0.73062	0.30367	1.0000
O	O38	1.0	0.18067	0.62776	0.35158	1.0000

O	O39	1.0	0.51434	0.84421	0.31191	1.0000
O	O40	1.0	0.50679	0.65128	0.34975	1.0000
O	O41	1.0	0.34173	0.96925	0.31338	1.0000
O	O42	1.0	0.13809	0.02538	0.35660	1.0000
O	O43	1.0	0.53061	0.03753	0.34453	1.0000
O	O44	1.0	0.67463	0.61961	0.81019	1.0000
O	O45	1.0	0.83030	0.65588	0.74072	1.0000
O	O46	1.0	0.82687	0.76565	0.82615	1.0000
O	O47	1.0	0.86977	0.55573	0.82480	1.0000
O	O48	1.0	0.50743	0.64743	0.75070	1.0000
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O	O50	1.0	0.47935	0.57255	0.84361	1.0000
O	O51	1.0	0.65488	0.28738	0.80774	1.0000
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O	O62	1.0	0.56162	0.85310	0.92217	1.0000
O	O63	1.0	0.67669	0.49456	0.00271	1.0000
O	O64	1.0	0.78341	0.52708	0.91640	1.0000
O	O65	1.0	0.58005	0.46303	0.91559	1.0000
O	O66	1.0	0.29351	0.64676	0.94043	1.0000
O	O67	1.0	0.17028	0.81441	0.92270	1.0000
O	O68	1.0	0.36665	0.80781	0.88744	1.0000
O	O69	1.0	0.16686	0.47853	0.93551	1.0000
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O	O73	1.0	0.97936	0.46157	0.89671	1.0000
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O	O75	1.0	0.34637	0.17531	0.51009	1.0000
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O	O92	1.0	0.49044	0.31493	0.74754	1.0000
O	O93	1.0	0.52442	0.23440	0.65625	1.0000
O	O94	1.0	0.48372	0.44202	0.67028	1.0000
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O	O107	1.0	0.50402	0.67555	0.25016	1.0000
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Al	Al3	1.0	0.53707	0.86176	0.12477	1.0000
Al	Al4	1.0	0.20570	0.96541	0.30781	1.0000
Si	Si1	1.0	0.33952	0.54283	0.06095	1.0000
Si	Si2	1.0	0.72721	0.78641	0.05937	1.0000
Si	Si3	1.0	0.72365	0.52903	0.05792	1.0000
Si	Si4	1.0	0.97327	0.78424	0.04764	1.0000
Si	Si5	1.0	0.96568	0.52751	0.05144	1.0000
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Si	Si8	1.0	0.27425	0.20322	0.56200	1.0000

Si	Si9	1.0	0.29053	0.45691	0.55722	1.0000
Si	Si10	1.0	0.02991	0.21302	0.54886	1.0000
Si	Si11	1.0	0.04649	0.47029	0.55446	1.0000
Si	Si12	1.0	0.21000	0.33759	0.31040	1.0000
Si	Si13	1.0	0.45855	0.35180	0.30512	1.0000
Si	Si14	1.0	0.46799	0.72563	0.30363	1.0000
Si	Si15	1.0	0.46781	0.96416	0.30330	1.0000
Si	Si16	1.0	0.14364	0.51881	0.38050	1.0000
Si	Si17	1.0	0.79975	0.65156	0.80094	1.0000
Si	Si18	1.0	0.54918	0.65336	0.80842	1.0000
Si	Si19	1.0	0.78269	0.28180	0.81214	1.0000
Si	Si20	1.0	0.52589	0.28158	0.80409	1.0000
Si	Si21	1.0	0.78425	0.04143	0.81143	1.0000
Si	Si22	1.0	0.52611	0.04344	0.80628	1.0000
Si	Si23	1.0	0.86112	0.47578	0.87378	1.0000
Si	Si24	1.0	0.65794	0.78615	0.94758	1.0000
Si	Si25	1.0	0.66797	0.53549	0.94463	1.0000
Si	Si26	1.0	0.29010	0.77403	0.93410	1.0000
Si	Si27	1.0	0.28650	0.51937	0.94824	1.0000
Si	Si28	1.0	0.04808	0.77744	0.93551	1.0000
Si	Si29	1.0	0.04589	0.52045	0.94088	1.0000
Si	Si30	1.0	0.48517	0.84971	0.87211	1.0000
Si	Si31	1.0	0.33699	0.19441	0.44861	1.0000
Si	Si32	1.0	0.34036	0.44839	0.44504	1.0000
Si	Si33	1.0	0.71296	0.22822	0.43624	1.0000
Si	Si34	1.0	0.71169	0.48379	0.44503	1.0000
Si	Si35	1.0	0.95502	0.22944	0.43852	1.0000
Si	Si36	1.0	0.95403	0.48530	0.44732	1.0000
Si	Si37	1.0	0.51874	0.14928	0.37298	1.0000
Si	Si38	1.0	0.54043	0.33566	0.69133	1.0000
Si	Si39	1.0	0.79261	0.72469	0.68928	1.0000
Si	Si40	1.0	0.53465	0.71176	0.69795	1.0000
Si	Si41	1.0	0.79008	0.96720	0.70104	1.0000
Si	Si42	1.0	0.53153	0.95420	0.69879	1.0000

Si	Si43	1.0	0.20422	0.66043	0.19489	1.0000
Si	Si44	1.0	0.45706	0.66036	0.19319	1.0000
Si	Si45	1.0	0.19743	0.28179	0.19810	1.0000
Si	Si46	1.0	0.45469	0.29173	0.19318	1.0000
Si	Si47	1.0	0.20077	0.03835	0.19512	1.0000
Si	Si48	1.0	0.45983	0.04763	0.19196	1.0000
Si	Si49	1.0	0.14253	0.47154	0.13081	1.0000
Si	Si50	1.0	0.16041	0.86000	0.12025	1.0000
Si	Si51	1.0	0.53395	0.47691	0.12508	1.0000
Si	Si52	1.0	0.84154	0.15777	0.62456	1.0000
Si	Si53	1.0	0.46987	0.53276	0.62695	1.0000
Si	Si54	1.0	0.14944	0.14199	0.37973	1.0000
Si	Si55	1.0	0.52883	0.53546	0.37382	1.0000
Si	Si56	1.0	0.85066	0.84352	0.87381	1.0000
Si	Si57	1.0	0.47656	0.46520	0.87848	1.0000
Si	Si58	1.0	0.79581	0.34634	0.70071	1.0000
Si	Si59	1.0	0.34281	0.79851	0.04639	1.0000
Si	Si60	1.0	0.21248	0.70855	0.30702	1.0000

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H	H3	1.0	0.52152	0.84307	0.03330	1.0000
H	H4	1.0	0.10696	0.82440	0.35239	1.0000
O	O1	1.0	0.32897	0.67252	0.05766	1.0000
O	O2	1.0	0.33378	0.82652	0.98670	1.0000
O	O3	1.0	0.26100	0.86522	0.08003	1.0000
O	O4	1.0	0.31658	0.49100	0.00627	1.0000

O	O5	1.0	0.25456	0.49377	0.10100	1.0000
O	O6	1.0	0.45951	0.51376	0.07758	1.0000
O	O7	1.0	0.72165	0.65739	0.06197	1.0000
O	O8	1.0	0.85152	0.82526	0.05431	1.0000
O	O9	1.0	0.66702	0.83939	0.10566	1.0000
O	O10	1.0	0.84494	0.48795	0.06379	1.0000
O	O11	1.0	0.65518	0.47378	0.10320	1.0000
O	O12	1.0	0.97749	0.65595	0.05341	1.0000
O	O13	1.0	0.05005	0.83634	0.09010	1.0000
O	O14	1.0	0.04306	0.47484	0.09258	1.0000
O	O15	1.0	0.62768	0.33495	0.55426	1.0000
O	O16	1.0	0.67814	0.17839	0.49150	1.0000
O	O17	1.0	0.73567	0.16360	0.58856	1.0000
O	O18	1.0	0.53305	0.14445	0.56154	1.0000
O	O19	1.0	0.66929	0.51237	0.50116	1.0000
O	O20	1.0	0.77045	0.47192	0.58846	1.0000
O	O21	1.0	0.56328	0.52357	0.58480	1.0000
O	O22	1.0	0.28240	0.33091	0.57036	1.0000
O	O23	1.0	0.15001	0.16659	0.55487	1.0000
O	O24	1.0	0.33048	0.14266	0.60763	1.0000
O	O25	1.0	0.17217	0.50423	0.55132	1.0000
O	O26	1.0	0.35307	0.52028	0.60130	1.0000
O	O27	1.0	0.03259	0.34081	0.55408	1.0000
O	O28	1.0	0.95058	0.15992	0.59152	1.0000
O	O29	1.0	0.99404	0.51787	0.60424	1.0000
O	O30	1.0	0.33257	0.38442	0.30958	1.0000
O	O31	1.0	0.16360	0.32657	0.25357	1.0000
O	O32	1.0	0.20677	0.22210	0.33816	1.0000
O	O33	1.0	0.13609	0.42188	0.34057	1.0000
O	O34	1.0	0.49425	0.34439	0.24628	1.0000
O	O35	1.0	0.47410	0.23874	0.33401	1.0000
O	O36	1.0	0.53181	0.44417	0.33069	1.0000
O	O37	1.0	0.33762	0.73062	0.30367	1.0000
O	O38	1.0	0.18067	0.62776	0.35158	1.0000

O	O39	1.0	0.51434	0.84421	0.31191	1.0000
O	O40	1.0	0.50679	0.65128	0.34975	1.0000
O	O41	1.0	0.34173	0.96925	0.31338	1.0000
O	O42	1.0	0.13809	0.02538	0.35660	1.0000
O	O43	1.0	0.53061	0.03753	0.34453	1.0000
O	O44	1.0	0.67463	0.61961	0.81019	1.0000
O	O45	1.0	0.83030	0.65588	0.74072	1.0000
O	O46	1.0	0.82687	0.76565	0.82615	1.0000
O	O47	1.0	0.86977	0.55573	0.82480	1.0000
O	O48	1.0	0.50743	0.64743	0.75070	1.0000
O	O49	1.0	0.53966	0.77390	0.82989	1.0000
O	O50	1.0	0.47935	0.57255	0.84361	1.0000
O	O51	1.0	0.65488	0.28738	0.80774	1.0000
O	O52	1.0	0.82197	0.16231	0.82478	1.0000
O	O53	1.0	0.82034	0.35898	0.85723	1.0000
O	O54	1.0	0.48586	0.16226	0.81857	1.0000
O	O55	1.0	0.47329	0.36049	0.84428	1.0000
O	O56	1.0	0.65502	0.03292	0.81172	1.0000
O	O57	1.0	0.83219	0.96481	0.85532	1.0000
O	O58	1.0	0.47105	0.96763	0.84915	1.0000
O	O59	1.0	0.63038	0.65957	0.94276	1.0000
O	O60	1.0	0.65996	0.82082	0.00713	1.0000
O	O61	1.0	0.77232	0.81285	0.92126	1.0000
O	O62	1.0	0.56162	0.85310	0.92217	1.0000
O	O63	1.0	0.67669	0.49456	0.00271	1.0000
O	O64	1.0	0.78341	0.52708	0.91640	1.0000
O	O65	1.0	0.58005	0.46303	0.91559	1.0000
O	O66	1.0	0.29351	0.64676	0.94043	1.0000
O	O67	1.0	0.17028	0.81441	0.92270	1.0000
O	O68	1.0	0.36665	0.80781	0.88744	1.0000
O	O69	1.0	0.16686	0.47853	0.93551	1.0000
O	O70	1.0	0.36765	0.46058	0.91103	1.0000
O	O71	1.0	0.03773	0.64868	0.93326	1.0000
O	O72	1.0	0.97268	0.83077	0.89279	1.0000

O	O73	1.0	0.97936	0.46157	0.89671	1.0000
O	O74	1.0	0.34224	0.32096	0.43537	1.0000
O	O75	1.0	0.34637	0.17531	0.51009	1.0000
O	O76	1.0	0.22437	0.14303	0.43061	1.0000
O	O77	1.0	0.43895	0.13829	0.42227	1.0000
O	O78	1.0	0.35662	0.47366	0.50439	1.0000
O	O79	1.0	0.22595	0.49278	0.42596	1.0000
O	O80	1.0	0.43591	0.50678	0.41457	1.0000
O	O81	1.0	0.70224	0.35600	0.43774	1.0000
O	O82	1.0	0.83406	0.19374	0.42378	1.0000
O	O83	1.0	0.63681	0.18179	0.39275	1.0000
O	O84	1.0	0.83370	0.52464	0.43711	1.0000
O	O85	1.0	0.64262	0.54380	0.40224	1.0000
O	O86	1.0	0.96486	0.35790	0.44061	1.0000
O	O87	1.0	0.03270	0.18633	0.39486	1.0000
O	O88	1.0	0.02802	0.54430	0.40448	1.0000
O	O89	1.0	0.66921	0.36239	0.69665	1.0000
O	O90	1.0	0.83415	0.32180	0.75805	1.0000
O	O91	1.0	0.84252	0.26187	0.66136	1.0000
O	O92	1.0	0.49044	0.31493	0.74754	1.0000
O	O93	1.0	0.52442	0.23440	0.65625	1.0000
O	O94	1.0	0.48372	0.44202	0.67028	1.0000
O	O95	1.0	0.66300	0.71788	0.68948	1.0000
O	O96	1.0	0.83503	0.84762	0.69285	1.0000
O	O97	1.0	0.84171	0.66644	0.64155	1.0000
O	O98	1.0	0.49012	0.83104	0.70203	1.0000
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O	O100	1.0	0.66162	0.96240	0.69989	1.0000
O	O101	1.0	0.83616	0.04857	0.65758	1.0000
O	O102	1.0	0.48813	0.00798	0.64842	1.0000
O	O103	1.0	0.32927	0.62766	0.19613	1.0000
O	O104	1.0	0.16220	0.68032	0.25277	1.0000
O	O105	1.0	0.18490	0.76658	0.16125	1.0000
O	O106	1.0	0.13130	0.56292	0.17371	1.0000

O	O107	1.0	0.50402	0.67555	0.25016	1.0000
O	O108	1.0	0.47064	0.76524	0.15926	1.0000
O	O109	1.0	0.52333	0.56100	0.17063	1.0000
O	O110	1.0	0.32546	0.29416	0.19135	1.0000
O	O111	1.0	0.15782	0.16020	0.19083	1.0000
O	O112	1.0	0.13955	0.35399	0.15554	1.0000
O	O113	1.0	0.49744	0.17223	0.18893	1.0000
O	O114	1.0	0.50194	0.35924	0.14536	1.0000
O	O115	1.0	0.32997	0.03949	0.18980	1.0000
O	O116	1.0	0.15046	0.97385	0.14699	1.0000
O	O117	1.0	0.51261	0.98696	0.14539	1.0000
O	O118	1.0	0.01634	0.81896	0.99154	1.0000
O	O119	1.0	0.99828	0.48613	0.99566	1.0000
O	O120	1.0	0.98424	0.17927	0.49363	1.0000
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O	O124	1.0	0.83038	0.01012	0.75600	1.0000
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Al	Al2	1.0	0.86561	0.53775	0.62354	1.0000
Al	Al3	1.0	0.53707	0.86176	0.12477	1.0000
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Si	Si1	1.0	0.33952	0.54283	0.06095	1.0000
Si	Si2	1.0	0.72721	0.78641	0.05937	1.0000
Si	Si3	1.0	0.72365	0.52903	0.05792	1.0000
Si	Si4	1.0	0.97327	0.78424	0.04764	1.0000
Si	Si5	1.0	0.96568	0.52751	0.05144	1.0000
Si	Si6	1.0	0.64982	0.20986	0.54903	1.0000
Si	Si7	1.0	0.66066	0.46201	0.55802	1.0000
Si	Si8	1.0	0.27425	0.20322	0.56200	1.0000

Si	Si9	1.0	0.29053	0.45691	0.55722	1.0000
Si	Si10	1.0	0.02991	0.21302	0.54886	1.0000
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Si	Si13	1.0	0.45855	0.35180	0.30512	1.0000
Si	Si14	1.0	0.46799	0.72563	0.30363	1.0000
Si	Si15	1.0	0.46781	0.96416	0.30330	1.0000
Si	Si16	1.0	0.14364	0.51881	0.38050	1.0000
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Si	Si51	1.0	0.53395	0.47691	0.12508	1.0000
Si	Si52	1.0	0.84154	0.15777	0.62456	1.0000
Si	Si53	1.0	0.46987	0.53276	0.62695	1.0000
Si	Si54	1.0	0.14944	0.14199	0.37973	1.0000
Si	Si55	1.0	0.52883	0.53546	0.37382	1.0000
Si	Si56	1.0	0.85066	0.84352	0.87381	1.0000
Si	Si57	1.0	0.47656	0.46520	0.87848	1.0000
Si	Si58	1.0	0.79581	0.34634	0.70071	1.0000
Si	Si59	1.0	0.34281	0.79851	0.04639	1.0000
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O	O7	1.0	0.72165	0.65739	0.06197	1.0000
O	O8	1.0	0.85152	0.82526	0.05431	1.0000
O	O9	1.0	0.66702	0.83939	0.10566	1.0000
O	O10	1.0	0.84494	0.48795	0.06379	1.0000
O	O11	1.0	0.65518	0.47378	0.10320	1.0000
O	O12	1.0	0.97749	0.65595	0.05341	1.0000
O	O13	1.0	0.05005	0.83634	0.09010	1.0000
O	O14	1.0	0.04306	0.47484	0.09258	1.0000
O	O15	1.0	0.62768	0.33495	0.55426	1.0000
O	O16	1.0	0.67814	0.17839	0.49150	1.0000
O	O17	1.0	0.73567	0.16360	0.58856	1.0000
O	O18	1.0	0.53305	0.14445	0.56154	1.0000
O	O19	1.0	0.66929	0.51237	0.50116	1.0000
O	O20	1.0	0.77045	0.47192	0.58846	1.0000
O	O21	1.0	0.56328	0.52357	0.58480	1.0000
O	O22	1.0	0.28240	0.33091	0.57036	1.0000
O	O23	1.0	0.15001	0.16659	0.55487	1.0000
O	O24	1.0	0.33048	0.14266	0.60763	1.0000
O	O25	1.0	0.17217	0.50423	0.55132	1.0000
O	O26	1.0	0.35307	0.52028	0.60130	1.0000
O	O27	1.0	0.03259	0.34081	0.55408	1.0000
O	O28	1.0	0.95058	0.15992	0.59152	1.0000
O	O29	1.0	0.99404	0.51787	0.60424	1.0000
O	O30	1.0	0.33257	0.38442	0.30958	1.0000
O	O31	1.0	0.16360	0.32657	0.25357	1.0000
O	O32	1.0	0.20677	0.22210	0.33816	1.0000
O	O33	1.0	0.13609	0.42188	0.34057	1.0000
O	O34	1.0	0.49425	0.34439	0.24628	1.0000
O	O35	1.0	0.47410	0.23874	0.33401	1.0000
O	O36	1.0	0.53181	0.44417	0.33069	1.0000
O	O37	1.0	0.33762	0.73062	0.30367	1.0000
O	O38	1.0	0.18067	0.62776	0.35158	1.0000

O	O39	1.0	0.51434	0.84421	0.31191	1.0000
O	O40	1.0	0.50679	0.65128	0.34975	1.0000
O	O41	1.0	0.34173	0.96925	0.31338	1.0000
O	O42	1.0	0.13809	0.02538	0.35660	1.0000
O	O43	1.0	0.53061	0.03753	0.34453	1.0000
O	O44	1.0	0.67463	0.61961	0.81019	1.0000
O	O45	1.0	0.83030	0.65588	0.74072	1.0000
O	O46	1.0	0.82687	0.76565	0.82615	1.0000
O	O47	1.0	0.86977	0.55573	0.82480	1.0000
O	O48	1.0	0.50743	0.64743	0.75070	1.0000
O	O49	1.0	0.53966	0.77390	0.82989	1.0000
O	O50	1.0	0.47935	0.57255	0.84361	1.0000
O	O51	1.0	0.65488	0.28738	0.80774	1.0000
O	O52	1.0	0.82197	0.16231	0.82478	1.0000
O	O53	1.0	0.82034	0.35898	0.85723	1.0000
O	O54	1.0	0.48586	0.16226	0.81857	1.0000
O	O55	1.0	0.47329	0.36049	0.84428	1.0000
O	O56	1.0	0.65502	0.03292	0.81172	1.0000
O	O57	1.0	0.83219	0.96481	0.85532	1.0000
O	O58	1.0	0.47105	0.96763	0.84915	1.0000
O	O59	1.0	0.63038	0.65957	0.94276	1.0000
O	O60	1.0	0.65996	0.82082	0.00713	1.0000
O	O61	1.0	0.77232	0.81285	0.92126	1.0000
O	O62	1.0	0.56162	0.85310	0.92217	1.0000
O	O63	1.0	0.67669	0.49456	0.00271	1.0000
O	O64	1.0	0.78341	0.52708	0.91640	1.0000
O	O65	1.0	0.58005	0.46303	0.91559	1.0000
O	O66	1.0	0.29351	0.64676	0.94043	1.0000
O	O67	1.0	0.17028	0.81441	0.92270	1.0000
O	O68	1.0	0.36665	0.80781	0.88744	1.0000
O	O69	1.0	0.16686	0.47853	0.93551	1.0000
O	O70	1.0	0.36765	0.46058	0.91103	1.0000
O	O71	1.0	0.03773	0.64868	0.93326	1.0000
O	O72	1.0	0.97268	0.83077	0.89279	1.0000

O	O73	1.0	0.97936	0.46157	0.89671	1.0000
O	O74	1.0	0.34224	0.32096	0.43537	1.0000
O	O75	1.0	0.34637	0.17531	0.51009	1.0000
O	O76	1.0	0.22437	0.14303	0.43061	1.0000
O	O77	1.0	0.43895	0.13829	0.42227	1.0000
O	O78	1.0	0.35662	0.47366	0.50439	1.0000
O	O79	1.0	0.22595	0.49278	0.42596	1.0000
O	O80	1.0	0.43591	0.50678	0.41457	1.0000
O	O81	1.0	0.70224	0.35600	0.43774	1.0000
O	O82	1.0	0.83406	0.19374	0.42378	1.0000
O	O83	1.0	0.63681	0.18179	0.39275	1.0000
O	O84	1.0	0.83370	0.52464	0.43711	1.0000
O	O85	1.0	0.64262	0.54380	0.40224	1.0000
O	O86	1.0	0.96486	0.35790	0.44061	1.0000
O	O87	1.0	0.03270	0.18633	0.39486	1.0000
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O	O89	1.0	0.66921	0.36239	0.69665	1.0000
O	O90	1.0	0.83415	0.32180	0.75805	1.0000
O	O91	1.0	0.84252	0.26187	0.66136	1.0000
O	O92	1.0	0.49044	0.31493	0.74754	1.0000
O	O93	1.0	0.52442	0.23440	0.65625	1.0000
O	O94	1.0	0.48372	0.44202	0.67028	1.0000
O	O95	1.0	0.66300	0.71788	0.68948	1.0000
O	O96	1.0	0.83503	0.84762	0.69285	1.0000
O	O97	1.0	0.84171	0.66644	0.64155	1.0000
O	O98	1.0	0.49012	0.83104	0.70203	1.0000
O	O99	1.0	0.47628	0.64987	0.65218	1.0000
O	O100	1.0	0.66162	0.96240	0.69989	1.0000
O	O101	1.0	0.83616	0.04857	0.65758	1.0000
O	O102	1.0	0.48813	0.00798	0.64842	1.0000
O	O103	1.0	0.32927	0.62766	0.19613	1.0000
O	O104	1.0	0.16220	0.68032	0.25277	1.0000
O	O105	1.0	0.18490	0.76658	0.16125	1.0000
O	O106	1.0	0.13130	0.56292	0.17371	1.0000

O	O107	1.0	0.50402	0.67555	0.25016	1.0000
O	O108	1.0	0.47064	0.76524	0.15926	1.0000
O	O109	1.0	0.52333	0.56100	0.17063	1.0000
O	O110	1.0	0.32546	0.29416	0.19135	1.0000
O	O111	1.0	0.15782	0.16020	0.19083	1.0000
O	O112	1.0	0.13955	0.35399	0.15554	1.0000
O	O113	1.0	0.49744	0.17223	0.18893	1.0000
O	O114	1.0	0.50194	0.35924	0.14536	1.0000
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O	O124	1.0	0.83038	0.01012	0.75600	1.0000
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O	O126	1.0	0.85497	0.46532	0.68684	1.0000
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Al	Al1	1.0	0.46221	0.13152	0.62504	1.0000
Al	Al2	1.0	0.86561	0.53775	0.62354	1.0000
Al	Al3	1.0	0.53707	0.86176	0.12477	1.0000
Al	Al4	1.0	0.20570	0.96541	0.30781	1.0000
Si	Si1	1.0	0.33952	0.54283	0.06095	1.0000
Si	Si2	1.0	0.72721	0.78641	0.05937	1.0000
Si	Si3	1.0	0.72365	0.52903	0.05792	1.0000
Si	Si4	1.0	0.97327	0.78424	0.04764	1.0000
Si	Si5	1.0	0.96568	0.52751	0.05144	1.0000
Si	Si6	1.0	0.64982	0.20986	0.54903	1.0000
Si	Si7	1.0	0.66066	0.46201	0.55802	1.0000
Si	Si8	1.0	0.27425	0.20322	0.56200	1.0000

Si	Si9	1.0	0.29053	0.45691	0.55722	1.0000
Si	Si10	1.0	0.02991	0.21302	0.54886	1.0000
Si	Si11	1.0	0.04649	0.47029	0.55446	1.0000
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Si	Si13	1.0	0.45855	0.35180	0.30512	1.0000
Si	Si14	1.0	0.46799	0.72563	0.30363	1.0000
Si	Si15	1.0	0.46781	0.96416	0.30330	1.0000
Si	Si16	1.0	0.14364	0.51881	0.38050	1.0000
Si	Si17	1.0	0.79975	0.65156	0.80094	1.0000
Si	Si18	1.0	0.54918	0.65336	0.80842	1.0000
Si	Si19	1.0	0.78269	0.28180	0.81214	1.0000
Si	Si20	1.0	0.52589	0.28158	0.80409	1.0000
Si	Si21	1.0	0.78425	0.04143	0.81143	1.0000
Si	Si22	1.0	0.52611	0.04344	0.80628	1.0000
Si	Si23	1.0	0.86112	0.47578	0.87378	1.0000
Si	Si24	1.0	0.65794	0.78615	0.94758	1.0000
Si	Si25	1.0	0.66797	0.53549	0.94463	1.0000
Si	Si26	1.0	0.29010	0.77403	0.93410	1.0000
Si	Si27	1.0	0.28650	0.51937	0.94824	1.0000
Si	Si28	1.0	0.04808	0.77744	0.93551	1.0000
Si	Si29	1.0	0.04589	0.52045	0.94088	1.0000
Si	Si30	1.0	0.48517	0.84971	0.87211	1.0000
Si	Si31	1.0	0.33699	0.19441	0.44861	1.0000
Si	Si32	1.0	0.34036	0.44839	0.44504	1.0000
Si	Si33	1.0	0.71296	0.22822	0.43624	1.0000
Si	Si34	1.0	0.71169	0.48379	0.44503	1.0000
Si	Si35	1.0	0.95502	0.22944	0.43852	1.0000
Si	Si36	1.0	0.95403	0.48530	0.44732	1.0000
Si	Si37	1.0	0.51874	0.14928	0.37298	1.0000
Si	Si38	1.0	0.54043	0.33566	0.69133	1.0000
Si	Si39	1.0	0.79261	0.72469	0.68928	1.0000
Si	Si40	1.0	0.53465	0.71176	0.69795	1.0000
Si	Si41	1.0	0.79008	0.96720	0.70104	1.0000
Si	Si42	1.0	0.53153	0.95420	0.69879	1.0000

Si	Si43	1.0	0.20422	0.66043	0.19489	1.0000
Si	Si44	1.0	0.45706	0.66036	0.19319	1.0000
Si	Si45	1.0	0.19743	0.28179	0.19810	1.0000
Si	Si46	1.0	0.45469	0.29173	0.19318	1.0000
Si	Si47	1.0	0.20077	0.03835	0.19512	1.0000
Si	Si48	1.0	0.45983	0.04763	0.19196	1.0000
Si	Si49	1.0	0.14253	0.47154	0.13081	1.0000
Si	Si50	1.0	0.16041	0.86000	0.12025	1.0000
Si	Si51	1.0	0.53395	0.47691	0.12508	1.0000
Si	Si52	1.0	0.84154	0.15777	0.62456	1.0000
Si	Si53	1.0	0.46987	0.53276	0.62695	1.0000
Si	Si54	1.0	0.14944	0.14199	0.37973	1.0000
Si	Si55	1.0	0.52883	0.53546	0.37382	1.0000
Si	Si56	1.0	0.85066	0.84352	0.87381	1.0000
Si	Si57	1.0	0.47656	0.46520	0.87848	1.0000
Si	Si58	1.0	0.79581	0.34634	0.70071	1.0000
Si	Si59	1.0	0.34281	0.79851	0.04639	1.0000
Si	Si60	1.0	0.21248	0.70855	0.30702	1.0000

AlSiAl-T2T7T7T9:

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O	O7	1.0	0.43806	0.50886	0.08196	1.0000
O	O8	1.0	0.70186	0.67378	0.06392	1.0000
O	O9	1.0	0.83071	0.84275	0.05853	1.0000
O	O10	1.0	0.64036	0.86421	0.09667	1.0000
O	O11	1.0	0.83050	0.50460	0.06303	1.0000
O	O12	1.0	0.64276	0.49125	0.10566	1.0000
O	O13	1.0	0.95915	0.67332	0.05668	1.0000
O	O14	1.0	0.02214	0.85552	0.09793	1.0000
O	O15	1.0	0.02461	0.49683	0.10171	1.0000
O	O16	1.0	0.64080	0.33009	0.54880	1.0000
O	O17	1.0	0.68442	0.16965	0.48634	1.0000
O	O18	1.0	0.73539	0.15172	0.58507	1.0000
O	O19	1.0	0.53596	0.14677	0.55635	1.0000
O	O20	1.0	0.68468	0.51174	0.50120	1.0000
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O	O27	1.0	0.35709	0.51416	0.60158	1.0000
O	O28	1.0	0.04379	0.32803	0.55320	1.0000
O	O29	1.0	0.96793	0.14407	0.59033	1.0000
O	O30	1.0	0.00038	0.49599	0.61062	1.0000
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O	O34	1.0	0.14672	0.42233	0.34373	1.0000
O	O35	1.0	0.49284	0.34044	0.24274	1.0000
O	O36	1.0	0.48451	0.22803	0.32679	1.0000
O	O37	1.0	0.54412	0.43531	0.32826	1.0000
O	O38	1.0	0.32841	0.71915	0.31259	1.0000

O	O39	1.0	0.14888	0.82966	0.31091	1.0000
O	O40	1.0	0.14988	0.63532	0.34690	1.0000
O	O41	1.0	0.49698	0.63288	0.35801	1.0000
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O	O45	1.0	0.67135	0.67480	0.81552	1.0000
O	O46	1.0	0.82175	0.64302	0.74405	1.0000
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O	O49	1.0	0.51977	0.64770	0.74655	1.0000
O	O50	1.0	0.47741	0.74707	0.83353	1.0000
O	O51	1.0	0.50825	0.53969	0.83066	1.0000
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O	O54	1.0	0.83751	0.34782	0.86423	1.0000
O	O55	1.0	0.51500	0.15487	0.81717	1.0000
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O	O59	1.0	0.46262	0.95740	0.83497	1.0000
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O	O62	1.0	0.77700	0.80227	0.91577	1.0000
O	O63	1.0	0.57251	0.85646	0.90789	1.0000
O	O64	1.0	0.65384	0.50658	0.00614	1.0000
O	O65	1.0	0.76554	0.50830	0.92233	1.0000
O	O66	1.0	0.55643	0.46127	0.92059	1.0000
O	O67	1.0	0.28829	0.66591	0.93341	1.0000
O	O68	1.0	0.16964	0.83921	0.94124	1.0000
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O	O70	1.0	0.16320	0.49481	0.93957	1.0000
O	O71	1.0	0.35141	0.48444	0.89544	1.0000
O	O72	1.0	0.04076	0.66798	0.94442	1.0000

O	O73	1.0	0.98140	0.84556	0.89848	1.0000
O	O74	1.0	0.97074	0.48824	0.90247	1.0000
O	O75	1.0	0.30528	0.32545	0.43847	1.0000
O	O76	1.0	0.35081	0.17153	0.50621	1.0000
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O	O81	1.0	0.46193	0.46497	0.41938	1.0000
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O	O87	1.0	0.97000	0.35032	0.44295	1.0000
O	O88	1.0	0.04621	0.18497	0.39418	1.0000
O	O89	1.0	0.05004	0.53558	0.41613	1.0000
O	O90	1.0	0.67272	0.35781	0.70154	1.0000
O	O91	1.0	0.83484	0.31787	0.76428	1.0000
O	O92	1.0	0.84515	0.25112	0.66853	1.0000
O	O93	1.0	0.49475	0.31269	0.74971	1.0000
O	O94	1.0	0.52922	0.23084	0.65725	1.0000
O	O95	1.0	0.49154	0.43990	0.67066	1.0000
O	O96	1.0	0.67151	0.71401	0.68274	1.0000
O	O97	1.0	0.84407	0.83523	0.70071	1.0000
O	O98	1.0	0.85936	0.65735	0.64603	1.0000
O	O99	1.0	0.50382	0.83179	0.69799	1.0000
O	O100	1.0	0.48348	0.64707	0.64851	1.0000
O	O101	1.0	0.67467	0.96367	0.69205	1.0000
O	O102	1.0	0.50186	0.00345	0.63921	1.0000
O	O103	1.0	0.34293	0.69260	0.18875	1.0000
O	O104	1.0	0.17573	0.66116	0.24910	1.0000
O	O105	1.0	0.15492	0.77307	0.16549	1.0000
O	O106	1.0	0.18363	0.56210	0.16232	1.0000

O	O107	1.0	0.49725	0.66654	0.25771	1.0000
O	O108	1.0	0.53765	0.76821	0.17231	1.0000
O	O109	1.0	0.50317	0.55598	0.17461	1.0000
O	O110	1.0	0.32517	0.29699	0.18473	1.0000
O	O111	1.0	0.15606	0.16923	0.19456	1.0000
O	O112	1.0	0.13418	0.35749	0.15319	1.0000
O	O113	1.0	0.49225	0.16436	0.18518	1.0000
O	O114	1.0	0.50708	0.35430	0.14338	1.0000
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O	O120	1.0	0.99370	0.16675	0.49156	1.0000
O	O121	1.0	0.98350	0.50819	0.51063	1.0000
O	O122	1.0	0.15184	0.99387	0.24944	1.0000
O	O123	1.0	0.49952	0.99280	0.24623	1.0000
O	O124	1.0	0.83580	0.01509	0.75507	1.0000
O	O125	1.0	0.50050	0.02165	0.74005	1.0000
O	O126	1.0	0.85730	0.45812	0.69192	1.0000
O	O127	1.0	0.50573	0.82854	0.32371	1.0000
O	O128	1.0	0.86132	0.02223	0.65532	1.0000
Al	Al1	1.0	0.47304	0.13119	0.62050	1.0000
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Al	Al3	1.0	0.45457	0.96632	0.30629	1.0000
Al	Al4	1.0	0.84918	0.15621	0.62159	1.0000
Si	Si1	1.0	0.32735	0.78586	0.05744	1.0000
Si	Si2	1.0	0.32577	0.53376	0.05449	1.0000
Si	Si3	1.0	0.70808	0.80178	0.05403	1.0000
Si	Si4	1.0	0.70799	0.54466	0.05939	1.0000
Si	Si5	1.0	0.95236	0.80246	0.05289	1.0000
Si	Si6	1.0	0.95316	0.54391	0.05586	1.0000
Si	Si7	1.0	0.52720	0.85417	0.12590	1.0000
Si	Si8	1.0	0.65722	0.20260	0.54432	1.0000

Si	Si9	1.0	0.66896	0.45713	0.55701	1.0000
Si	Si10	1.0	0.28211	0.19909	0.55885	1.0000
Si	Si11	1.0	0.29244	0.45571	0.55611	1.0000
Si	Si12	1.0	0.04029	0.19904	0.54752	1.0000
Si	Si13	1.0	0.04986	0.45753	0.55829	1.0000
Si	Si14	1.0	0.21734	0.34164	0.30970	1.0000
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Si	Si21	1.0	0.78067	0.28381	0.81786	1.0000
Si	Si22	1.0	0.53094	0.28110	0.80664	1.0000
Si	Si23	1.0	0.78237	0.03395	0.81106	1.0000
Si	Si24	1.0	0.53353	0.03366	0.79915	1.0000
Si	Si25	1.0	0.85165	0.47249	0.88021	1.0000
Si	Si26	1.0	0.65826	0.78680	0.93966	1.0000
Si	Si27	1.0	0.64956	0.53418	0.94635	1.0000
Si	Si28	1.0	0.28993	0.79333	0.94385	1.0000
Si	Si29	1.0	0.28565	0.53777	0.94114	1.0000
Si	Si30	1.0	0.04746	0.79757	0.94595	1.0000
Si	Si31	1.0	0.04321	0.53858	0.94756	1.0000
Si	Si32	1.0	0.46982	0.85178	0.86970	1.0000
Si	Si33	1.0	0.33820	0.20023	0.44596	1.0000
Si	Si34	1.0	0.34466	0.45002	0.44401	1.0000
Si	Si35	1.0	0.72437	0.22279	0.43306	1.0000
Si	Si36	1.0	0.72582	0.48021	0.44504	1.0000
Si	Si37	1.0	0.96456	0.22156	0.43781	1.0000
Si	Si38	1.0	0.96299	0.47809	0.45180	1.0000
Si	Si39	1.0	0.52679	0.15230	0.37297	1.0000
Si	Si40	1.0	0.54527	0.33229	0.69334	1.0000
Si	Si41	1.0	0.79905	0.71288	0.69149	1.0000
Si	Si42	1.0	0.54418	0.70981	0.69373	1.0000

Si	Si43	1.0	0.54323	0.95505	0.69095	1.0000
Si	Si44	1.0	0.21424	0.67214	0.19085	1.0000
Si	Si45	1.0	0.46949	0.67080	0.19720	1.0000
Si	Si46	1.0	0.19826	0.29167	0.19632	1.0000
Si	Si47	1.0	0.45384	0.28705	0.18937	1.0000
Si	Si48	1.0	0.19539	0.04619	0.19739	1.0000
Si	Si49	1.0	0.45350	0.04081	0.19434	1.0000
Si	Si50	1.0	0.14242	0.47014	0.12335	1.0000
Si	Si51	1.0	0.13916	0.86643	0.12344	1.0000
Si	Si52	1.0	0.52202	0.47766	0.12630	1.0000
Si	Si53	1.0	0.47577	0.52630	0.62551	1.0000
Si	Si54	1.0	0.15795	0.13945	0.37373	1.0000
Si	Si55	1.0	0.53895	0.51591	0.37656	1.0000
Si	Si56	1.0	0.86332	0.84199	0.87384	1.0000
Si	Si57	1.0	0.46917	0.45798	0.87459	1.0000
Si	Si58	1.0	0.79913	0.33828	0.70584	1.0000
Si	Si59	1.0	0.45420	0.70439	0.31206	1.0000
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AlSiAl-T7T7T7T9:

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O	O7	1.0	0.72008	0.65823	0.06147	1.0000
O	O8	1.0	0.85087	0.82528	0.05574	1.0000
O	O9	1.0	0.66722	0.83953	0.10675	1.0000
O	O10	1.0	0.84233	0.48834	0.06262	1.0000
O	O11	1.0	0.65578	0.47597	0.10417	1.0000
O	O12	1.0	0.97686	0.65569	0.05673	1.0000
O	O13	1.0	0.04897	0.83681	0.09291	1.0000
O	O14	1.0	0.04131	0.46897	0.09015	1.0000
O	O15	1.0	0.63189	0.32984	0.55061	1.0000
O	O16	1.0	0.68032	0.17135	0.48833	1.0000
O	O17	1.0	0.73243	0.15543	0.58657	1.0000
O	O18	1.0	0.53234	0.14354	0.55838	1.0000
O	O19	1.0	0.68100	0.50678	0.50040	1.0000
O	O20	1.0	0.76761	0.46840	0.59129	1.0000
O	O21	1.0	0.56095	0.51661	0.58060	1.0000
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O	O24	1.0	0.33534	0.14477	0.60541	1.0000
O	O25	1.0	0.16890	0.50085	0.55030	1.0000
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O	O29	1.0	0.99422	0.50925	0.60555	1.0000
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O	O31	1.0	0.16950	0.33456	0.25333	1.0000
O	O32	1.0	0.20179	0.23027	0.33803	1.0000
O	O33	1.0	0.14414	0.43382	0.33997	1.0000
O	O34	1.0	0.49647	0.34966	0.24410	1.0000
O	O35	1.0	0.48828	0.24049	0.32961	1.0000
O	O36	1.0	0.53828	0.44863	0.32857	1.0000
O	O37	1.0	0.33061	0.71817	0.30723	1.0000
O	O38	1.0	0.15815	0.83668	0.31399	1.0000

O	O39	1.0	0.15663	0.64443	0.35045	1.0000
O	O40	1.0	0.50192	0.84179	0.31308	1.0000
O	O41	1.0	0.50395	0.65105	0.35372	1.0000
O	O42	1.0	0.32964	0.96534	0.30707	1.0000
O	O43	1.0	0.14815	0.02837	0.34838	1.0000
O	O44	1.0	0.50895	0.03498	0.34772	1.0000
O	O45	1.0	0.67163	0.62540	0.81061	1.0000
O	O46	1.0	0.83159	0.64937	0.74318	1.0000
O	O47	1.0	0.83005	0.76419	0.82755	1.0000
O	O48	1.0	0.86322	0.55214	0.82738	1.0000
O	O49	1.0	0.50566	0.64960	0.74895	1.0000
O	O50	1.0	0.53095	0.77380	0.82963	1.0000
O	O51	1.0	0.47703	0.57050	0.84065	1.0000
O	O52	1.0	0.65285	0.28391	0.81004	1.0000
O	O53	1.0	0.82317	0.16330	0.82600	1.0000
O	O54	1.0	0.81589	0.35667	0.86263	1.0000
O	O55	1.0	0.48248	0.16148	0.81553	1.0000
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O	O58	1.0	0.83011	0.96442	0.85635	1.0000
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O	O63	1.0	0.56198	0.85417	0.92170	1.0000
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O	O66	1.0	0.57878	0.46569	0.91406	1.0000
O	O67	1.0	0.29295	0.65099	0.93849	1.0000
O	O68	1.0	0.16939	0.82002	0.92561	1.0000
O	O69	1.0	0.36383	0.81701	0.88930	1.0000
O	O70	1.0	0.16756	0.48179	0.93835	1.0000
O	O71	1.0	0.36517	0.46431	0.90864	1.0000
O	O72	1.0	0.03956	0.65189	0.93254	1.0000

O	O73	1.0	0.97193	0.83536	0.89560	1.0000
O	O74	1.0	0.98034	0.46354	0.89674	1.0000
O	O75	1.0	0.31743	0.32766	0.43506	1.0000
O	O76	1.0	0.35106	0.18078	0.50748	1.0000
O	O77	1.0	0.23496	0.13477	0.42552	1.0000
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O	O81	1.0	0.44837	0.49162	0.41606	1.0000
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O	O89	1.0	0.03141	0.54164	0.40846	1.0000
O	O90	1.0	0.67014	0.36669	0.69961	1.0000
O	O91	1.0	0.83247	0.33035	0.76337	1.0000
O	O92	1.0	0.84152	0.25540	0.66945	1.0000
O	O93	1.0	0.49087	0.31738	0.74695	1.0000
O	O94	1.0	0.52923	0.23447	0.65609	1.0000
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O	O102	1.0	0.49166	0.01007	0.64671	1.0000
O	O103	1.0	0.32963	0.62536	0.19394	1.0000
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O	O109	1.0	0.52556	0.55724	0.17392	1.0000
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O	O127	1.0	0.46606	0.83987	0.06418	1.0000
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Al	Al2	1.0	0.86683	0.53103	0.62545	1.0000
Al	Al3	1.0	0.53837	0.85913	0.12763	1.0000
Al	Al4	1.0	0.84603	0.16032	0.62313	1.0000
Si	Si1	1.0	0.34065	0.54469	0.06105	1.0000
Si	Si2	1.0	0.72629	0.78712	0.06002	1.0000
Si	Si3	1.0	0.72098	0.52984	0.05796	1.0000
Si	Si4	1.0	0.97256	0.78362	0.05020	1.0000
Si	Si5	1.0	0.96320	0.52781	0.05128	1.0000
Si	Si6	1.0	0.65211	0.20359	0.54614	1.0000
Si	Si7	1.0	0.66303	0.45623	0.55665	1.0000
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Si	Si9	1.0	0.28925	0.45799	0.55594	1.0000
Si	Si10	1.0	0.03458	0.20410	0.54853	1.0000
Si	Si11	1.0	0.04456	0.46179	0.55515	1.0000
Si	Si12	1.0	0.21384	0.34552	0.31087	1.0000
Si	Si13	1.0	0.46560	0.35495	0.30352	1.0000
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Si	Si15	1.0	0.45951	0.72018	0.30677	1.0000
Si	Si16	1.0	0.20040	0.95712	0.30437	1.0000
Si	Si17	1.0	0.45898	0.96126	0.30328	1.0000
Si	Si18	1.0	0.14427	0.53285	0.37968	1.0000
Si	Si19	1.0	0.79820	0.64992	0.80298	1.0000
Si	Si20	1.0	0.54527	0.65460	0.80722	1.0000
Si	Si21	1.0	0.78085	0.28300	0.81528	1.0000
Si	Si22	1.0	0.52418	0.28120	0.80331	1.0000
Si	Si23	1.0	0.78423	0.04302	0.81306	1.0000
Si	Si24	1.0	0.52620	0.04337	0.80501	1.0000
Si	Si25	1.0	0.85889	0.47449	0.87677	1.0000
Si	Si26	1.0	0.65696	0.78705	0.94819	1.0000
Si	Si27	1.0	0.66541	0.53637	0.94540	1.0000
Si	Si28	1.0	0.28945	0.77858	0.93553	1.0000
Si	Si29	1.0	0.28850	0.52404	0.94753	1.0000
Si	Si30	1.0	0.04798	0.78029	0.93760	1.0000
Si	Si31	1.0	0.04634	0.52402	0.94103	1.0000
Si	Si32	1.0	0.48294	0.85249	0.87232	1.0000
Si	Si33	1.0	0.33714	0.20248	0.44656	1.0000
Si	Si34	1.0	0.33970	0.45460	0.44368	1.0000
Si	Si35	1.0	0.71231	0.22353	0.43367	1.0000
Si	Si36	1.0	0.71202	0.47311	0.44319	1.0000
Si	Si37	1.0	0.96176	0.22266	0.43836	1.0000
Si	Si38	1.0	0.96026	0.47191	0.44742	1.0000
Si	Si39	1.0	0.52213	0.15237	0.37132	1.0000
Si	Si40	1.0	0.54311	0.33686	0.69105	1.0000
Si	Si41	1.0	0.79530	0.71600	0.69158	1.0000
Si	Si42	1.0	0.53713	0.70977	0.69601	1.0000

Si	Si43	1.0	0.53465	0.95416	0.69622	1.0000
Si	Si44	1.0	0.20486	0.66050	0.19403	1.0000
Si	Si45	1.0	0.45774	0.65686	0.19558	1.0000
Si	Si46	1.0	0.19971	0.28735	0.19806	1.0000
Si	Si47	1.0	0.45657	0.29296	0.19197	1.0000
Si	Si48	1.0	0.20113	0.04495	0.19540	1.0000
Si	Si49	1.0	0.46009	0.04863	0.19333	1.0000
Si	Si50	1.0	0.14237	0.47147	0.12789	1.0000
Si	Si51	1.0	0.16022	0.86207	0.12239	1.0000
Si	Si52	1.0	0.53513	0.47750	0.12641	1.0000
Si	Si53	1.0	0.47154	0.52991	0.62421	1.0000
Si	Si54	1.0	0.15404	0.14149	0.37692	1.0000
Si	Si55	1.0	0.53377	0.53433	0.37462	1.0000
Si	Si56	1.0	0.85026	0.84382	0.87532	1.0000
Si	Si57	1.0	0.47467	0.46575	0.87684	1.0000
Si	Si58	1.0	0.79663	0.34598	0.70455	1.0000
Si	Si59	1.0	0.34057	0.79907	0.04881	1.0000
Si	Si60	1.0	0.79229	0.95689	0.70495	1.0000

AlSiAl-T7T7T9T9

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CRYSTAL DATA

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_cell_length_c	26.238811				
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_cell_angle_beta	91.547363				
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_cell_volume	4111.041693				
_space_group_name_H-M_alt	'P 1'				
_space_group_IT_number	1				

loop_

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'x, y, z'

loop_

_atom_site_label

_atom_site_occupancy

_atom_site_fract_x

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_atom_site_adp_type

_atom_site_U_iso_or_equiv

_atom_site_type_symbol

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H3	1.0	0.073344	0.975749	0.358140	Uiso	? H

H4	1.0	0.861723	0.968176	0.679698	Uiso	? H
O1	1.0	0.314449	0.653612	0.059594	Uiso	? O
O2	1.0	0.333772	0.815777	-0.005220	Uiso	? O
O3	1.0	0.225350	0.840728	0.079210	Uiso	? O
O4	1.0	0.436122	0.821576	0.082961	Uiso	? O
O5	1.0	0.330204	0.499560	0.988775	Uiso	? O
O6	1.0	0.220965	0.465668	0.070668	Uiso	? O
O7	1.0	0.433732	0.480241	0.076683	Uiso	? O
O8	1.0	0.690123	0.676951	0.064612	Uiso	? O
O9	1.0	0.826819	0.838987	0.061977	Uiso	? O
O10	1.0	0.638636	0.867124	0.099565	Uiso	? O
O11	1.0	0.822928	0.510394	0.058617	Uiso	? O
O12	1.0	0.638999	0.489012	0.102982	Uiso	? O
O13	1.0	0.960942	0.672088	0.056732	Uiso	? O
O14	1.0	0.019968	0.856930	0.097594	Uiso	? O
O15	1.0	0.017321	0.485342	0.096059	Uiso	? O
O16	1.0	0.670668	0.324658	0.554131	Uiso	? O
O17	1.0	0.696457	0.159321	0.491137	Uiso	? O
O18	1.0	0.757252	0.139551	0.590472	Uiso	? O
O19	1.0	0.555141	0.149884	0.562406	Uiso	? O
O20	1.0	0.700530	0.500478	0.501436	Uiso	? O
O21	1.0	0.773786	0.485905	0.597653	Uiso	? O
O22	1.0	0.565615	0.504831	0.576507	Uiso	? O
O23	1.0	0.298360	0.323133	0.571971	Uiso	? O
O24	1.0	0.176514	0.151394	0.554913	Uiso	? O
O25	1.0	0.361889	0.134648	0.608923	Uiso	? O
O26	1.0	0.176624	0.493632	0.553583	Uiso	? O
O27	1.0	0.362320	0.513547	0.602681	Uiso	? O
O28	1.0	0.051993	0.322957	0.560008	Uiso	? O
O29	1.0	0.986706	0.141254	0.599622	Uiso	? O
O30	1.0	0.004322	0.503578	0.609078	Uiso	? O
O31	1.0	0.345319	0.372452	0.314195	Uiso	? O
O32	1.0	0.184203	0.348220	0.247967	Uiso	? O
O33	1.0	0.203627	0.214938	0.326643	Uiso	? O

O34	1.0	0.148209	0.420259	0.340332	Uiso	? O
O35	1.0	0.494283	0.337364	0.244991	Uiso	? O
O36	1.0	0.498097	0.224974	0.329925	Uiso	? O
O37	1.0	0.544849	0.434118	0.330358	Uiso	? O
O38	1.0	0.330528	0.702068	0.311213	Uiso	? O
O39	1.0	0.157080	0.819767	0.302355	Uiso	? O
O40	1.0	0.148201	0.632776	0.346790	Uiso	? O
O41	1.0	0.497426	0.829071	0.316175	Uiso	? O
O42	1.0	0.507439	0.636795	0.356483	Uiso	? O
O43	1.0	0.326126	0.956406	0.308652	Uiso	? O
O44	1.0	0.505477	0.022333	0.355051	Uiso	? O
O45	1.0	0.648216	0.673730	0.807454	Uiso	? O
O46	1.0	0.821010	0.657195	0.747967	Uiso	? O
O47	1.0	0.839347	0.724957	0.844366	Uiso	? O
O48	1.0	0.797689	0.523808	0.824065	Uiso	? O
O49	1.0	0.491405	0.675624	0.736771	Uiso	? O
O50	1.0	0.471424	0.783055	0.822746	Uiso	? O
O51	1.0	0.464738	0.570489	0.821966	Uiso	? O
O52	1.0	0.665866	0.280266	0.810643	Uiso	? O
O53	1.0	0.827424	0.143254	0.817385	Uiso	? O
O54	1.0	0.840730	0.332281	0.863420	Uiso	? O
O55	1.0	0.484562	0.175243	0.812644	Uiso	? O
O56	1.0	0.492488	0.368020	0.849757	Uiso	? O
O57	1.0	0.645415	0.034720	0.829106	Uiso	? O
O58	1.0	0.832624	0.931740	0.824027	Uiso	? O
O59	1.0	0.452081	0.985061	0.852567	Uiso	? O
O60	1.0	0.677114	0.674032	0.936838	Uiso	? O
O61	1.0	0.656997	0.839203	0.999631	Uiso	? O
O62	1.0	0.752383	0.861139	0.910565	Uiso	? O
O63	1.0	0.542511	0.837144	0.915111	Uiso	? O
O64	1.0	0.640986	0.516363	0.003099	Uiso	? O
O65	1.0	0.745521	0.478361	0.919515	Uiso	? O
O66	1.0	0.535305	0.523553	0.915632	Uiso	? O
O67	1.0	0.272312	0.663109	0.930112	Uiso	? O

O68	1.0	0.153713	0.840105	0.939896	Uiso	? O
O69	1.0	0.335426	0.845639	0.894336	Uiso	? O
O70	1.0	0.147284	0.495603	0.932875	Uiso	? O
O71	1.0	0.335589	0.480828	0.888650	Uiso	? O
O72	1.0	0.025219	0.672461	0.938883	Uiso	? O
O73	1.0	0.962020	0.857417	0.897068	Uiso	? O
O74	1.0	0.950875	0.497421	0.895735	Uiso	? O
O75	1.0	0.321687	0.318980	0.437009	Uiso	? O
O76	1.0	0.367210	0.172637	0.510729	Uiso	? O
O77	1.0	0.265067	0.117952	0.423146	Uiso	? O
O78	1.0	0.471762	0.168900	0.427530	Uiso	? O
O79	1.0	0.357277	0.472106	0.504697	Uiso	? O
O80	1.0	0.256229	0.516920	0.416120	Uiso	? O
O81	1.0	0.462334	0.475551	0.420233	Uiso	? O
O82	1.0	0.687809	0.336696	0.435827	Uiso	? O
O83	1.0	0.849403	0.198520	0.426193	Uiso	? O
O84	1.0	0.660016	0.149490	0.389898	Uiso	? O
O85	1.0	0.849598	0.473198	0.431087	Uiso	? O
O86	1.0	0.659715	0.533914	0.402901	Uiso	? O
O87	1.0	0.011250	0.333260	0.442175	Uiso	? O
O88	1.0	0.039821	0.144178	0.400049	Uiso	? O
O89	1.0	0.044180	0.529342	0.412362	Uiso	? O
O90	1.0	0.686201	0.371297	0.703549	Uiso	? O
O91	1.0	0.849289	0.318321	0.763274	Uiso	? O
O92	1.0	0.857578	0.269580	0.663831	Uiso	? O
O93	1.0	0.504535	0.340714	0.749313	Uiso	? O
O94	1.0	0.527344	0.272046	0.653218	Uiso	? O
O95	1.0	0.514524	0.478526	0.674345	Uiso	? O
O96	1.0	0.667968	0.705302	0.684019	Uiso	? O
O97	1.0	0.822909	0.851384	0.694757	Uiso	? O
O98	1.0	0.864071	0.667205	0.650599	Uiso	? O
O99	1.0	0.515111	0.850632	0.683360	Uiso	? O
O100	1.0	0.487358	0.666841	0.634296	Uiso	? O
O101	1.0	0.686170	0.936462	0.730182	Uiso	? O

O102	1.0	0.559874	0.050917	0.659865	Uiso	? O
O103	1.0	0.338197	0.688365	0.186864	Uiso	? O
O104	1.0	0.174987	0.643625	0.246810	Uiso	? O
O105	1.0	0.152199	0.778754	0.169416	Uiso	? O
O106	1.0	0.173405	0.569305	0.153991	Uiso	? O
O107	1.0	0.497454	0.657010	0.255396	Uiso	? O
O108	1.0	0.532767	0.756365	0.168758	Uiso	? O
O109	1.0	0.492240	0.547405	0.169695	Uiso	? O
O110	1.0	0.331921	0.290757	0.181459	Uiso	? O
O111	1.0	0.158728	0.171618	0.191118	Uiso	? O
O112	1.0	0.142081	0.359174	0.148901	Uiso	? O
O113	1.0	0.500712	0.159393	0.189701	Uiso	? O
O114	1.0	0.518665	0.345051	0.145057	Uiso	? O
O115	1.0	0.327288	0.040374	0.196208	Uiso	? O
O116	1.0	0.151939	0.984499	0.145079	Uiso	? O
O117	1.0	0.498155	0.964391	0.153380	Uiso	? O
O118	1.0	-0.016240	0.840981	-0.002780	Uiso	? O
O119	1.0	0.985196	0.503731	0.996026	Uiso	? O
O120	1.0	-0.003397	0.160355	0.499473	Uiso	? O
O121	1.0	0.986792	0.493985	0.508192	Uiso	? O
O122	1.0	0.155615	0.994952	0.246479	Uiso	? O
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O124	1.0	0.735889	0.035092	0.740843	Uiso	? O
O125	1.0	0.498446	0.002426	0.754585	Uiso	? O
O126	1.0	0.871728	0.469367	0.695468	Uiso	? O
O127	1.0	0.142281	0.002409	0.347486	Uiso	? O
O128	1.0	0.881352	0.045650	0.679847	Uiso	? O
Al1	1.0	0.494868	0.151661	0.626192	Uiso	? Al
Al2	1.0	0.881394	0.535662	0.631251	Uiso	? Al
Al3	1.0	0.166244	0.136954	0.377249	Uiso	? Al
Al4	1.0	0.868198	0.146922	0.632329	Uiso	? Al
Si1	1.0	0.327713	0.782548	0.054464	Uiso	? Si
Si2	1.0	0.325482	0.525310	0.049277	Uiso	? Si
Si3	1.0	0.703202	0.804688	0.055925	Uiso	? Si

Si4	1.0	0.698994	0.548355	0.057249	Uiso	? Si
Si5	1.0	0.948278	0.801182	0.053139	Uiso	? Si
Si6	1.0	0.946337	0.543519	0.051627	Uiso	? Si
Si7	1.0	0.525078	0.851748	0.126592	Uiso	? Si
Si8	1.0	0.679661	0.195815	0.549890	Uiso	? Si
Si9	1.0	0.679497	0.454709	0.558566	Uiso	? Si
Si10	1.0	0.297356	0.194152	0.563355	Uiso	? Si
Si11	1.0	0.297883	0.449363	0.558123	Uiso	? Si
Si12	1.0	0.052212	0.193136	0.554441	Uiso	? Si
Si13	1.0	0.054171	0.452948	0.559058	Uiso	? Si
Si14	1.0	0.219875	0.335992	0.308201	Uiso	? Si
Si15	1.0	0.470005	0.341587	0.305426	Uiso	? Si
Si16	1.0	0.203279	0.697139	0.302002	Uiso	? Si
Si17	1.0	0.459204	0.705837	0.309631	Uiso	? Si
Si18	1.0	0.457161	0.951547	0.308582	Uiso	? Si
Si19	1.0	0.150234	0.521775	0.379149	Uiso	? Si
Si20	1.0	0.774891	0.646427	0.805235	Uiso	? Si
Si21	1.0	0.518983	0.674751	0.797232	Uiso	? Si
Si22	1.0	0.794685	0.270230	0.813269	Uiso	? Si
Si23	1.0	0.537010	0.292780	0.804722	Uiso	? Si
Si24	1.0	0.763991	0.034220	0.806299	Uiso	? Si
Si25	1.0	0.519262	0.050932	0.811730	Uiso	? Si
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Si27	1.0	0.656508	0.802596	0.940333	Uiso	? Si
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Si29	1.0	0.273639	0.790566	0.940346	Uiso	? Si
Si30	1.0	0.270954	0.534089	0.935242	Uiso	? Si
Si31	1.0	0.031199	0.801709	0.943340	Uiso	? Si
Si32	1.0	0.027727	0.542793	0.941131	Uiso	? Si
Si33	1.0	0.451980	0.861076	0.871161	Uiso	? Si
Si34	1.0	0.353188	0.193672	0.449010	Uiso	? Si
Si35	1.0	0.349026	0.445613	0.444416	Uiso	? Si
Si36	1.0	0.724111	0.211415	0.436100	Uiso	? Si
Si37	1.0	0.725298	0.460441	0.444194	Uiso	? Si

Si38	1.0	0.974914	0.207780	0.442293	Uiso	? Si
Si39	1.0	0.972700	0.456637	0.449237	Uiso	? Si
Si40	1.0	0.533427	0.142390	0.375300	Uiso	? Si
Si41	1.0	0.557531	0.362158	0.693699	Uiso	? Si
Si42	1.0	0.795110	0.724695	0.693145	Uiso	? Si
Si43	1.0	0.540401	0.722532	0.684384	Uiso	? Si
Si44	1.0	0.556624	0.964627	0.702943	Uiso	? Si
Si45	1.0	0.209978	0.668757	0.188861	Uiso	? Si
Si46	1.0	0.465152	0.661737	0.195139	Uiso	? Si
Si47	1.0	0.205177	0.292778	0.193316	Uiso	? Si
Si48	1.0	0.460499	0.283154	0.190878	Uiso	? Si
Si49	1.0	0.198781	0.048851	0.194223	Uiso	? Si
Si50	1.0	0.456303	0.039897	0.198574	Uiso	? Si
Si51	1.0	0.138756	0.470118	0.117609	Uiso	? Si
Si52	1.0	0.138656	0.864183	0.122806	Uiso	? Si
Si53	1.0	0.520319	0.466386	0.123438	Uiso	? Si
Si54	1.0	0.483928	0.538631	0.620788	Uiso	? Si
Si55	1.0	0.542016	0.519310	0.377427	Uiso	? Si
Si56	1.0	0.845896	0.843078	0.869518	Uiso	? Si
Si57	1.0	0.457180	0.485776	0.868596	Uiso	? Si
Si58	1.0	0.813128	0.348718	0.704885	Uiso	? Si
Si59	1.0	0.200473	0.940125	0.298314	Uiso	? Si

T1T7T7T7T7:

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_cell_length_c 26.4417
_cell_angle_alpha 89.8792
_cell_angle_beta 89.9276
_cell_angle_gamma 91.0103

_space_group_name_H-M_alt "P 1"
_space_group_IT_number 1

loop_

_space_group_symop_operation_xyz
'x, y, z'

loop_

_atom_site_type_symbol
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_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
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H H2 1.0 0.85965 0.51665 0.71693 1.0000
H H3 1.0 0.52013 0.86151 0.03291 1.0000
H H4 1.0 0.12802 0.82433 0.36097 1.0000
H H5 1.0 0.13835 0.48349 0.21708 1.0000
O O1 1.0 0.37345 0.66924 0.05050 1.0000
O O2 1.0 0.32596 0.83116 0.98915 1.0000
O O3 1.0 0.26162 0.83493 0.08589 1.0000

O	O4	1.0	0.31111	0.48805	0.00575	1.0000
O	O5	1.0	0.23847	0.53778	0.09710	1.0000
O	O6	1.0	0.44211	0.48244	0.08140	1.0000
O	O7	1.0	0.71956	0.66107	0.05924	1.0000
O	O8	1.0	0.84964	0.83138	0.05467	1.0000
O	O9	1.0	0.66672	0.83984	0.10599	1.0000
O	O10	1.0	0.83336	0.48713	0.05254	1.0000
O	O11	1.0	0.64927	0.47926	0.10024	1.0000
O	O12	1.0	0.96583	0.65771	0.05233	1.0000
O	O13	1.0	0.04850	0.83487	0.09185	1.0000
O	O14	1.0	0.01459	0.48080	0.10092	1.0000
O	O15	1.0	0.62821	0.33244	0.55159	1.0000
O	O16	1.0	0.67490	0.17192	0.49002	1.0000
O	O17	1.0	0.73640	0.16297	0.58719	1.0000
O	O18	1.0	0.53268	0.14157	0.56061	1.0000
O	O19	1.0	0.68262	0.51550	0.50511	1.0000
O	O20	1.0	0.76550	0.46523	0.59449	1.0000
O	O21	1.0	0.55957	0.51843	0.58356	1.0000
O	O22	1.0	0.28049	0.33466	0.56003	1.0000
O	O23	1.0	0.14860	0.16650	0.55302	1.0000
O	O24	1.0	0.32966	0.15381	0.60571	1.0000
O	O25	1.0	0.16875	0.50980	0.55254	1.0000
O	O26	1.0	0.35148	0.51616	0.60134	1.0000
O	O27	1.0	0.03340	0.34155	0.55280	1.0000
O	O28	1.0	0.95033	0.16235	0.59116	1.0000
O	O29	1.0	0.98912	0.51810	0.60291	1.0000
O	O30	1.0	0.33031	0.37892	0.31009	1.0000
O	O31	1.0	0.17114	0.34119	0.24349	1.0000
O	O32	1.0	0.18497	0.22491	0.32762	1.0000
O	O33	1.0	0.13304	0.43205	0.33058	1.0000
O	O34	1.0	0.49703	0.34790	0.24938	1.0000
O	O35	1.0	0.46419	0.22377	0.33057	1.0000
O	O36	1.0	0.52896	0.42528	0.33985	1.0000
O	O37	1.0	0.35147	0.72191	0.30730	1.0000

O	O38	1.0	0.19516	0.62620	0.35903	1.0000
O	O39	1.0	0.52751	0.83795	0.31673	1.0000
O	O40	1.0	0.52971	0.63769	0.34187	1.0000
O	O41	1.0	0.35661	0.96445	0.31673	1.0000
O	O42	1.0	0.15649	0.02901	0.36095	1.0000
O	O43	1.0	0.54580	0.03330	0.34677	1.0000
O	O44	1.0	0.66821	0.62124	0.81004	1.0000
O	O45	1.0	0.82602	0.65690	0.74225	1.0000
O	O46	1.0	0.82137	0.76585	0.82810	1.0000
O	O47	1.0	0.86346	0.55625	0.82653	1.0000
O	O48	1.0	0.50272	0.65253	0.74940	1.0000
O	O49	1.0	0.53388	0.77567	0.83069	1.0000
O	O50	1.0	0.46950	0.57440	0.84006	1.0000
O	O51	1.0	0.65132	0.29420	0.80816	1.0000
O	O52	1.0	0.81398	0.16381	0.82601	1.0000
O	O53	1.0	0.81720	0.36023	0.85905	1.0000
O	O54	1.0	0.48747	0.16247	0.81894	1.0000
O	O55	1.0	0.46479	0.36198	0.84153	1.0000
O	O56	1.0	0.65233	0.02652	0.81309	1.0000
O	O57	1.0	0.83624	0.96691	0.85344	1.0000
O	O58	1.0	0.46385	0.96894	0.84816	1.0000
O	O59	1.0	0.62749	0.66762	0.93920	1.0000
O	O60	1.0	0.65757	0.82668	0.00696	1.0000
O	O61	1.0	0.76956	0.82379	0.92202	1.0000
O	O62	1.0	0.55884	0.86160	0.92209	1.0000
O	O63	1.0	0.65482	0.50215	0.00036	1.0000
O	O64	1.0	0.77939	0.53011	0.91865	1.0000
O	O65	1.0	0.57768	0.46936	0.90959	1.0000
O	O66	1.0	0.29226	0.64897	0.94258	1.0000
O	O67	1.0	0.16701	0.81430	0.92314	1.0000
O	O68	1.0	0.36344	0.81085	0.88980	1.0000
O	O69	1.0	0.16495	0.48193	0.93251	1.0000
O	O70	1.0	0.36543	0.46372	0.91034	1.0000
O	O71	1.0	0.03305	0.64999	0.93622	1.0000

O	O72	1.0	0.96995	0.83088	0.89418	1.0000
O	O73	1.0	0.97337	0.46360	0.90019	1.0000
O	O74	1.0	0.38020	0.32838	0.44012	1.0000
O	O75	1.0	0.34368	0.16980	0.50709	1.0000
O	O76	1.0	0.22715	0.18261	0.42422	1.0000
O	O77	1.0	0.43651	0.13156	0.42020	1.0000
O	O78	1.0	0.34915	0.49293	0.50175	1.0000
O	O79	1.0	0.22256	0.46130	0.42163	1.0000
O	O80	1.0	0.42296	0.52825	0.41077	1.0000
O	O81	1.0	0.71234	0.35508	0.44367	1.0000
O	O82	1.0	0.83096	0.18823	0.42242	1.0000
O	O83	1.0	0.63119	0.19650	0.39183	1.0000
O	O84	1.0	0.83562	0.52662	0.43445	1.0000
O	O85	1.0	0.63622	0.53684	0.40841	1.0000
O	O86	1.0	0.96131	0.35511	0.43804	1.0000
O	O87	1.0	0.02878	0.18054	0.39351	1.0000
O	O88	1.0	0.03142	0.53941	0.40291	1.0000
O	O89	1.0	0.66936	0.36471	0.69799	1.0000
O	O90	1.0	0.83242	0.32129	0.75947	1.0000
O	O91	1.0	0.83999	0.26019	0.66233	1.0000
O	O92	1.0	0.48889	0.30979	0.74586	1.0000
O	O93	1.0	0.52777	0.23879	0.65319	1.0000
O	O94	1.0	0.48425	0.44427	0.67128	1.0000
O	O95	1.0	0.66035	0.71750	0.68920	1.0000
O	O96	1.0	0.83086	0.84835	0.69396	1.0000
O	O97	1.0	0.84017	0.66538	0.64328	1.0000
O	O98	1.0	0.48854	0.83347	0.69873	1.0000
O	O99	1.0	0.47515	0.65022	0.65026	1.0000
O	O100	1.0	0.65868	0.96661	0.69593	1.0000
O	O101	1.0	0.83692	0.04705	0.65590	1.0000
O	O102	1.0	0.48016	0.01277	0.64833	1.0000
O	O103	1.0	0.33066	0.63164	0.19927	1.0000
O	O104	1.0	0.16969	0.67732	0.26037	1.0000
O	O105	1.0	0.16190	0.74234	0.16365	1.0000

O	O106	1.0	0.51164	0.68623	0.24553	1.0000
O	O107	1.0	0.46638	0.76435	0.15435	1.0000
O	O108	1.0	0.51650	0.55876	0.16854	1.0000
O	O109	1.0	0.33810	0.28287	0.19099	1.0000
O	O110	1.0	0.16850	0.15065	0.19407	1.0000
O	O111	1.0	0.15989	0.33570	0.14445	1.0000
O	O112	1.0	0.51139	0.16753	0.19808	1.0000
O	O113	1.0	0.52136	0.35135	0.15014	1.0000
O	O114	1.0	0.34150	0.03438	0.19500	1.0000
O	O115	1.0	0.16462	0.95597	0.15273	1.0000
O	O116	1.0	0.52097	0.98868	0.14773	1.0000
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O	O118	1.0	0.01072	0.48596	0.99979	1.0000
O	O119	1.0	0.98099	0.17895	0.49270	1.0000
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O	O121	1.0	0.17377	0.97624	0.25191	1.0000
O	O122	1.0	0.51391	0.98792	0.24849	1.0000
O	O123	1.0	0.82459	0.01576	0.75470	1.0000
O	O124	1.0	0.48819	0.01337	0.74930	1.0000
O	O125	1.0	0.85819	0.46393	0.68899	1.0000
O	O126	1.0	0.46614	0.86036	0.06049	1.0000
O	O127	1.0	0.17730	0.82472	0.33240	1.0000
O	O128	1.0	0.13939	0.53719	0.18944	1.0000
Al	Al1	1.0	0.46001	0.13612	0.62375	1.0000
Al	Al2	1.0	0.86371	0.53596	0.62589	1.0000
Al	Al3	1.0	0.53743	0.86434	0.12394	1.0000
Al	Al4	1.0	0.22086	0.96431	0.31250	1.0000
Al	Al5	1.0	0.13797	0.46457	0.12603	1.0000
Si	Si1	1.0	0.33894	0.54350	0.05982	1.0000
Si	Si2	1.0	0.72583	0.79016	0.05852	1.0000
Si	Si3	1.0	0.71411	0.53269	0.05356	1.0000
Si	Si4	1.0	0.96984	0.78591	0.04837	1.0000
Si	Si5	1.0	0.95714	0.52779	0.05239	1.0000
Si	Si6	1.0	0.64958	0.20672	0.54770	1.0000

Si	Si7	1.0	0.66146	0.45883	0.55979	1.0000
Si	Si8	1.0	0.27283	0.20563	0.55806	1.0000
Si	Si9	1.0	0.28751	0.46301	0.55455	1.0000
Si	Si10	1.0	0.02871	0.21345	0.54777	1.0000
Si	Si11	1.0	0.04425	0.47142	0.55368	1.0000
Si	Si12	1.0	0.20554	0.34161	0.30321	1.0000
Si	Si13	1.0	0.45553	0.34329	0.30729	1.0000
Si	Si14	1.0	0.48180	0.72132	0.30247	1.0000
Si	Si15	1.0	0.48218	0.95742	0.30630	1.0000
Si	Si16	1.0	0.14603	0.51222	0.37873	1.0000
Si	Si17	1.0	0.79409	0.65195	0.80231	1.0000
Si	Si18	1.0	0.54321	0.65621	0.80744	1.0000
Si	Si19	1.0	0.77856	0.28421	0.81341	1.0000
Si	Si20	1.0	0.52303	0.28237	0.80331	1.0000
Si	Si21	1.0	0.78107	0.04202	0.81129	1.0000
Si	Si22	1.0	0.52431	0.04253	0.80635	1.0000
Si	Si23	1.0	0.85667	0.47789	0.87612	1.0000
Si	Si24	1.0	0.65500	0.79398	0.94702	1.0000
Si	Si25	1.0	0.66004	0.54204	0.94215	1.0000
Si	Si26	1.0	0.28656	0.77617	0.93602	1.0000
Si	Si27	1.0	0.28388	0.52067	0.94808	1.0000
Si	Si28	1.0	0.04525	0.77883	0.93720	1.0000
Si	Si29	1.0	0.04502	0.52174	0.94325	1.0000
Si	Si30	1.0	0.48040	0.85296	0.87278	1.0000
Si	Si31	1.0	0.34527	0.20286	0.44693	1.0000
Si	Si32	1.0	0.34380	0.45246	0.44376	1.0000
Si	Si33	1.0	0.71236	0.22774	0.43659	1.0000
Si	Si34	1.0	0.71627	0.48351	0.44814	1.0000
Si	Si35	1.0	0.95182	0.22604	0.43708	1.0000
Si	Si36	1.0	0.95440	0.48313	0.44532	1.0000
Si	Si37	1.0	0.51909	0.14613	0.37228	1.0000
Si	Si38	1.0	0.54133	0.33697	0.69095	1.0000
Si	Si39	1.0	0.78956	0.72458	0.69055	1.0000
Si	Si40	1.0	0.53201	0.71358	0.69644	1.0000

Si	Si41	1.0	0.78696	0.96913	0.69981	1.0000
Si	Si42	1.0	0.52865	0.95734	0.69707	1.0000
Si	Si43	1.0	0.45789	0.66282	0.19056	1.0000
Si	Si44	1.0	0.20892	0.27419	0.19153	1.0000
Si	Si45	1.0	0.46659	0.28674	0.19662	1.0000
Si	Si46	1.0	0.21244	0.02882	0.19932	1.0000
Si	Si47	1.0	0.47128	0.04336	0.19658	1.0000
Si	Si48	1.0	0.15863	0.84318	0.12371	1.0000
Si	Si49	1.0	0.53134	0.46895	0.12514	1.0000
Si	Si50	1.0	0.84121	0.15765	0.62407	1.0000
Si	Si51	1.0	0.46852	0.53115	0.62655	1.0000
Si	Si52	1.0	0.14923	0.15175	0.37658	1.0000
Si	Si53	1.0	0.52896	0.53075	0.37523	1.0000
Si	Si54	1.0	0.84921	0.84671	0.87445	1.0000
Si	Si55	1.0	0.47012	0.46818	0.87535	1.0000
Si	Si56	1.0	0.79539	0.34580	0.70202	1.0000
Si	Si57	1.0	0.35020	0.79469	0.04676	1.0000
Si	Si58	1.0	0.22642	0.70586	0.31385	1.0000
Si	Si59	1.0	0.20517	0.65372	0.20190	1.0000

T1T7T7T7T9:

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H	H2	1.0	0.85659	0.52627	0.71536	1.0000
H	H3	1.0	0.09398	0.97324	0.37117	1.0000
H	H4	1.0	0.17543	0.89137	0.89746	1.0000
H	H5	1.0	0.16122	0.46921	0.21287	1.0000
O	O1	1.0	0.37439	0.67160	0.05435	1.0000
O	O2	1.0	0.32706	0.83755	0.99532	1.0000
O	O3	1.0	0.23316	0.81782	0.08498	1.0000

O	O4	1.0	0.43753	0.86948	0.07809	1.0000
O	O5	1.0	0.33234	0.49574	0.00076	1.0000
O	O6	1.0	0.22873	0.53373	0.08695	1.0000
O	O7	1.0	0.43318	0.47760	0.08570	1.0000
O	O8	1.0	0.70404	0.67362	0.06058	1.0000
O	O9	1.0	0.83879	0.84033	0.05883	1.0000
O	O10	1.0	0.64673	0.86038	0.09637	1.0000
O	O11	1.0	0.82452	0.50008	0.06056	1.0000
O	O12	1.0	0.63907	0.49522	0.10520	1.0000
O	O13	1.0	0.95795	0.66642	0.06071	1.0000
O	O14	1.0	0.02598	0.84633	0.10162	1.0000
O	O15	1.0	0.01004	0.48110	0.10455	1.0000
O	O16	1.0	0.64123	0.33416	0.55411	1.0000
O	O17	1.0	0.67026	0.16650	0.49329	1.0000
O	O18	1.0	0.74053	0.15954	0.58859	1.0000
O	O19	1.0	0.53340	0.15225	0.56643	1.0000
O	O20	1.0	0.69103	0.50957	0.50099	1.0000
O	O21	1.0	0.75818	0.48626	0.59575	1.0000
O	O22	1.0	0.55276	0.51871	0.57418	1.0000
O	O23	1.0	0.28090	0.34603	0.55809	1.0000
O	O24	1.0	0.15444	0.17239	0.56144	1.0000
O	O25	1.0	0.33571	0.17660	0.61367	1.0000
O	O26	1.0	0.16495	0.51796	0.54727	1.0000
O	O27	1.0	0.34831	0.53256	0.59544	1.0000
O	O28	1.0	0.03698	0.34375	0.55041	1.0000
O	O29	1.0	0.95368	0.17135	0.59639	1.0000
O	O30	1.0	0.98530	0.52003	0.59752	1.0000
O	O31	1.0	0.34287	0.36789	0.30198	1.0000
O	O32	1.0	0.18154	0.34022	0.23761	1.0000
O	O33	1.0	0.19325	0.21927	0.32169	1.0000
O	O34	1.0	0.14854	0.43020	0.32419	1.0000
O	O35	1.0	0.51060	0.30497	0.24830	1.0000
O	O36	1.0	0.46900	0.21622	0.33845	1.0000
O	O37	1.0	0.53720	0.41780	0.33182	1.0000

O	O38	1.0	0.35087	0.70393	0.30788	1.0000
O	O39	1.0	0.17940	0.82041	0.32294	1.0000
O	O40	1.0	0.18923	0.62491	0.35954	1.0000
O	O41	1.0	0.51467	0.83356	0.31668	1.0000
O	O42	1.0	0.53813	0.62988	0.33693	1.0000
O	O43	1.0	0.34337	0.96110	0.31881	1.0000
O	O44	1.0	0.52780	0.01824	0.35825	1.0000
O	O45	1.0	0.67508	0.64751	0.81362	1.0000
O	O46	1.0	0.82649	0.65489	0.74161	1.0000
O	O47	1.0	0.84283	0.78011	0.82021	1.0000
O	O48	1.0	0.86313	0.56668	0.83120	1.0000
O	O49	1.0	0.52013	0.64596	0.74517	1.0000
O	O50	1.0	0.51319	0.77854	0.82359	1.0000
O	O51	1.0	0.48353	0.56975	0.83581	1.0000
O	O52	1.0	0.64257	0.29772	0.81119	1.0000
O	O53	1.0	0.80760	0.17080	0.82686	1.0000
O	O54	1.0	0.81203	0.36793	0.85874	1.0000
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O	O56	1.0	0.45697	0.35928	0.84753	1.0000
O	O57	1.0	0.64124	0.04226	0.81095	1.0000
O	O58	1.0	0.81332	0.97238	0.85704	1.0000
O	O59	1.0	0.45545	0.97565	0.84595	1.0000
O	O60	1.0	0.61504	0.66948	0.94005	1.0000
O	O61	1.0	0.66827	0.83610	0.99828	1.0000
O	O62	1.0	0.77633	0.79902	0.91458	1.0000
O	O63	1.0	0.57493	0.86685	0.91082	1.0000
O	O64	1.0	0.64980	0.50769	0.00451	1.0000
O	O65	1.0	0.76424	0.52833	0.91965	1.0000
O	O66	1.0	0.55808	0.47099	0.91759	1.0000
O	O67	1.0	0.27135	0.66063	0.94660	1.0000
O	O68	1.0	0.37118	0.81701	0.89588	1.0000
O	O69	1.0	0.15776	0.48255	0.94157	1.0000
O	O70	1.0	0.34801	0.48914	0.90151	1.0000
O	O71	1.0	0.03351	0.65478	0.93614	1.0000

O	O72	1.0	0.97339	0.85745	0.89183	1.0000
O	O73	1.0	0.96391	0.46575	0.90628	1.0000
O	O74	1.0	0.38398	0.32735	0.44497	1.0000
O	O75	1.0	0.34784	0.17230	0.51456	1.0000
O	O76	1.0	0.24528	0.16800	0.42610	1.0000
O	O77	1.0	0.45470	0.13446	0.43268	1.0000
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O	O81	1.0	0.71133	0.34241	0.44149	1.0000
O	O82	1.0	0.83485	0.17052	0.43107	1.0000
O	O83	1.0	0.64467	0.17395	0.39247	1.0000
O	O84	1.0	0.83618	0.51103	0.42732	1.0000
O	O85	1.0	0.63525	0.52340	0.40523	1.0000
O	O86	1.0	0.96173	0.34001	0.43965	1.0000
O	O87	1.0	0.02873	0.15948	0.39791	1.0000
O	O88	1.0	0.03028	0.51768	0.39624	1.0000
O	O89	1.0	0.66513	0.38408	0.69679	1.0000
O	O90	1.0	0.82120	0.32975	0.75978	1.0000
O	O91	1.0	0.83126	0.26792	0.66307	1.0000
O	O92	1.0	0.48680	0.34224	0.74855	1.0000
O	O93	1.0	0.53603	0.23074	0.66592	1.0000
O	O94	1.0	0.47593	0.43577	0.66039	1.0000
O	O95	1.0	0.66980	0.71879	0.68233	1.0000
O	O96	1.0	0.83294	0.85319	0.69754	1.0000
O	O97	1.0	0.85808	0.67546	0.64397	1.0000
O	O98	1.0	0.49509	0.82901	0.69599	1.0000
O	O99	1.0	0.48503	0.64722	0.64666	1.0000
O	O100	1.0	0.65827	0.96949	0.69575	1.0000
O	O101	1.0	0.84014	0.05297	0.66017	1.0000
O	O102	1.0	0.47887	0.01136	0.64670	1.0000
O	O103	1.0	0.33049	0.66132	0.19018	1.0000
O	O104	1.0	0.17422	0.65772	0.25962	1.0000
O	O105	1.0	0.14017	0.73438	0.16655	1.0000

O	O106	1.0	0.50838	0.69314	0.24256	1.0000
O	O107	1.0	0.50880	0.73186	0.14493	1.0000
O	O108	1.0	0.49497	0.53315	0.17810	1.0000
O	O109	1.0	0.34680	0.27045	0.18759	1.0000
O	O110	1.0	0.17562	0.14620	0.19203	1.0000
O	O111	1.0	0.17036	0.32964	0.13871	1.0000
O	O112	1.0	0.51351	0.14461	0.18239	1.0000
O	O113	1.0	0.52990	0.33934	0.14798	1.0000
O	O114	1.0	0.34315	0.01639	0.19626	1.0000
O	O115	1.0	0.16333	0.94635	0.15799	1.0000
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O	O121	1.0	0.17743	0.98190	0.25609	1.0000
O	O122	1.0	0.50693	0.00744	0.25841	1.0000
O	O123	1.0	0.81806	0.01941	0.75782	1.0000
O	O124	1.0	0.48180	0.00699	0.74706	1.0000
O	O125	1.0	0.85828	0.47117	0.68815	1.0000
O	O126	1.0	0.15494	0.01098	0.35612	1.0000
O	O127	1.0	0.17459	0.83903	0.92509	1.0000
O	O128	1.0	0.15915	0.52591	0.18568	1.0000
Al	Al1	1.0	0.46355	0.14239	0.62968	1.0000
Al	Al2	1.0	0.86571	0.54469	0.62469	1.0000
Al	Al3	1.0	0.15744	0.15518	0.37728	1.0000
Al	Al4	1.0	0.03456	0.79085	0.94108	1.0000
Al	Al5	1.0	0.13847	0.45946	0.12187	1.0000
Si	Si1	1.0	0.34224	0.79699	0.05410	1.0000
Si	Si2	1.0	0.33973	0.54433	0.05771	1.0000
Si	Si3	1.0	0.71658	0.80179	0.05319	1.0000
Si	Si4	1.0	0.70531	0.54431	0.05746	1.0000
Si	Si5	1.0	0.95991	0.79562	0.05401	1.0000
Si	Si6	1.0	0.94935	0.53644	0.05813	1.0000

Si	Si7	1.0	0.52928	0.85059	0.12067	1.0000
Si	Si8	1.0	0.65265	0.20686	0.55062	1.0000
Si	Si9	1.0	0.66338	0.46379	0.55745	1.0000
Si	Si10	1.0	0.27689	0.21667	0.56377	1.0000
Si	Si11	1.0	0.28490	0.47463	0.54989	1.0000
Si	Si12	1.0	0.03404	0.21483	0.55183	1.0000
Si	Si13	1.0	0.04260	0.47404	0.54890	1.0000
Si	Si14	1.0	0.21668	0.33536	0.29784	1.0000
Si	Si15	1.0	0.46515	0.32624	0.30490	1.0000
Si	Si16	1.0	0.22375	0.70011	0.31269	1.0000
Si	Si17	1.0	0.47844	0.71392	0.30121	1.0000
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Si	Si19	1.0	0.14888	0.50455	0.37453	1.0000
Si	Si20	1.0	0.80171	0.66329	0.80260	1.0000
Si	Si21	1.0	0.54805	0.66051	0.80445	1.0000
Si	Si22	1.0	0.77035	0.29154	0.81434	1.0000
Si	Si23	1.0	0.51484	0.29215	0.80371	1.0000
Si	Si24	1.0	0.76976	0.05003	0.81285	1.0000
Si	Si25	1.0	0.51397	0.04907	0.80248	1.0000
Si	Si26	1.0	0.85063	0.48336	0.87930	1.0000
Si	Si27	1.0	0.65989	0.79271	0.94086	1.0000
Si	Si28	1.0	0.64795	0.54354	0.94530	1.0000
Si	Si29	1.0	0.27660	0.52992	0.94787	1.0000
Si	Si30	1.0	0.03717	0.52886	0.94758	1.0000
Si	Si31	1.0	0.48110	0.85849	0.86901	1.0000
Si	Si32	1.0	0.35302	0.20090	0.45359	1.0000
Si	Si33	1.0	0.34491	0.45050	0.44079	1.0000
Si	Si34	1.0	0.71630	0.21397	0.43952	1.0000
Si	Si35	1.0	0.71824	0.47144	0.44425	1.0000
Si	Si36	1.0	0.95674	0.20990	0.44145	1.0000
Si	Si37	1.0	0.95438	0.46913	0.44087	1.0000
Si	Si38	1.0	0.52369	0.13836	0.38053	1.0000
Si	Si39	1.0	0.53969	0.34570	0.69208	1.0000
Si	Si40	1.0	0.79743	0.72883	0.69003	1.0000

Si	Si41	1.0	0.54287	0.71043	0.69207	1.0000
Si	Si42	1.0	0.78578	0.97336	0.70248	1.0000
Si	Si43	1.0	0.52885	0.95488	0.69525	1.0000
Si	Si44	1.0	0.46054	0.65494	0.18890	1.0000
Si	Si45	1.0	0.21788	0.26999	0.18694	1.0000
Si	Si46	1.0	0.47494	0.26641	0.19187	1.0000
Si	Si47	1.0	0.21514	0.02433	0.19960	1.0000
Si	Si48	1.0	0.47157	0.02725	0.20002	1.0000
Si	Si49	1.0	0.14128	0.83676	0.12702	1.0000
Si	Si50	1.0	0.52424	0.46240	0.12811	1.0000
Si	Si51	1.0	0.84220	0.16271	0.62711	1.0000
Si	Si52	1.0	0.46687	0.53287	0.61955	1.0000
Si	Si53	1.0	0.53244	0.51990	0.36958	1.0000
Si	Si54	1.0	0.85403	0.85313	0.87114	1.0000
Si	Si55	1.0	0.46307	0.47284	0.87597	1.0000
Si	Si56	1.0	0.78942	0.35675	0.70180	1.0000
Si	Si57	1.0	0.21859	0.94140	0.31041	1.0000
Si	Si58	1.0	0.29358	0.78587	0.94188	1.0000
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T2T2T7T7T9:

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O	O6	1.0	0.22998	0.46296	0.07964	1.0000
O	O7	1.0	0.43953	0.50408	0.08015	1.0000
O	O8	1.0	0.69658	0.67351	0.06392	1.0000
O	O9	1.0	0.82749	0.84055	0.05248	1.0000
O	O10	1.0	0.64308	0.86572	0.09620	1.0000
O	O11	1.0	0.83540	0.51191	0.06710	1.0000
O	O12	1.0	0.64342	0.48731	0.10349	1.0000
O	O13	1.0	0.96438	0.67823	0.05636	1.0000
O	O14	1.0	0.01038	0.86459	0.09847	1.0000
O	O15	1.0	0.02721	0.50530	0.10444	1.0000
O	O16	1.0	0.64009	0.33055	0.55212	1.0000
O	O17	1.0	0.68840	0.16928	0.49047	1.0000
O	O18	1.0	0.73975	0.15716	0.58844	1.0000
O	O19	1.0	0.53885	0.14535	0.55962	1.0000
O	O20	1.0	0.67840	0.50826	0.50048	1.0000
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O	O23	1.0	0.28338	0.32720	0.56921	1.0000
O	O24	1.0	0.15400	0.15682	0.55763	1.0000
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O	O29	1.0	0.95333	0.15672	0.59163	1.0000
O	O30	1.0	0.99925	0.50053	0.60961	1.0000
O	O31	1.0	0.34227	0.37801	0.31123	1.0000
O	O32	1.0	0.17128	0.34857	0.25372	1.0000
O	O33	1.0	0.20421	0.22132	0.33224	1.0000
O	O34	1.0	0.14975	0.42602	0.34535	1.0000
O	O35	1.0	0.49567	0.32897	0.24463	1.0000
O	O36	1.0	0.48627	0.23167	0.33304	1.0000
O	O37	1.0	0.54158	0.43802	0.32678	1.0000

O	O38	1.0	0.33507	0.72606	0.31360	1.0000
O	O39	1.0	0.15276	0.82914	0.31066	1.0000
O	O40	1.0	0.16110	0.64005	0.35223	1.0000
O	O41	1.0	0.50308	0.63661	0.35675	1.0000
O	O42	1.0	0.32008	0.96250	0.31063	1.0000
O	O43	1.0	0.13534	0.02270	0.35000	1.0000
O	O44	1.0	0.51896	0.02929	0.35427	1.0000
O	O45	1.0	0.67841	0.68883	0.81214	1.0000
O	O46	1.0	0.82877	0.65696	0.74115	1.0000
O	O47	1.0	0.87352	0.75521	0.82890	1.0000
O	O48	1.0	0.83380	0.54418	0.82229	1.0000
O	O49	1.0	0.52594	0.64234	0.74609	1.0000
O	O50	1.0	0.47976	0.74542	0.83124	1.0000
O	O51	1.0	0.52990	0.54157	0.83219	1.0000
O	O52	1.0	0.65243	0.29039	0.81191	1.0000
O	O53	1.0	0.81254	0.15441	0.82644	1.0000
O	O54	1.0	0.82811	0.34969	0.85876	1.0000
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O	O57	1.0	0.65096	0.02284	0.80629	1.0000
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O	O61	1.0	0.65295	0.82556	0.99714	1.0000
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O	O63	1.0	0.57518	0.85217	0.90576	1.0000
O	O64	1.0	0.66939	0.50525	0.00468	1.0000
O	O65	1.0	0.77110	0.51407	0.91721	1.0000
O	O66	1.0	0.56529	0.45675	0.92219	1.0000
O	O67	1.0	0.27704	0.66621	0.93770	1.0000
O	O68	1.0	0.17091	0.84759	0.93952	1.0000
O	O69	1.0	0.36183	0.84112	0.89986	1.0000
O	O70	1.0	0.36588	0.49706	0.89480	1.0000
O	O71	1.0	0.04082	0.67853	0.93923	1.0000

O	O72	1.0	0.97873	0.86217	0.89977	1.0000
O	O73	1.0	0.97274	0.48153	0.89393	1.0000
O	O74	1.0	0.31091	0.32142	0.43728	1.0000
O	O75	1.0	0.34188	0.17080	0.50830	1.0000
O	O76	1.0	0.24377	0.12655	0.42059	1.0000
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O	O78	1.0	0.35855	0.47214	0.50461	1.0000
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O	O82	1.0	0.84539	0.18498	0.42326	1.0000
O	O83	1.0	0.64976	0.17294	0.39125	1.0000
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O	O87	1.0	0.04538	0.18247	0.39626	1.0000
O	O88	1.0	0.04275	0.53749	0.41369	1.0000
O	O89	1.0	0.66892	0.35718	0.69765	1.0000
O	O90	1.0	0.83051	0.31124	0.75934	1.0000
O	O91	1.0	0.84323	0.25968	0.66132	1.0000
O	O92	1.0	0.49145	0.31820	0.74952	1.0000
O	O93	1.0	0.52487	0.22804	0.65871	1.0000
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O	O96	1.0	0.84210	0.84534	0.69179	1.0000
O	O97	1.0	0.85739	0.66167	0.64283	1.0000
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O	O101	1.0	0.84335	0.04562	0.65725	1.0000
O	O102	1.0	0.49844	0.00018	0.64064	1.0000
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O	O105	1.0	0.15304	0.77315	0.17438	1.0000

O	O106	1.0	0.18756	0.56163	0.16550	1.0000
O	O107	1.0	0.50039	0.66472	0.25646	1.0000
O	O108	1.0	0.53773	0.77082	0.17209	1.0000
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O	O113	1.0	0.48249	0.16316	0.18149	1.0000
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O	O127	1.0	0.17119	0.48774	0.93027	1.0000
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Al	Al2	1.0	0.87118	0.53013	0.62646	1.0000
Al	Al3	1.0	0.45541	0.96729	0.30468	1.0000
Al	Al4	1.0	0.03344	0.54333	0.94447	1.0000
Al	Al5	1.0	0.13524	0.85757	0.12415	1.0000
Si	Si1	1.0	0.33086	0.78632	0.05720	1.0000
Si	Si2	1.0	0.32630	0.53303	0.05496	1.0000
Si	Si3	1.0	0.70559	0.80066	0.05220	1.0000
Si	Si4	1.0	0.71276	0.54554	0.05948	1.0000
Si	Si5	1.0	0.95222	0.80703	0.05195	1.0000
Si	Si6	1.0	0.95839	0.54877	0.05648	1.0000

Si	Si7	1.0	0.52852	0.85296	0.12407	1.0000
Si	Si8	1.0	0.65821	0.20462	0.54748	1.0000
Si	Si9	1.0	0.66689	0.45872	0.55742	1.0000
Si	Si10	1.0	0.27666	0.19857	0.56182	1.0000
Si	Si11	1.0	0.29178	0.45378	0.55710	1.0000
Si	Si12	1.0	0.03537	0.20447	0.54964	1.0000
Si	Si13	1.0	0.04951	0.46181	0.55754	1.0000
Si	Si14	1.0	0.21665	0.34296	0.31113	1.0000
Si	Si15	1.0	0.46651	0.34304	0.30385	1.0000
Si	Si16	1.0	0.20632	0.71232	0.30691	1.0000
Si	Si17	1.0	0.19373	0.95251	0.30629	1.0000
Si	Si18	1.0	0.15257	0.52923	0.38271	1.0000
Si	Si19	1.0	0.80365	0.66224	0.80194	1.0000
Si	Si20	1.0	0.55334	0.65534	0.80543	1.0000
Si	Si21	1.0	0.78014	0.27630	0.81434	1.0000
Si	Si22	1.0	0.52454	0.27775	0.80548	1.0000
Si	Si23	1.0	0.77907	0.03401	0.80999	1.0000
Si	Si24	1.0	0.52371	0.03745	0.79912	1.0000
Si	Si25	1.0	0.85334	0.47311	0.87363	1.0000
Si	Si26	1.0	0.65835	0.78357	0.93921	1.0000
Si	Si27	1.0	0.65847	0.53373	0.94538	1.0000
Si	Si28	1.0	0.28753	0.79552	0.94441	1.0000
Si	Si29	1.0	0.04756	0.80544	0.94460	1.0000
Si	Si30	1.0	0.47182	0.84767	0.86880	1.0000
Si	Si31	1.0	0.33703	0.19600	0.44771	1.0000
Si	Si32	1.0	0.34450	0.44640	0.44520	1.0000
Si	Si33	1.0	0.72416	0.21951	0.43566	1.0000
Si	Si34	1.0	0.72183	0.47614	0.44490	1.0000
Si	Si35	1.0	0.96464	0.22182	0.43977	1.0000
Si	Si36	1.0	0.96093	0.47817	0.45156	1.0000
Si	Si37	1.0	0.52691	0.14802	0.37597	1.0000
Si	Si38	1.0	0.54064	0.33210	0.69270	1.0000
Si	Si39	1.0	0.80009	0.72249	0.68795	1.0000
Si	Si40	1.0	0.54530	0.70863	0.69369	1.0000

Si	Si41	1.0	0.79527	0.96459	0.69972	1.0000
Si	Si42	1.0	0.53834	0.95128	0.69275	1.0000
Si	Si43	1.0	0.21544	0.67164	0.19471	1.0000
Si	Si44	1.0	0.47059	0.67180	0.19613	1.0000
Si	Si45	1.0	0.19763	0.29898	0.19835	1.0000
Si	Si46	1.0	0.45273	0.28711	0.19000	1.0000
Si	Si47	1.0	0.44908	0.03896	0.19098	1.0000
Si	Si48	1.0	0.14307	0.47474	0.12547	1.0000
Si	Si49	1.0	0.52327	0.47738	0.12501	1.0000
Si	Si50	1.0	0.84511	0.15455	0.62474	1.0000
Si	Si51	1.0	0.47294	0.52722	0.62552	1.0000
Si	Si52	1.0	0.15724	0.13878	0.37491	1.0000
Si	Si53	1.0	0.53809	0.51762	0.37529	1.0000
Si	Si54	1.0	0.86304	0.84192	0.87494	1.0000
Si	Si55	1.0	0.48338	0.46132	0.87486	1.0000
Si	Si56	1.0	0.79481	0.34081	0.70249	1.0000
Si	Si57	1.0	0.45998	0.70673	0.31047	1.0000
Si	Si58	1.0	0.29458	0.54099	0.94056	1.0000
Si	Si59	1.0	0.19485	0.05280	0.20082	1.0000

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O	O6	1.0	0.22388	0.53150	0.08764	1.0000
O	O7	1.0	0.42620	0.46972	0.09026	1.0000
O	O8	1.0	0.71056	0.65918	0.05948	1.0000
O	O9	1.0	0.83438	0.83256	0.05501	1.0000
O	O10	1.0	0.65026	0.83726	0.10225	1.0000
O	O11	1.0	0.83289	0.48817	0.06139	1.0000
O	O12	1.0	0.63979	0.47488	0.09557	1.0000
O	O13	1.0	0.95854	0.66146	0.05436	1.0000
O	O14	1.0	0.02389	0.84334	0.09598	1.0000
O	O15	1.0	0.02051	0.48811	0.10352	1.0000
O	O16	1.0	0.62834	0.33154	0.55325	1.0000
O	O17	1.0	0.68114	0.16994	0.49295	1.0000
O	O18	1.0	0.73762	0.16147	0.58975	1.0000
O	O19	1.0	0.53621	0.13965	0.56201	1.0000
O	O20	1.0	0.66888	0.51302	0.50289	1.0000
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O	O23	1.0	0.28286	0.32971	0.56039	1.0000
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O	O26	1.0	0.17018	0.50601	0.55437	1.0000
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O	O30	1.0	0.99056	0.52221	0.60323	1.0000
O	O31	1.0	0.33666	0.37503	0.30595	1.0000
O	O32	1.0	0.17135	0.33336	0.24450	1.0000
O	O33	1.0	0.16862	0.26168	0.33880	1.0000
O	O34	1.0	0.50423	0.30791	0.25440	1.0000
O	O35	1.0	0.46071	0.22459	0.34363	1.0000
O	O36	1.0	0.53239	0.42728	0.33432	1.0000
O	O37	1.0	0.34925	0.74244	0.30289	1.0000

O	O38	1.0	0.16991	0.84835	0.30987	1.0000
O	O39	1.0	0.19707	0.66506	0.36220	1.0000
O	O40	1.0	0.51576	0.63773	0.34548	1.0000
O	O41	1.0	0.33756	0.98095	0.30834	1.0000
O	O42	1.0	0.15170	0.04831	0.34320	1.0000
O	O43	1.0	0.54041	0.02861	0.35091	1.0000
O	O44	1.0	0.66929	0.62727	0.81313	1.0000
O	O45	1.0	0.82032	0.64914	0.74158	1.0000
O	O46	1.0	0.83132	0.76338	0.82533	1.0000
O	O47	1.0	0.86344	0.55099	0.82566	1.0000
O	O48	1.0	0.50835	0.64394	0.74866	1.0000
O	O49	1.0	0.51993	0.77338	0.82751	1.0000
O	O50	1.0	0.47262	0.56956	0.83984	1.0000
O	O51	1.0	0.65373	0.31411	0.81188	1.0000
O	O52	1.0	0.79805	0.15930	0.82606	1.0000
O	O53	1.0	0.83264	0.35218	0.85905	1.0000
O	O54	1.0	0.50639	0.16176	0.82047	1.0000
O	O55	1.0	0.45990	0.35730	0.84192	1.0000
O	O56	1.0	0.65072	0.00669	0.81372	1.0000
O	O57	1.0	0.83805	0.96377	0.85426	1.0000
O	O58	1.0	0.45571	0.96870	0.84586	1.0000
O	O59	1.0	0.62136	0.66107	0.93762	1.0000
O	O60	1.0	0.65567	0.82288	0.00192	1.0000
O	O61	1.0	0.76419	0.81229	0.91732	1.0000
O	O62	1.0	0.55558	0.85736	0.91732	1.0000
O	O63	1.0	0.66626	0.49669	0.99853	1.0000
O	O64	1.0	0.77226	0.52236	0.91418	1.0000
O	O65	1.0	0.56817	0.46159	0.91317	1.0000
O	O66	1.0	0.28478	0.64699	0.94148	1.0000
O	O67	1.0	0.16426	0.81930	0.93003	1.0000
O	O68	1.0	0.35572	0.81155	0.88970	1.0000
O	O69	1.0	0.16240	0.47598	0.94124	1.0000
O	O70	1.0	0.35613	0.46304	0.90677	1.0000
O	O71	1.0	0.03742	0.65101	0.94281	1.0000

O	O72	1.0	0.96848	0.82592	0.89637	1.0000
O	O73	1.0	0.97307	0.46918	0.90339	1.0000
O	O74	1.0	0.37438	0.31660	0.44423	1.0000
O	O75	1.0	0.33396	0.15687	0.50930	1.0000
O	O76	1.0	0.24221	0.15637	0.41859	1.0000
O	O77	1.0	0.45099	0.12357	0.43084	1.0000
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O	O79	1.0	0.23090	0.45975	0.41759	1.0000
O	O80	1.0	0.43550	0.50935	0.41430	1.0000
O	O81	1.0	0.70867	0.35170	0.44340	1.0000
O	O82	1.0	0.83670	0.18675	0.42562	1.0000
O	O83	1.0	0.63978	0.18513	0.39455	1.0000
O	O84	1.0	0.83427	0.52174	0.43960	1.0000
O	O85	1.0	0.64397	0.53483	0.40350	1.0000
O	O86	1.0	0.96672	0.35337	0.43760	1.0000
O	O87	1.0	0.03492	0.16808	0.40087	1.0000
O	O88	1.0	0.02330	0.54449	0.40287	1.0000
O	O89	1.0	0.67024	0.36339	0.69730	1.0000
O	O90	1.0	0.83133	0.31766	0.75985	1.0000
O	O91	1.0	0.84152	0.25720	0.66396	1.0000
O	O92	1.0	0.49458	0.30682	0.74674	1.0000
O	O93	1.0	0.52984	0.23549	0.65427	1.0000
O	O94	1.0	0.48375	0.44192	0.67195	1.0000
O	O95	1.0	0.65826	0.71721	0.68719	1.0000
O	O96	1.0	0.83016	0.84348	0.69609	1.0000
O	O97	1.0	0.83766	0.66347	0.64313	1.0000
O	O98	1.0	0.48738	0.83124	0.70224	1.0000
O	O99	1.0	0.47185	0.64933	0.65099	1.0000
O	O100	1.0	0.65827	0.96205	0.69755	1.0000
O	O101	1.0	0.83589	0.04258	0.65787	1.0000
O	O102	1.0	0.48306	0.00799	0.64796	1.0000
O	O103	1.0	0.33449	0.64285	0.19373	1.0000
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O	O107	1.0	0.51032	0.67977	0.24684	1.0000
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O	O109	1.0	0.52413	0.57536	0.16318	1.0000
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O	O114	1.0	0.53804	0.36385	0.15982	1.0000
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O	O116	1.0	0.52622	0.98356	0.14022	1.0000
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O	O120	1.0	0.99368	0.51208	0.50252	1.0000
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Al	Al2	1.0	0.86391	0.53499	0.62450	1.0000
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Al	Al4	1.0	0.14799	0.84149	0.12304	1.0000
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Si	Si2	1.0	0.33852	0.53923	0.05948	1.0000
Si	Si3	1.0	0.71337	0.78833	0.05442	1.0000
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Si	Si5	1.0	0.95675	0.79178	0.05072	1.0000
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Si	Si7	1.0	0.52842	0.86383	0.11729	1.0000
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Si	Si9	1.0	0.66043	0.45915	0.55907	1.0000
Si	Si10	1.0	0.27209	0.20039	0.56060	1.0000
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Si	Si12	1.0	0.02904	0.21224	0.55259	1.0000
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Si	Si16	1.0	0.21146	0.97192	0.30297	1.0000
Si	Si17	1.0	0.79481	0.64947	0.80211	1.0000
Si	Si18	1.0	0.54259	0.65361	0.80726	1.0000
Si	Si19	1.0	0.77842	0.28435	0.81414	1.0000
Si	Si20	1.0	0.52867	0.28451	0.80457	1.0000
Si	Si21	1.0	0.77682	0.03492	0.81199	1.0000
Si	Si22	1.0	0.52585	0.03820	0.80614	1.0000
Si	Si23	1.0	0.85912	0.47375	0.87565	1.0000
Si	Si24	1.0	0.64975	0.78840	0.94323	1.0000
Si	Si25	1.0	0.65690	0.53588	0.94037	1.0000
Si	Si26	1.0	0.28487	0.77609	0.93778	1.0000
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Si	Si41	1.0	0.78589	0.96490	0.70145	1.0000
Si	Si42	1.0	0.52880	0.95480	0.69805	1.0000
Si	Si43	1.0	0.20683	0.66158	0.20207	1.0000
Si	Si44	1.0	0.46059	0.67080	0.18983	1.0000
Si	Si45	1.0	0.21758	0.29766	0.18972	1.0000
Si	Si46	1.0	0.46828	0.28854	0.19633	1.0000
Si	Si47	1.0	0.46737	0.03886	0.18744	1.0000
Si	Si48	1.0	0.13796	0.48636	0.12808	1.0000
Si	Si49	1.0	0.53043	0.47225	0.12652	1.0000
Si	Si50	1.0	0.84197	0.15402	0.62646	1.0000
Si	Si51	1.0	0.46880	0.52983	0.62717	1.0000
Si	Si52	1.0	0.15045	0.15759	0.37568	1.0000
Si	Si53	1.0	0.53129	0.52408	0.37517	1.0000
Si	Si54	1.0	0.85001	0.84117	0.87368	1.0000
Si	Si55	1.0	0.46556	0.46386	0.87553	1.0000
Si	Si56	1.0	0.79576	0.34407	0.70239	1.0000
Si	Si57	1.0	0.47288	0.71496	0.30207	1.0000
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O	O6	1.0	0.23171	0.46868	0.08377	1.0000
O	O7	1.0	0.43794	0.51733	0.08656	1.0000
O	O8	1.0	0.69941	0.66041	0.06618	1.0000
O	O9	1.0	0.83013	0.82883	0.05815	1.0000
O	O10	1.0	0.64698	0.84792	0.10501	1.0000
O	O11	1.0	0.83061	0.49408	0.06065	1.0000
O	O12	1.0	0.64097	0.46800	0.09669	1.0000
O	O13	1.0	0.96173	0.66285	0.05625	1.0000
O	O14	1.0	0.02048	0.84510	0.09904	1.0000
O	O15	1.0	0.02129	0.47999	0.09778	1.0000
O	O16	1.0	0.63641	0.33119	0.55129	1.0000
O	O17	1.0	0.69081	0.17029	0.49050	1.0000
O	O18	1.0	0.74005	0.15974	0.58856	1.0000
O	O19	1.0	0.54050	0.14163	0.55856	1.0000
O	O20	1.0	0.67537	0.50908	0.50010	1.0000
O	O21	1.0	0.77546	0.47041	0.58751	1.0000
O	O22	1.0	0.56687	0.51780	0.58384	1.0000
O	O23	1.0	0.28549	0.32832	0.56871	1.0000
O	O24	1.0	0.15311	0.16103	0.55748	1.0000
O	O25	1.0	0.33759	0.14020	0.60528	1.0000
O	O26	1.0	0.17508	0.50251	0.55197	1.0000
O	O27	1.0	0.35799	0.51640	0.60136	1.0000
O	O28	1.0	0.03809	0.33721	0.55540	1.0000
O	O29	1.0	0.95354	0.15670	0.59118	1.0000
O	O30	1.0	0.99907	0.51424	0.60701	1.0000
O	O31	1.0	0.34158	0.37721	0.31122	1.0000
O	O32	1.0	0.16899	0.34598	0.25449	1.0000
O	O33	1.0	0.20513	0.21941	0.33234	1.0000
O	O34	1.0	0.14883	0.42333	0.34591	1.0000
O	O35	1.0	0.49593	0.32893	0.24509	1.0000
O	O36	1.0	0.48713	0.23220	0.33350	1.0000
O	O37	1.0	0.54029	0.43937	0.32694	1.0000

O	O38	1.0	0.33390	0.72667	0.30930	1.0000
O	O39	1.0	0.15090	0.82878	0.31075	1.0000
O	O40	1.0	0.16482	0.63717	0.34972	1.0000
O	O41	1.0	0.49766	0.63760	0.35780	1.0000
O	O42	1.0	0.31859	0.96253	0.31002	1.0000
O	O43	1.0	0.13332	0.02230	0.34874	1.0000
O	O44	1.0	0.51740	0.02863	0.35410	1.0000
O	O45	1.0	0.67045	0.63486	0.81036	1.0000
O	O46	1.0	0.82363	0.64905	0.73872	1.0000
O	O47	1.0	0.83322	0.77234	0.82040	1.0000
O	O48	1.0	0.86139	0.55776	0.82415	1.0000
O	O49	1.0	0.51010	0.65126	0.74717	1.0000
O	O50	1.0	0.51511	0.77453	0.82912	1.0000
O	O51	1.0	0.47654	0.56755	0.83641	1.0000
O	O52	1.0	0.65966	0.32798	0.80976	1.0000
O	O53	1.0	0.79910	0.16854	0.82363	1.0000
O	O54	1.0	0.84116	0.35943	0.85734	1.0000
O	O55	1.0	0.52674	0.16508	0.81912	1.0000
O	O56	1.0	0.46345	0.35614	0.84155	1.0000
O	O57	1.0	0.66171	0.00295	0.81272	1.0000
O	O58	1.0	0.46621	0.97449	0.84594	1.0000
O	O59	1.0	0.62040	0.66475	0.93675	1.0000
O	O60	1.0	0.64931	0.82026	0.00539	1.0000
O	O61	1.0	0.76798	0.81616	0.92263	1.0000
O	O62	1.0	0.56108	0.86265	0.91824	1.0000
O	O63	1.0	0.66409	0.50416	0.99902	1.0000
O	O64	1.0	0.77332	0.52474	0.91442	1.0000
O	O65	1.0	0.56919	0.46538	0.91237	1.0000
O	O66	1.0	0.28944	0.65417	0.93325	1.0000
O	O67	1.0	0.17516	0.83099	0.94284	1.0000
O	O68	1.0	0.35759	0.83133	0.89330	1.0000
O	O69	1.0	0.16525	0.48470	0.94245	1.0000
O	O70	1.0	0.35587	0.46561	0.90347	1.0000
O	O71	1.0	0.04572	0.66204	0.94398	1.0000

O	O72	1.0	0.98806	0.84247	0.89865	1.0000
O	O73	1.0	0.97867	0.48496	0.89946	1.0000
O	O74	1.0	0.30918	0.32096	0.43729	1.0000
O	O75	1.0	0.34047	0.17003	0.50766	1.0000
O	O76	1.0	0.24437	0.12429	0.41994	1.0000
O	O77	1.0	0.45460	0.16528	0.42713	1.0000
O	O78	1.0	0.35888	0.47332	0.50431	1.0000
O	O79	1.0	0.25002	0.52033	0.42149	1.0000
O	O80	1.0	0.45499	0.46963	0.41724	1.0000
O	O81	1.0	0.71141	0.34850	0.43747	1.0000
O	O82	1.0	0.84599	0.18720	0.42281	1.0000
O	O83	1.0	0.64976	0.17092	0.39172	1.0000
O	O84	1.0	0.84118	0.51838	0.43699	1.0000
O	O85	1.0	0.65141	0.53535	0.40083	1.0000
O	O86	1.0	0.97367	0.35318	0.44200	1.0000
O	O87	1.0	0.04618	0.18164	0.39663	1.0000
O	O88	1.0	0.03992	0.54156	0.41096	1.0000
O	O89	1.0	0.67385	0.36086	0.69591	1.0000
O	O90	1.0	0.83788	0.32132	0.75747	1.0000
O	O91	1.0	0.84704	0.26017	0.66135	1.0000
O	O92	1.0	0.49836	0.30797	0.74565	1.0000
O	O93	1.0	0.52806	0.24059	0.65159	1.0000
O	O94	1.0	0.49060	0.44716	0.67181	1.0000
O	O95	1.0	0.66462	0.72299	0.68570	1.0000
O	O96	1.0	0.84008	0.84535	0.69452	1.0000
O	O97	1.0	0.84384	0.66621	0.64039	1.0000
O	O98	1.0	0.49325	0.83608	0.70007	1.0000
O	O99	1.0	0.48041	0.65306	0.64887	1.0000
O	O100	1.0	0.66804	0.96341	0.69868	1.0000
O	O101	1.0	0.84272	0.04527	0.65666	1.0000
O	O102	1.0	0.49785	0.01166	0.64657	1.0000
O	O103	1.0	0.34482	0.64088	0.18995	1.0000
O	O104	1.0	0.17812	0.65645	0.25112	1.0000
O	O105	1.0	0.19201	0.78321	0.17095	1.0000

O	O106	1.0	0.15292	0.57323	0.16252	1.0000
O	O107	1.0	0.50186	0.65752	0.25754	1.0000
O	O108	1.0	0.51324	0.77137	0.17513	1.0000
O	O109	1.0	0.53560	0.55836	0.17267	1.0000
O	O110	1.0	0.32321	0.30035	0.18978	1.0000
O	O111	1.0	0.15569	0.17257	0.19667	1.0000
O	O112	1.0	0.13343	0.36129	0.15637	1.0000
O	O113	1.0	0.48344	0.16287	0.18174	1.0000
O	O114	1.0	0.50202	0.35611	0.14570	1.0000
O	O115	1.0	0.31868	0.03088	0.18861	1.0000
O	O116	1.0	0.49596	0.97013	0.14348	1.0000
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O	O120	1.0	0.98902	0.51453	0.50727	1.0000
O	O121	1.0	0.15136	0.99461	0.24996	1.0000
O	O122	1.0	0.49314	0.99589	0.24382	1.0000
O	O123	1.0	0.83516	0.01641	0.75458	1.0000
O	O124	1.0	0.49796	0.02039	0.74805	1.0000
O	O125	1.0	0.85626	0.46643	0.68695	1.0000
O	O126	1.0	0.51112	0.82985	0.31873	1.0000
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Al	Al2	1.0	0.86949	0.53585	0.62381	1.0000
Al	Al3	1.0	0.45393	0.96678	0.30425	1.0000
Al	Al4	1.0	0.14920	0.85736	0.12018	1.0000
Al	Al5	1.0	0.85999	0.83785	0.87626	1.0000
Si	Si1	1.0	0.33495	0.79052	0.05311	1.0000
Si	Si2	1.0	0.32634	0.53972	0.05839	1.0000
Si	Si3	1.0	0.70721	0.78932	0.05812	1.0000
Si	Si4	1.0	0.70894	0.53336	0.05494	1.0000
Si	Si5	1.0	0.95415	0.79292	0.05341	1.0000
Si	Si6	1.0	0.95225	0.53429	0.05328	1.0000

Si	Si7	1.0	0.52541	0.84939	0.12604	1.0000
Si	Si8	1.0	0.65828	0.20529	0.54716	1.0000
Si	Si9	1.0	0.66633	0.45914	0.55687	1.0000
Si	Si10	1.0	0.27675	0.19972	0.56106	1.0000
Si	Si11	1.0	0.29382	0.45509	0.55705	1.0000
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Si	Si13	1.0	0.05039	0.46740	0.55675	1.0000
Si	Si14	1.0	0.21628	0.34117	0.31142	1.0000
Si	Si15	1.0	0.46622	0.34313	0.30410	1.0000
Si	Si16	1.0	0.20481	0.71236	0.30460	1.0000
Si	Si17	1.0	0.19231	0.95203	0.30519	1.0000
Si	Si18	1.0	0.15165	0.52905	0.38182	1.0000
Si	Si19	1.0	0.79650	0.65766	0.79976	1.0000
Si	Si20	1.0	0.54331	0.65779	0.80627	1.0000
Si	Si21	1.0	0.78358	0.29542	0.81215	1.0000
Si	Si22	1.0	0.53611	0.28915	0.80324	1.0000
Si	Si23	1.0	0.53643	0.03999	0.80558	1.0000
Si	Si24	1.0	0.86186	0.48330	0.87447	1.0000
Si	Si25	1.0	0.65260	0.79136	0.94548	1.0000
Si	Si26	1.0	0.65690	0.54064	0.94051	1.0000
Si	Si27	1.0	0.29421	0.78246	0.94124	1.0000
Si	Si28	1.0	0.28699	0.52795	0.94529	1.0000
Si	Si29	1.0	0.05101	0.79259	0.94571	1.0000
Si	Si30	1.0	0.04617	0.53316	0.94648	1.0000
Si	Si31	1.0	0.47567	0.85794	0.87248	1.0000
Si	Si32	1.0	0.33646	0.19530	0.44730	1.0000
Si	Si33	1.0	0.34265	0.44644	0.44516	1.0000
Si	Si34	1.0	0.72449	0.22003	0.43549	1.0000
Si	Si35	1.0	0.72003	0.47721	0.44477	1.0000
Si	Si36	1.0	0.96534	0.22432	0.43920	1.0000
Si	Si37	1.0	0.96127	0.48112	0.44988	1.0000
Si	Si38	1.0	0.52666	0.14748	0.37609	1.0000
Si	Si39	1.0	0.54560	0.33699	0.69013	1.0000
Si	Si40	1.0	0.79351	0.72342	0.68842	1.0000

Si	Si41	1.0	0.53732	0.71545	0.69537	1.0000
Si	Si42	1.0	0.79570	0.96633	0.70010	1.0000
Si	Si43	1.0	0.53824	0.95801	0.69715	1.0000
Si	Si44	1.0	0.21693	0.66671	0.19240	1.0000
Si	Si45	1.0	0.47202	0.65785	0.19719	1.0000
Si	Si46	1.0	0.19630	0.29664	0.19926	1.0000
Si	Si47	1.0	0.45151	0.28623	0.19081	1.0000
Si	Si48	1.0	0.44996	0.03842	0.19073	1.0000
Si	Si49	1.0	0.13579	0.47279	0.12491	1.0000
Si	Si50	1.0	0.52784	0.47526	0.12525	1.0000
Si	Si51	1.0	0.84591	0.15519	0.62443	1.0000
Si	Si52	1.0	0.47496	0.53236	0.62630	1.0000
Si	Si53	1.0	0.15716	0.13736	0.37463	1.0000
Si	Si54	1.0	0.53553	0.51863	0.37559	1.0000
Si	Si55	1.0	0.46791	0.46576	0.87398	1.0000
Si	Si56	1.0	0.80010	0.34681	0.70033	1.0000
Si	Si57	1.0	0.45854	0.70509	0.30984	1.0000
Si	Si58	1.0	0.19517	0.05033	0.19948	1.0000
Si	Si59	1.0	0.78256	0.04476	0.80841	1.0000

T7T7T7T7T9:

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H H3 1.0 0.52546 0.85544 0.03561 1.0000
H H4 1.0 0.13385 0.48529 0.21722 1.0000
H H5 1.0 0.90343 0.02333 0.86972 1.0000
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O	O6	1.0	0.44504	0.48098	0.07952	1.0000
O	O7	1.0	0.72231	0.65751	0.05702	1.0000
O	O8	1.0	0.84913	0.82967	0.05653	1.0000
O	O9	1.0	0.66763	0.82972	0.10948	1.0000
O	O10	1.0	0.83635	0.48423	0.05319	1.0000
O	O11	1.0	0.65073	0.47804	0.09964	1.0000
O	O12	1.0	0.96708	0.65699	0.05320	1.0000
O	O13	1.0	0.04863	0.83473	0.09318	1.0000
O	O14	1.0	0.01828	0.47867	0.09943	1.0000
O	O15	1.0	0.62569	0.32831	0.55122	1.0000
O	O16	1.0	0.67543	0.16746	0.48947	1.0000
O	O17	1.0	0.73752	0.16119	0.58630	1.0000
O	O18	1.0	0.53409	0.13647	0.56047	1.0000
O	O19	1.0	0.67502	0.51052	0.50458	1.0000
O	O20	1.0	0.76893	0.45912	0.59103	1.0000
O	O21	1.0	0.56361	0.51470	0.58721	1.0000
O	O22	1.0	0.28179	0.33748	0.56031	1.0000
O	O23	1.0	0.14997	0.16904	0.55453	1.0000
O	O24	1.0	0.33161	0.15665	0.60534	1.0000
O	O25	1.0	0.16974	0.51203	0.55370	1.0000
O	O26	1.0	0.35412	0.51872	0.60051	1.0000
O	O27	1.0	0.03404	0.34337	0.55404	1.0000
O	O28	1.0	0.95114	0.16411	0.59188	1.0000
O	O29	1.0	0.98811	0.52450	0.60103	1.0000
O	O30	1.0	0.33404	0.37855	0.30968	1.0000
O	O31	1.0	0.17404	0.34254	0.24350	1.0000
O	O32	1.0	0.18194	0.23536	0.32944	1.0000
O	O33	1.0	0.13960	0.44454	0.32779	1.0000
O	O34	1.0	0.49916	0.34680	0.24867	1.0000
O	O35	1.0	0.46997	0.22563	0.33096	1.0000
O	O36	1.0	0.53181	0.42788	0.33837	1.0000
O	O37	1.0	0.34800	0.70382	0.30878	1.0000

O	O38	1.0	0.18705	0.83670	0.32600	1.0000
O	O39	1.0	0.18055	0.64166	0.35965	1.0000
O	O40	1.0	0.51112	0.83707	0.31621	1.0000
O	O41	1.0	0.53459	0.64094	0.34322	1.0000
O	O42	1.0	0.34824	0.97496	0.31390	1.0000
O	O43	1.0	0.16177	0.03352	0.35208	1.0000
O	O44	1.0	0.53698	0.03021	0.34780	1.0000
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O	O46	1.0	0.82539	0.65120	0.73826	1.0000
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O	O49	1.0	0.49764	0.65826	0.75086	1.0000
O	O50	1.0	0.53933	0.77564	0.83338	1.0000
O	O51	1.0	0.47097	0.57574	0.84077	1.0000
O	O52	1.0	0.65297	0.29691	0.80801	1.0000
O	O53	1.0	0.81835	0.17132	0.82279	1.0000
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O	O60	1.0	0.65407	0.82637	0.01058	1.0000
O	O61	1.0	0.76333	0.82174	0.92440	1.0000
O	O62	1.0	0.55416	0.85938	0.92640	1.0000
O	O63	1.0	0.65984	0.49486	0.99964	1.0000
O	O64	1.0	0.77822	0.53663	0.91732	1.0000
O	O65	1.0	0.57917	0.46833	0.90929	1.0000
O	O66	1.0	0.29363	0.64931	0.94284	1.0000
O	O67	1.0	0.17186	0.81949	0.92744	1.0000
O	O68	1.0	0.36378	0.81054	0.88972	1.0000
O	O69	1.0	0.16624	0.48220	0.93185	1.0000
O	O70	1.0	0.36709	0.46364	0.91056	1.0000
O	O71	1.0	0.03986	0.65365	0.93760	1.0000

O	O72	1.0	0.97862	0.83584	0.89520	1.0000
O	O73	1.0	0.97401	0.47120	0.89886	1.0000
O	O74	1.0	0.36945	0.33104	0.43836	1.0000
O	O75	1.0	0.34247	0.17249	0.50663	1.0000
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O	O77	1.0	0.44304	0.13862	0.42196	1.0000
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O	O87	1.0	0.03176	0.17077	0.39479	1.0000
O	O88	1.0	0.02583	0.53558	0.40067	1.0000
O	O89	1.0	0.66780	0.37062	0.69724	1.0000
O	O90	1.0	0.83181	0.32940	0.75769	1.0000
O	O91	1.0	0.83640	0.26070	0.66220	1.0000
O	O92	1.0	0.49159	0.30400	0.74537	1.0000
O	O93	1.0	0.53080	0.24175	0.65137	1.0000
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O	O95	1.0	0.65743	0.72119	0.69141	1.0000
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O	O97	1.0	0.82949	0.66548	0.63925	1.0000
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O	O101	1.0	0.83680	0.04716	0.65524	1.0000
O	O102	1.0	0.47796	0.01787	0.65127	1.0000
O	O103	1.0	0.32968	0.62763	0.19936	1.0000
O	O104	1.0	0.16753	0.67857	0.25976	1.0000
O	O105	1.0	0.16489	0.74033	0.16275	1.0000

O	O106	1.0	0.50998	0.68091	0.24648	1.0000
O	O107	1.0	0.46327	0.76547	0.15739	1.0000
O	O108	1.0	0.51636	0.55926	0.16706	1.0000
O	O109	1.0	0.33969	0.28263	0.19028	1.0000
O	O110	1.0	0.17106	0.15104	0.19491	1.0000
O	O111	1.0	0.16014	0.33380	0.14459	1.0000
O	O112	1.0	0.51219	0.16743	0.19673	1.0000
O	O113	1.0	0.52169	0.35131	0.14918	1.0000
O	O114	1.0	0.34363	0.03261	0.19360	1.0000
O	O115	1.0	0.16385	0.95342	0.15534	1.0000
O	O116	1.0	0.52618	0.98638	0.14849	1.0000
O	O117	1.0	0.01601	0.82477	0.99510	1.0000
O	O118	1.0	0.01053	0.48666	0.99840	1.0000
O	O119	1.0	0.98433	0.17842	0.49378	1.0000
O	O120	1.0	0.99506	0.51464	0.50017	1.0000
O	O121	1.0	0.17980	0.98191	0.25379	1.0000
O	O122	1.0	0.51130	0.99041	0.24909	1.0000
O	O123	1.0	0.82424	0.01538	0.75333	1.0000
O	O124	1.0	0.49353	0.01192	0.75216	1.0000
O	O125	1.0	0.85638	0.46800	0.68626	1.0000
O	O126	1.0	0.46936	0.85722	0.06270	1.0000
O	O127	1.0	0.13772	0.53700	0.18906	1.0000
O	O128	1.0	0.84718	0.98142	0.85331	1.0000
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Al	Al2	1.0	0.86129	0.53675	0.62279	1.0000
Al	Al3	1.0	0.53890	0.85985	0.12590	1.0000
Al	Al4	1.0	0.13946	0.46301	0.12610	1.0000
Al	Al5	1.0	0.84979	0.83811	0.87491	1.0000
Si	Si1	1.0	0.34027	0.54199	0.05996	1.0000
Si	Si2	1.0	0.72617	0.78653	0.06010	1.0000
Si	Si3	1.0	0.71696	0.52889	0.05286	1.0000
Si	Si4	1.0	0.96989	0.78551	0.04960	1.0000
Si	Si5	1.0	0.95911	0.52689	0.05196	1.0000
Si	Si6	1.0	0.64985	0.20306	0.54710	1.0000

Si	Si7	1.0	0.66070	0.45426	0.55955	1.0000
Si	Si8	1.0	0.27390	0.20850	0.55820	1.0000
Si	Si9	1.0	0.28846	0.46576	0.55425	1.0000
Si	Si10	1.0	0.03022	0.21512	0.54880	1.0000
Si	Si11	1.0	0.04577	0.47355	0.55320	1.0000
Si	Si12	1.0	0.20830	0.34867	0.30300	1.0000
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Si	Si24	1.0	0.85765	0.48628	0.87505	1.0000
Si	Si25	1.0	0.65226	0.79233	0.95021	1.0000
Si	Si26	1.0	0.65973	0.54178	0.94268	1.0000
Si	Si27	1.0	0.29004	0.77700	0.93743	1.0000
Si	Si28	1.0	0.28451	0.52110	0.94805	1.0000
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Si	Si31	1.0	0.48236	0.85174	0.87540	1.0000
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Si	Si35	1.0	0.71466	0.47851	0.44828	1.0000
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Si	Si41	1.0	0.52927	0.71585	0.69762	1.0000
Si	Si42	1.0	0.78619	0.96786	0.69800	1.0000
Si	Si43	1.0	0.52843	0.95887	0.69810	1.0000
Si	Si44	1.0	0.45598	0.66066	0.19135	1.0000
Si	Si45	1.0	0.21093	0.27517	0.19169	1.0000
Si	Si46	1.0	0.46783	0.28707	0.19569	1.0000
Si	Si47	1.0	0.21574	0.03014	0.19898	1.0000
Si	Si48	1.0	0.47330	0.04333	0.19594	1.0000
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Si	Si51	1.0	0.84089	0.15817	0.62368	1.0000
Si	Si52	1.0	0.46853	0.53060	0.62792	1.0000
Si	Si53	1.0	0.15186	0.15292	0.37462	1.0000
Si	Si54	1.0	0.53189	0.53209	0.37504	1.0000
Si	Si55	1.0	0.47157	0.46923	0.87552	1.0000
Si	Si56	1.0	0.79382	0.35140	0.70017	1.0000
Si	Si57	1.0	0.35308	0.79452	0.04804	1.0000
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T7T7T7T9T9:

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O	O11	1.0	0.66249	0.47101	0.10405	1.0000
O	O12	1.0	0.98141	0.65333	0.05442	1.0000
O	O13	1.0	0.05341	0.83122	0.09363	1.0000
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O	O15	1.0	0.62558	0.32982	0.55240	1.0000
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O	O18	1.0	0.53237	0.14024	0.56187	1.0000
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O	O32	1.0	0.20493	0.22195	0.33109	1.0000
O	O33	1.0	0.14206	0.42538	0.33933	1.0000
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O	O36	1.0	0.53762	0.44656	0.32758	1.0000
O	O37	1.0	0.32613	0.71697	0.30402	1.0000

O	O38	1.0	0.15045	0.82801	0.30907	1.0000
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O	O40	1.0	0.49406	0.84073	0.31451	1.0000
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O	O50	1.0	0.48137	0.57719	0.84474	1.0000
O	O51	1.0	0.65893	0.28855	0.80583	1.0000
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O	O54	1.0	0.49179	0.16515	0.81972	1.0000
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O	O57	1.0	0.47866	0.97205	0.85382	1.0000
O	O58	1.0	0.63205	0.65984	0.94748	1.0000
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O	O60	1.0	0.77103	0.81706	0.92630	1.0000
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O	O66	1.0	0.17875	0.82384	0.93017	1.0000
O	O67	1.0	0.36891	0.81307	0.88924	1.0000
O	O68	1.0	0.16837	0.47891	0.93969	1.0000
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O	O70	1.0	0.04932	0.65538	0.93417	1.0000
O	O71	1.0	0.98489	0.84016	0.89550	1.0000

O	O72	1.0	0.98505	0.47392	0.89211	1.0000
O	O73	1.0	0.30766	0.32501	0.43933	1.0000
O	O74	1.0	0.34751	0.17988	0.51140	1.0000
O	O75	1.0	0.24575	0.12382	0.42665	1.0000
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O	O91	1.0	0.49142	0.31380	0.74670	1.0000
O	O92	1.0	0.53380	0.23741	0.65536	1.0000
O	O93	1.0	0.47599	0.44138	0.66930	1.0000
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O	O104	1.0	0.19542	0.77204	0.16468	1.0000
O	O105	1.0	0.13372	0.56930	0.16131	1.0000

O	O106	1.0	0.49855	0.66843	0.25360	1.0000
O	O107	1.0	0.47460	0.75808	0.16302	1.0000
O	O108	1.0	0.52903	0.55401	0.17323	1.0000
O	O109	1.0	0.32931	0.29373	0.18656	1.0000
O	O110	1.0	0.16044	0.16527	0.19066	1.0000
O	O111	1.0	0.14113	0.35564	0.15276	1.0000
O	O112	1.0	0.49939	0.16953	0.18971	1.0000
O	O113	1.0	0.50932	0.35421	0.14357	1.0000
O	O114	1.0	0.33132	0.03804	0.19113	1.0000
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O	O116	1.0	0.51875	0.97817	0.15330	1.0000
O	O117	1.0	0.01943	0.82061	0.99515	1.0000
O	O118	1.0	0.98541	0.49105	0.98999	1.0000
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O	O126	1.0	0.47272	0.83869	0.06625	1.0000
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Al	Al2	1.0	0.86006	0.54027	0.62085	1.0000
Al	Al3	1.0	0.54249	0.85413	0.12988	1.0000
Al	Al4	1.0	0.85450	0.83726	0.87579	1.0000
Al	Al5	1.0	0.15478	0.14421	0.37901	1.0000
Si	Si1	1.0	0.34935	0.54033	0.06042	1.0000
Si	Si2	1.0	0.73038	0.78336	0.06261	1.0000
Si	Si3	1.0	0.73003	0.52542	0.05861	1.0000
Si	Si4	1.0	0.97623	0.78207	0.05004	1.0000
Si	Si5	1.0	0.96845	0.52535	0.04837	1.0000
Si	Si6	1.0	0.64840	0.20446	0.54719	1.0000

Si	Si7	1.0	0.65795	0.45682	0.55679	1.0000
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Si	Si9	1.0	0.28690	0.46538	0.55529	1.0000
Si	Si10	1.0	0.02912	0.21548	0.55184	1.0000
Si	Si11	1.0	0.04248	0.47351	0.55384	1.0000
Si	Si12	1.0	0.21452	0.34012	0.30851	1.0000
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Si	Si14	1.0	0.19809	0.70794	0.30224	1.0000
Si	Si15	1.0	0.45518	0.71790	0.30625	1.0000
Si	Si16	1.0	0.45206	0.96176	0.30721	1.0000
Si	Si17	1.0	0.13910	0.52581	0.37786	1.0000
Si	Si18	1.0	0.79682	0.65624	0.79772	1.0000
Si	Si19	1.0	0.54801	0.65768	0.80846	1.0000
Si	Si20	1.0	0.78661	0.29062	0.80986	1.0000
Si	Si21	1.0	0.52961	0.28391	0.80316	1.0000
Si	Si22	1.0	0.52973	0.04437	0.80941	1.0000
Si	Si23	1.0	0.86354	0.48346	0.87199	1.0000
Si	Si24	1.0	0.65964	0.78731	0.95197	1.0000
Si	Si25	1.0	0.67131	0.53651	0.94586	1.0000
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Si	Si29	1.0	0.04845	0.52688	0.93929	1.0000
Si	Si30	1.0	0.48885	0.85212	0.87558	1.0000
Si	Si31	1.0	0.33610	0.19984	0.44992	1.0000
Si	Si32	1.0	0.33262	0.45250	0.44372	1.0000
Si	Si33	1.0	0.70731	0.22086	0.43483	1.0000
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Si	Si36	1.0	0.95462	0.47222	0.44600	1.0000
Si	Si37	1.0	0.51857	0.15342	0.37426	1.0000
Si	Si38	1.0	0.54051	0.33979	0.69085	1.0000
Si	Si39	1.0	0.78678	0.72509	0.68790	1.0000
Si	Si40	1.0	0.52946	0.71434	0.69880	1.0000

Si	Si41	1.0	0.78671	0.96696	0.69912	1.0000
Si	Si42	1.0	0.52808	0.95644	0.70011	1.0000
Si	Si43	1.0	0.20703	0.65563	0.19132	1.0000
Si	Si44	1.0	0.45851	0.65195	0.19535	1.0000
Si	Si45	1.0	0.20178	0.28805	0.19592	1.0000
Si	Si46	1.0	0.45815	0.29076	0.19133	1.0000
Si	Si47	1.0	0.20307	0.04421	0.19334	1.0000
Si	Si48	1.0	0.46133	0.04625	0.19592	1.0000
Si	Si49	1.0	0.14962	0.46829	0.12375	1.0000
Si	Si50	1.0	0.16513	0.85879	0.12154	1.0000
Si	Si51	1.0	0.54148	0.47368	0.12575	1.0000
Si	Si52	1.0	0.83968	0.15917	0.62441	1.0000
Si	Si53	1.0	0.46726	0.53291	0.62601	1.0000
Si	Si54	1.0	0.52759	0.53080	0.37404	1.0000
Si	Si55	1.0	0.47896	0.46897	0.87847	1.0000
Si	Si56	1.0	0.79297	0.35453	0.69932	1.0000
Si	Si57	1.0	0.34940	0.79522	0.04948	1.0000
Si	Si58	1.0	0.78619	0.05065	0.80795	1.0000
Si	Si59	1.0	0.19637	0.94693	0.30032	1.0000

AlSiAl-T2T7T7T9T9:

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H H4 1.0 0.05959 0.02670 0.14026 1.0000
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O O2 1.0 0.34844 0.81257 0.99189 1.0000
O O3 1.0 0.24663 0.87167 0.07558 1.0000

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O	O6	1.0	0.22542	0.47150	0.08327	1.0000
O	O7	1.0	0.43280	0.51889	0.08936	1.0000
O	O8	1.0	0.69393	0.66549	0.06540	1.0000
O	O9	1.0	0.83099	0.82922	0.05864	1.0000
O	O10	1.0	0.64548	0.85444	0.10361	1.0000
O	O11	1.0	0.82594	0.49847	0.05988	1.0000
O	O12	1.0	0.63775	0.47283	0.09765	1.0000
O	O13	1.0	0.96271	0.66226	0.05664	1.0000
O	O14	1.0	0.02193	0.84724	0.09732	1.0000
O	O15	1.0	0.01501	0.47937	0.09978	1.0000
O	O16	1.0	0.64051	0.33229	0.55090	1.0000
O	O17	1.0	0.69776	0.17366	0.48944	1.0000
O	O18	1.0	0.74365	0.16081	0.58833	1.0000
O	O19	1.0	0.54480	0.14203	0.55549	1.0000
O	O20	1.0	0.68177	0.50982	0.49986	1.0000
O	O21	1.0	0.77662	0.47251	0.58933	1.0000
O	O22	1.0	0.56725	0.51892	0.58164	1.0000
O	O23	1.0	0.28774	0.32531	0.56963	1.0000
O	O24	1.0	0.15577	0.15755	0.55683	1.0000
O	O25	1.0	0.34207	0.13477	0.60390	1.0000
O	O26	1.0	0.17468	0.49786	0.55135	1.0000
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O	O29	1.0	0.95669	0.15102	0.59253	1.0000
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O	O31	1.0	0.34319	0.38131	0.31224	1.0000
O	O32	1.0	0.17046	0.35130	0.25511	1.0000
O	O33	1.0	0.20728	0.22107	0.33142	1.0000
O	O34	1.0	0.14892	0.42410	0.34759	1.0000
O	O35	1.0	0.49546	0.33109	0.24490	1.0000
O	O36	1.0	0.48780	0.23349	0.33293	1.0000
O	O37	1.0	0.54419	0.44011	0.32689	1.0000

O	O38	1.0	0.33046	0.72580	0.31079	1.0000
O	O39	1.0	0.14757	0.83008	0.31154	1.0000
O	O40	1.0	0.15859	0.63802	0.35012	1.0000
O	O41	1.0	0.49582	0.63610	0.35834	1.0000
O	O42	1.0	0.31641	0.96316	0.31041	1.0000
O	O43	1.0	0.13090	0.02524	0.34849	1.0000
O	O44	1.0	0.51795	0.03054	0.35374	1.0000
O	O45	1.0	0.67031	0.63591	0.81491	1.0000
O	O46	1.0	0.82329	0.65157	0.74254	1.0000
O	O47	1.0	0.83615	0.76785	0.82658	1.0000
O	O48	1.0	0.86237	0.55516	0.82663	1.0000
O	O49	1.0	0.51515	0.65215	0.74812	1.0000
O	O50	1.0	0.52118	0.78636	0.82707	1.0000
O	O51	1.0	0.47051	0.58442	0.84005	1.0000
O	O52	1.0	0.65593	0.29019	0.80926	1.0000
O	O53	1.0	0.82364	0.16332	0.82709	1.0000
O	O54	1.0	0.82302	0.36002	0.85960	1.0000
O	O55	1.0	0.46833	0.37373	0.83683	1.0000
O	O56	1.0	0.66049	0.02916	0.81290	1.0000
O	O57	1.0	0.84453	0.96790	0.85549	1.0000
O	O58	1.0	0.45138	0.97859	0.84884	1.0000
O	O59	1.0	0.62301	0.66987	0.93666	1.0000
O	O60	1.0	0.65499	0.82777	0.00351	1.0000
O	O61	1.0	0.76861	0.81956	0.91919	1.0000
O	O62	1.0	0.55881	0.86663	0.91801	1.0000
O	O63	1.0	0.65641	0.50794	0.99967	1.0000
O	O64	1.0	0.77691	0.52871	0.91810	1.0000
O	O65	1.0	0.57172	0.47148	0.91067	1.0000
O	O66	1.0	0.28310	0.64899	0.93593	1.0000
O	O67	1.0	0.16819	0.82518	0.93703	1.0000
O	O68	1.0	0.35764	0.81732	0.89185	1.0000
O	O69	1.0	0.16468	0.47638	0.94363	1.0000
O	O70	1.0	0.35741	0.46403	0.90436	1.0000
O	O71	1.0	0.04254	0.65355	0.94235	1.0000

O	O72	1.0	0.97452	0.82920	0.89746	1.0000
O	O73	1.0	0.97710	0.47193	0.90076	1.0000
O	O74	1.0	0.31031	0.32152	0.43587	1.0000
O	O75	1.0	0.34281	0.17081	0.50671	1.0000
O	O76	1.0	0.25053	0.12314	0.41808	1.0000
O	O77	1.0	0.45971	0.16850	0.42725	1.0000
O	O78	1.0	0.35972	0.47038	0.50422	1.0000
O	O79	1.0	0.26112	0.52447	0.41876	1.0000
O	O80	1.0	0.46316	0.46587	0.41856	1.0000
O	O81	1.0	0.71496	0.35126	0.43545	1.0000
O	O82	1.0	0.85007	0.18947	0.42062	1.0000
O	O83	1.0	0.65336	0.17270	0.39033	1.0000
O	O84	1.0	0.84643	0.52073	0.43593	1.0000
O	O85	1.0	0.65587	0.53963	0.40036	1.0000
O	O86	1.0	0.97575	0.35358	0.44502	1.0000
O	O87	1.0	0.05227	0.18683	0.39803	1.0000
O	O88	1.0	0.04952	0.54140	0.41724	1.0000
O	O89	1.0	0.67545	0.35554	0.69609	1.0000
O	O90	1.0	0.83609	0.32010	0.76009	1.0000
O	O91	1.0	0.85150	0.25735	0.66278	1.0000
O	O92	1.0	0.49660	0.30539	0.74267	1.0000
O	O93	1.0	0.53296	0.23192	0.64999	1.0000
O	O94	1.0	0.49338	0.44002	0.66825	1.0000
O	O95	1.0	0.66764	0.71872	0.68477	1.0000
O	O96	1.0	0.84262	0.84431	0.69634	1.0000
O	O97	1.0	0.85256	0.66330	0.64441	1.0000
O	O98	1.0	0.49373	0.83353	0.69815	1.0000
O	O99	1.0	0.48139	0.64799	0.65002	1.0000
O	O100	1.0	0.66821	0.95757	0.70098	1.0000
O	O101	1.0	0.84071	0.04311	0.65795	1.0000
O	O102	1.0	0.51076	0.00104	0.63871	1.0000
O	O103	1.0	0.34217	0.64364	0.19034	1.0000
O	O104	1.0	0.17452	0.65815	0.25161	1.0000
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O	O106	1.0	0.14947	0.57639	0.16251	1.0000
O	O107	1.0	0.49997	0.66350	0.25797	1.0000
O	O108	1.0	0.51354	0.76922	0.17275	1.0000
O	O109	1.0	0.53213	0.55610	0.17536	1.0000
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O	O111	1.0	0.15070	0.17548	0.19881	1.0000
O	O112	1.0	0.13275	0.36344	0.15720	1.0000
O	O113	1.0	0.48478	0.16193	0.18282	1.0000
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O	O118	1.0	0.99338	0.48811	0.00048	1.0000
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O	O127	1.0	0.12820	0.99638	0.14997	1.0000
O	O128	1.0	0.48086	0.17341	0.81943	1.0000
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Al	Al2	1.0	0.87293	0.53313	0.62655	1.0000
Al	Al3	1.0	0.45237	0.96712	0.30475	1.0000
Al	Al4	1.0	0.14906	0.86071	0.12081	1.0000
Al	Al5	1.0	0.52561	0.03625	0.80141	1.0000
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Si	Si2	1.0	0.32310	0.54049	0.05911	1.0000
Si	Si3	1.0	0.70666	0.79408	0.05748	1.0000
Si	Si4	1.0	0.70377	0.53801	0.05523	1.0000
Si	Si5	1.0	0.95467	0.79195	0.05284	1.0000
Si	Si6	1.0	0.94959	0.53392	0.05394	1.0000

Si	Si7	1.0	0.52328	0.85014	0.12465	1.0000
Si	Si8	1.0	0.66309	0.20650	0.54622	1.0000
Si	Si9	1.0	0.66961	0.46036	0.55668	1.0000
Si	Si10	1.0	0.27975	0.19678	0.56078	1.0000
Si	Si11	1.0	0.29441	0.45180	0.55694	1.0000
Si	Si12	1.0	0.03560	0.20408	0.55068	1.0000
Si	Si13	1.0	0.05027	0.46224	0.55905	1.0000
Si	Si14	1.0	0.21753	0.34414	0.31224	1.0000
Si	Si15	1.0	0.46770	0.34530	0.30419	1.0000
Si	Si16	1.0	0.20084	0.71326	0.30546	1.0000
Si	Si17	1.0	0.18957	0.95292	0.30556	1.0000
Si	Si18	1.0	0.15510	0.53049	0.38323	1.0000
Si	Si19	1.0	0.79687	0.65507	0.80311	1.0000
Si	Si20	1.0	0.54411	0.66618	0.80738	1.0000
Si	Si21	1.0	0.78544	0.28226	0.81421	1.0000
Si	Si22	1.0	0.78766	0.04089	0.81247	1.0000
Si	Si23	1.0	0.85883	0.47931	0.87655	1.0000
Si	Si24	1.0	0.65189	0.79691	0.94403	1.0000
Si	Si25	1.0	0.65762	0.54530	0.94118	1.0000
Si	Si26	1.0	0.28902	0.77777	0.93964	1.0000
Si	Si27	1.0	0.28576	0.52290	0.94678	1.0000
Si	Si28	1.0	0.04556	0.78359	0.94385	1.0000
Si	Si29	1.0	0.04465	0.52451	0.94701	1.0000
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Si	Si31	1.0	0.33986	0.19642	0.44649	1.0000
Si	Si32	1.0	0.34766	0.44590	0.44462	1.0000
Si	Si33	1.0	0.72858	0.22277	0.43402	1.0000
Si	Si34	1.0	0.72481	0.47966	0.44400	1.0000
Si	Si35	1.0	0.96818	0.22512	0.44014	1.0000
Si	Si36	1.0	0.96415	0.48139	0.45296	1.0000
Si	Si37	1.0	0.52935	0.14945	0.37550	1.0000
Si	Si38	1.0	0.54810	0.33055	0.68715	1.0000
Si	Si39	1.0	0.79673	0.72290	0.69044	1.0000
Si	Si40	1.0	0.53988	0.71413	0.69503	1.0000

Si	Si41	1.0	0.79609	0.96518	0.70286	1.0000
Si	Si42	1.0	0.53814	0.95660	0.69382	1.0000
Si	Si43	1.0	0.21373	0.66917	0.19300	1.0000
Si	Si44	1.0	0.47006	0.65924	0.19762	1.0000
Si	Si45	1.0	0.19508	0.29849	0.20029	1.0000
Si	Si46	1.0	0.45127	0.28534	0.19103	1.0000
Si	Si47	1.0	0.44727	0.03817	0.19107	1.0000
Si	Si48	1.0	0.13168	0.47457	0.12570	1.0000
Si	Si49	1.0	0.52485	0.47573	0.12689	1.0000
Si	Si50	1.0	0.84800	0.15200	0.62561	1.0000
Si	Si51	1.0	0.47633	0.52999	0.62501	1.0000
Si	Si52	1.0	0.16015	0.13936	0.37422	1.0000
Si	Si53	1.0	0.53923	0.51881	0.37590	1.0000
Si	Si54	1.0	0.85514	0.84649	0.87516	1.0000
Si	Si55	1.0	0.46803	0.47701	0.87378	1.0000
Si	Si56	1.0	0.80211	0.34196	0.70212	1.0000
Si	Si57	1.0	0.45595	0.70590	0.31121	1.0000
Si	Si58	1.0	0.19126	0.05341	0.20038	1.0000
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O O2 1.0 0.32810 0.83326 0.98639 1.0000
O O3 1.0 0.26756 0.84449 0.08432 1.0000

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O	O6	1.0	0.44139	0.48647	0.08085	1.0000
O	O7	1.0	0.71624	0.66040	0.05817	1.0000
O	O8	1.0	0.84341	0.83287	0.04944	1.0000
O	O9	1.0	0.66491	0.83949	0.10492	1.0000
O	O10	1.0	0.83270	0.48752	0.05259	1.0000
O	O11	1.0	0.64804	0.47842	0.09995	1.0000
O	O12	1.0	0.96221	0.66046	0.05180	1.0000
O	O13	1.0	0.03643	0.84349	0.09080	1.0000
O	O14	1.0	0.01434	0.48380	0.10066	1.0000
O	O15	1.0	0.63155	0.33029	0.55189	1.0000
O	O16	1.0	0.67790	0.16915	0.49021	1.0000
O	O17	1.0	0.73763	0.16011	0.58756	1.0000
O	O18	1.0	0.53447	0.13979	0.56064	1.0000
O	O19	1.0	0.68571	0.51252	0.50515	1.0000
O	O20	1.0	0.76458	0.46687	0.59556	1.0000
O	O21	1.0	0.55812	0.51583	0.58221	1.0000
O	O22	1.0	0.28066	0.33571	0.56150	1.0000
O	O23	1.0	0.14996	0.16596	0.55444	1.0000
O	O24	1.0	0.33181	0.15388	0.60605	1.0000
O	O25	1.0	0.16870	0.50998	0.55148	1.0000
O	O26	1.0	0.35031	0.51909	0.60164	1.0000
O	O27	1.0	0.03451	0.34051	0.55348	1.0000
O	O28	1.0	0.95080	0.16146	0.59172	1.0000
O	O29	1.0	0.98981	0.51726	0.60342	1.0000
O	O30	1.0	0.33501	0.38287	0.30965	1.0000
O	O31	1.0	0.17090	0.35238	0.24528	1.0000
O	O32	1.0	0.18438	0.23523	0.32838	1.0000
O	O33	1.0	0.14030	0.44497	0.33204	1.0000
O	O34	1.0	0.50129	0.34595	0.24928	1.0000
O	O35	1.0	0.46766	0.22797	0.33224	1.0000
O	O36	1.0	0.53377	0.42939	0.33882	1.0000
O	O37	1.0	0.35140	0.71531	0.30862	1.0000

O	O38	1.0	0.18221	0.83433	0.32684	1.0000
O	O39	1.0	0.19439	0.64049	0.36446	1.0000
O	O40	1.0	0.51952	0.83986	0.31625	1.0000
O	O41	1.0	0.53468	0.64161	0.34264	1.0000
O	O42	1.0	0.34768	0.96942	0.31529	1.0000
O	O43	1.0	0.16344	0.03366	0.35380	1.0000
O	O44	1.0	0.53719	0.03361	0.34588	1.0000
O	O45	1.0	0.66893	0.61935	0.81001	1.0000
O	O46	1.0	0.82682	0.65562	0.74218	1.0000
O	O47	1.0	0.81886	0.76815	0.82686	1.0000
O	O48	1.0	0.86535	0.55876	0.82737	1.0000
O	O49	1.0	0.50490	0.64838	0.74862	1.0000
O	O50	1.0	0.53473	0.77601	0.82817	1.0000
O	O51	1.0	0.46996	0.57507	0.84054	1.0000
O	O52	1.0	0.64829	0.29298	0.80793	1.0000
O	O53	1.0	0.81201	0.16510	0.82705	1.0000
O	O54	1.0	0.81273	0.36269	0.85870	1.0000
O	O55	1.0	0.48275	0.16274	0.81867	1.0000
O	O56	1.0	0.46152	0.36276	0.84088	1.0000
O	O57	1.0	0.64923	0.02911	0.81392	1.0000
O	O58	1.0	0.83146	0.96764	0.85520	1.0000
O	O59	1.0	0.45997	0.96764	0.84714	1.0000
O	O60	1.0	0.62243	0.66496	0.93860	1.0000
O	O61	1.0	0.65057	0.82476	0.00570	1.0000
O	O62	1.0	0.76818	0.81875	0.92203	1.0000
O	O63	1.0	0.55809	0.86026	0.91964	1.0000
O	O64	1.0	0.65391	0.49964	0.00002	1.0000
O	O65	1.0	0.77847	0.53175	0.91881	1.0000
O	O66	1.0	0.57785	0.46594	0.90897	1.0000
O	O67	1.0	0.28742	0.64866	0.94276	1.0000
O	O68	1.0	0.16645	0.81538	0.92143	1.0000
O	O69	1.0	0.36315	0.80478	0.88741	1.0000
O	O70	1.0	0.16399	0.47922	0.93221	1.0000
O	O71	1.0	0.36589	0.46450	0.91129	1.0000

O	O72	1.0	0.03362	0.64933	0.93406	1.0000
O	O73	1.0	0.96854	0.83004	0.89259	1.0000
O	O74	1.0	0.97157	0.46094	0.90070	1.0000
O	O75	1.0	0.37617	0.32999	0.43930	1.0000
O	O76	1.0	0.34302	0.17176	0.50733	1.0000
O	O77	1.0	0.23184	0.17520	0.42251	1.0000
O	O78	1.0	0.44163	0.13486	0.42207	1.0000
O	O79	1.0	0.35277	0.49290	0.50268	1.0000
O	O80	1.0	0.22351	0.46917	0.42356	1.0000
O	O81	1.0	0.42564	0.52857	0.41069	1.0000
O	O82	1.0	0.70672	0.35182	0.44211	1.0000
O	O83	1.0	0.83493	0.18877	0.42283	1.0000
O	O84	1.0	0.63772	0.18699	0.39099	1.0000
O	O85	1.0	0.83664	0.51868	0.43345	1.0000
O	O86	1.0	0.63815	0.53844	0.40918	1.0000
O	O87	1.0	0.96997	0.35260	0.43700	1.0000
O	O88	1.0	0.03210	0.17261	0.39397	1.0000
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O	O90	1.0	0.66846	0.36658	0.69806	1.0000
O	O91	1.0	0.83021	0.32129	0.75951	1.0000
O	O92	1.0	0.83914	0.26157	0.66215	1.0000
O	O93	1.0	0.48719	0.31007	0.74535	1.0000
O	O94	1.0	0.53025	0.23698	0.65338	1.0000
O	O95	1.0	0.48288	0.44268	0.67014	1.0000
O	O96	1.0	0.66230	0.71871	0.68920	1.0000
O	O97	1.0	0.83271	0.84904	0.69527	1.0000
O	O98	1.0	0.84279	0.66698	0.64338	1.0000
O	O99	1.0	0.48901	0.83199	0.69963	1.0000
O	O100	1.0	0.47878	0.64991	0.64954	1.0000
O	O101	1.0	0.65902	0.96552	0.69639	1.0000
O	O102	1.0	0.83776	0.04801	0.65758	1.0000
O	O103	1.0	0.48144	0.01057	0.64799	1.0000
O	O104	1.0	0.33053	0.62803	0.20169	1.0000
O	O105	1.0	0.16941	0.66709	0.26498	1.0000

O	O106	1.0	0.16463	0.74761	0.17109	1.0000
O	O107	1.0	0.51245	0.68667	0.24571	1.0000
O	O108	1.0	0.46469	0.76297	0.15453	1.0000
O	O109	1.0	0.51622	0.55813	0.16905	1.0000
O	O110	1.0	0.33671	0.28493	0.19392	1.0000
O	O111	1.0	0.16447	0.16039	0.19969	1.0000
O	O112	1.0	0.15929	0.34013	0.14562	1.0000
O	O113	1.0	0.50695	0.16717	0.19606	1.0000
O	O114	1.0	0.51681	0.35173	0.14890	1.0000
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O	O117	1.0	0.01438	0.82285	0.99130	1.0000
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O	O121	1.0	0.17814	0.98357	0.25577	1.0000
O	O122	1.0	0.50332	0.98900	0.24750	1.0000
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O	O125	1.0	0.85772	0.46516	0.68941	1.0000
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Al	Al2	1.0	0.86435	0.53676	0.62623	1.0000
Al	Al3	1.0	0.53439	0.86147	0.12214	1.0000
Al	Al4	1.0	0.13689	0.47047	0.12690	1.0000
Al	Al5	1.0	0.15576	0.83796	0.12228	1.0000
Si	Si1	1.0	0.33756	0.54711	0.05944	1.0000
Si	Si2	1.0	0.72179	0.78959	0.05664	1.0000
Si	Si3	1.0	0.71297	0.53180	0.05301	1.0000
Si	Si4	1.0	0.96544	0.78954	0.04683	1.0000
Si	Si5	1.0	0.95605	0.53055	0.05221	1.0000
Si	Si6	1.0	0.65195	0.20438	0.54793	1.0000

Si	Si7	1.0	0.66241	0.45748	0.56001	1.0000
Si	Si8	1.0	0.27379	0.20651	0.55907	1.0000
Si	Si9	1.0	0.28775	0.46418	0.55492	1.0000
Si	Si10	1.0	0.03015	0.21238	0.54859	1.0000
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Si	Si13	1.0	0.45970	0.34646	0.30739	1.0000
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Si	Si16	1.0	0.21911	0.95557	0.31313	1.0000
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Si	Si19	1.0	0.79442	0.65221	0.80235	1.0000
Si	Si20	1.0	0.54416	0.65477	0.80682	1.0000
Si	Si21	1.0	0.77555	0.28494	0.81351	1.0000
Si	Si22	1.0	0.51994	0.28243	0.80293	1.0000
Si	Si23	1.0	0.77811	0.04315	0.81269	1.0000
Si	Si24	1.0	0.52135	0.04312	0.80620	1.0000
Si	Si25	1.0	0.85583	0.47879	0.87639	1.0000
Si	Si26	1.0	0.65149	0.79139	0.94570	1.0000
Si	Si27	1.0	0.65829	0.54019	0.94184	1.0000
Si	Si28	1.0	0.28555	0.77588	0.93456	1.0000
Si	Si29	1.0	0.28190	0.52025	0.94842	1.0000
Si	Si30	1.0	0.04470	0.77867	0.93554	1.0000
Si	Si31	1.0	0.04454	0.52124	0.94269	1.0000
Si	Si32	1.0	0.47898	0.85095	0.87077	1.0000
Si	Si33	1.0	0.34657	0.20388	0.44731	1.0000
Si	Si34	1.0	0.34458	0.45569	0.44428	1.0000
Si	Si35	1.0	0.71479	0.22440	0.43648	1.0000
Si	Si36	1.0	0.71661	0.48029	0.44788	1.0000
Si	Si37	1.0	0.95641	0.22363	0.43735	1.0000
Si	Si38	1.0	0.95636	0.48050	0.44542	1.0000
Si	Si39	1.0	0.52094	0.14727	0.37290	1.0000
Si	Si40	1.0	0.54107	0.33668	0.69061	1.0000

Si	Si41	1.0	0.79145	0.72527	0.69086	1.0000
Si	Si42	1.0	0.53395	0.71251	0.69633	1.0000
Si	Si43	1.0	0.78705	0.96931	0.70115	1.0000
Si	Si44	1.0	0.52903	0.95614	0.69719	1.0000
Si	Si45	1.0	0.45615	0.66182	0.19128	1.0000
Si	Si46	1.0	0.20809	0.28464	0.19409	1.0000
Si	Si47	1.0	0.46596	0.28823	0.19649	1.0000
Si	Si48	1.0	0.46767	0.04323	0.19433	1.0000
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Si	Si50	1.0	0.84167	0.15740	0.62484	1.0000
Si	Si51	1.0	0.46852	0.53089	0.62589	1.0000
Si	Si52	1.0	0.15298	0.15449	0.37478	1.0000
Si	Si53	1.0	0.53214	0.53361	0.37540	1.0000
Si	Si54	1.0	0.84704	0.84614	0.87439	1.0000
Si	Si55	1.0	0.46949	0.46799	0.87545	1.0000
Si	Si56	1.0	0.79438	0.34704	0.70207	1.0000
Si	Si57	1.0	0.35080	0.79889	0.04474	1.0000
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T1T1T7T7T7T7

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H H4 1.0 0.12925 0.82259 0.36134 1.0000
H H5 1.0 0.13894 0.48109 0.21718 1.0000
H H6 1.0 0.17868 0.86993 0.88888 1.0000
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O O2 1.0 0.32669 0.82895 0.98891 1.0000

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O	O5	1.0	0.23749	0.53713	0.09709	1.0000
O	O6	1.0	0.44144	0.48225	0.08187	1.0000
O	O7	1.0	0.71850	0.66161	0.05920	1.0000
O	O8	1.0	0.85042	0.83165	0.05615	1.0000
O	O9	1.0	0.66491	0.84015	0.10561	1.0000
O	O10	1.0	0.83289	0.48718	0.05199	1.0000
O	O11	1.0	0.64911	0.47865	0.09977	1.0000
O	O12	1.0	0.96498	0.65771	0.05230	1.0000
O	O13	1.0	0.04549	0.83084	0.09680	1.0000
O	O14	1.0	0.01289	0.48143	0.10172	1.0000
O	O15	1.0	0.62977	0.33313	0.55211	1.0000
O	O16	1.0	0.67432	0.17186	0.49044	1.0000
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O	O19	1.0	0.68446	0.51604	0.50490	1.0000
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O	O21	1.0	0.55805	0.51892	0.58210	1.0000
O	O22	1.0	0.28092	0.33636	0.56070	1.0000
O	O23	1.0	0.14809	0.16818	0.55358	1.0000
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O	O25	1.0	0.16825	0.51105	0.55168	1.0000
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O	O27	1.0	0.03236	0.34288	0.55322	1.0000
O	O28	1.0	0.94979	0.16390	0.59212	1.0000
O	O29	1.0	0.98900	0.52057	0.60275	1.0000
O	O30	1.0	0.33057	0.37797	0.31055	1.0000
O	O31	1.0	0.17151	0.34158	0.24378	1.0000
O	O32	1.0	0.18324	0.22488	0.32775	1.0000
O	O33	1.0	0.13388	0.43274	0.33082	1.0000
O	O34	1.0	0.49692	0.34824	0.24968	1.0000
O	O35	1.0	0.46455	0.22306	0.33077	1.0000
O	O36	1.0	0.52958	0.42451	0.34020	1.0000

O	O37	1.0	0.35346	0.72143	0.30738	1.0000
O	O38	1.0	0.19834	0.62618	0.36028	1.0000
O	O39	1.0	0.52926	0.83801	0.31683	1.0000
O	O40	1.0	0.53194	0.63706	0.34116	1.0000
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O	O42	1.0	0.15827	0.02867	0.36160	1.0000
O	O43	1.0	0.54601	0.03296	0.34737	1.0000
O	O44	1.0	0.67112	0.61675	0.80944	1.0000
O	O45	1.0	0.82882	0.65654	0.74248	1.0000
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O	O48	1.0	0.50472	0.65058	0.74933	1.0000
O	O49	1.0	0.54194	0.77643	0.82899	1.0000
O	O50	1.0	0.47116	0.57681	0.84050	1.0000
O	O51	1.0	0.64635	0.28834	0.80648	1.0000
O	O52	1.0	0.81357	0.16877	0.82655	1.0000
O	O53	1.0	0.80620	0.36810	0.85776	1.0000
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O	O61	1.0	0.77614	0.81891	0.92219	1.0000
O	O62	1.0	0.56774	0.86578	0.92012	1.0000
O	O63	1.0	0.65352	0.50318	0.00040	1.0000
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O	O65	1.0	0.57837	0.47032	0.90968	1.0000
O	O66	1.0	0.28047	0.64649	0.94292	1.0000
O	O67	1.0	0.37457	0.80221	0.89013	1.0000
O	O68	1.0	0.16382	0.47081	0.93315	1.0000
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O	O71	1.0	0.97255	0.84034	0.88809	1.0000
O	O72	1.0	0.96953	0.45452	0.90207	1.0000
O	O73	1.0	0.38255	0.32909	0.44053	1.0000
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O	O89	1.0	0.82892	0.32529	0.75937	1.0000
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O	O91	1.0	0.48463	0.31333	0.74551	1.0000
O	O92	1.0	0.52820	0.23609	0.65446	1.0000
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O	O95	1.0	0.83098	0.85116	0.69596	1.0000
O	O96	1.0	0.84293	0.66941	0.64383	1.0000
O	O97	1.0	0.48845	0.83204	0.69913	1.0000
O	O98	1.0	0.47803	0.64969	0.65023	1.0000
O	O99	1.0	0.65686	0.96768	0.69673	1.0000
O	O100	1.0	0.83550	0.04920	0.65703	1.0000
O	O101	1.0	0.47858	0.01091	0.64793	1.0000
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O	O104	1.0	0.16767	0.74217	0.16549	1.0000

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O	O106	1.0	0.46370	0.76388	0.15416	1.0000
O	O107	1.0	0.51879	0.55965	0.16831	1.0000
O	O108	1.0	0.33824	0.28273	0.19117	1.0000
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O	O112	1.0	0.52126	0.35175	0.15038	1.0000
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O	O121	1.0	0.51599	0.98872	0.24897	1.0000
O	O122	1.0	0.82152	0.01986	0.75571	1.0000
O	O123	1.0	0.48326	0.01273	0.74870	1.0000
O	O124	1.0	0.85664	0.46714	0.68884	1.0000
O	O125	1.0	0.46503	0.86056	0.06054	1.0000
O	O126	1.0	0.17850	0.82366	0.33274	1.0000
O	O127	1.0	0.13966	0.53595	0.18996	1.0000
O	O128	1.0	0.17731	0.82151	0.91777	1.0000
Al	Al1	1.0	0.45931	0.13525	0.62393	1.0000
Al	Al2	1.0	0.86390	0.53948	0.62599	1.0000
Al	Al3	1.0	0.53634	0.86423	0.12427	1.0000
Al	Al4	1.0	0.22154	0.96390	0.31284	1.0000
Al	Al5	1.0	0.13634	0.46433	0.12627	1.0000
Al	Al6	1.0	0.03690	0.77856	0.93735	1.0000
Si	Si1	1.0	0.33828	0.54222	0.06008	1.0000
Si	Si2	1.0	0.72667	0.79092	0.05871	1.0000
Si	Si3	1.0	0.71414	0.53311	0.05331	1.0000
Si	Si4	1.0	0.97175	0.78697	0.04986	1.0000

Si	Si5	1.0	0.95722	0.52790	0.05248	1.0000
Si	Si6	1.0	0.64965	0.20709	0.54806	1.0000
Si	Si7	1.0	0.66176	0.46033	0.55962	1.0000
Si	Si8	1.0	0.27266	0.20706	0.55839	1.0000
Si	Si9	1.0	0.28710	0.46487	0.55424	1.0000
Si	Si10	1.0	0.02807	0.21455	0.54841	1.0000
Si	Si11	1.0	0.04349	0.47295	0.55359	1.0000
Si	Si12	1.0	0.20548	0.34165	0.30346	1.0000
Si	Si13	1.0	0.45577	0.34276	0.30756	1.0000
Si	Si14	1.0	0.48375	0.72124	0.30220	1.0000
Si	Si15	1.0	0.48326	0.95721	0.30654	1.0000
Si	Si16	1.0	0.14765	0.51201	0.37923	1.0000
Si	Si17	1.0	0.79643	0.65374	0.80271	1.0000
Si	Si18	1.0	0.54738	0.65496	0.80690	1.0000
Si	Si19	1.0	0.77394	0.28753	0.81298	1.0000
Si	Si20	1.0	0.51770	0.28280	0.80262	1.0000
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Si	Si22	1.0	0.51861	0.04502	0.80539	1.0000
Si	Si23	1.0	0.85612	0.48071	0.87714	1.0000
Si	Si24	1.0	0.66001	0.79488	0.94687	1.0000
Si	Si25	1.0	0.65978	0.54414	0.94252	1.0000
Si	Si26	1.0	0.28020	0.51625	0.94846	1.0000
Si	Si27	1.0	0.04445	0.51662	0.94345	1.0000
Si	Si28	1.0	0.48918	0.85243	0.87150	1.0000
Si	Si29	1.0	0.34570	0.20376	0.44719	1.0000
Si	Si30	1.0	0.34499	0.45292	0.44376	1.0000
Si	Si31	1.0	0.71233	0.22742	0.43699	1.0000
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Si	Si33	1.0	0.95198	0.22537	0.43772	1.0000
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Si	Si35	1.0	0.51907	0.14594	0.37267	1.0000
Si	Si36	1.0	0.53928	0.33728	0.69067	1.0000
Si	Si37	1.0	0.79174	0.72655	0.69154	1.0000
Si	Si38	1.0	0.53389	0.71286	0.69660	1.0000

Si	Si39	1.0	0.78525	0.97151	0.70108	1.0000
Si	Si40	1.0	0.52680	0.95674	0.69697	1.0000
Si	Si41	1.0	0.45860	0.66231	0.19068	1.0000
Si	Si42	1.0	0.20894	0.27422	0.19180	1.0000
Si	Si43	1.0	0.46678	0.28707	0.19692	1.0000
Si	Si44	1.0	0.21304	0.02887	0.20022	1.0000
Si	Si45	1.0	0.47205	0.04381	0.19735	1.0000
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Si	Si47	1.0	0.53169	0.46910	0.12511	1.0000
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Si	Si49	1.0	0.46800	0.53160	0.62553	1.0000
Si	Si50	1.0	0.14955	0.15157	0.37699	1.0000
Si	Si51	1.0	0.53003	0.53080	0.37508	1.0000
Si	Si52	1.0	0.84982	0.85034	0.87271	1.0000
Si	Si53	1.0	0.47100	0.46998	0.87560	1.0000
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Si	Si55	1.0	0.34947	0.79347	0.04737	1.0000
Si	Si56	1.0	0.22850	0.70494	0.31451	1.0000
Si	Si57	1.0	0.20729	0.65129	0.20312	1.0000
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O	O8	1.0	0.84970	0.82763	0.05751	1.0000
O	O9	1.0	0.66818	0.83106	0.11001	1.0000
O	O10	1.0	0.83714	0.48382	0.05232	1.0000
O	O11	1.0	0.65247	0.47176	0.09895	1.0000
O	O12	1.0	0.96874	0.65590	0.05347	1.0000
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O	O33	1.0	0.13182	0.43511	0.33028	1.0000
O	O34	1.0	0.49479	0.34915	0.24875	1.0000
O	O35	1.0	0.46090	0.22262	0.32871	1.0000
O	O36	1.0	0.52773	0.42332	0.33955	1.0000

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O	O39	1.0	0.19379	0.63130	0.35758	1.0000
O	O40	1.0	0.52521	0.83488	0.31498	1.0000
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O	O48	1.0	0.86286	0.56515	0.82614	1.0000
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O	O50	1.0	0.53837	0.77719	0.83383	1.0000
O	O51	1.0	0.47050	0.57700	0.84086	1.0000
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O	O53	1.0	0.81867	0.17322	0.82318	1.0000
O	O54	1.0	0.81522	0.36885	0.85871	1.0000
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O	O66	1.0	0.29443	0.64960	0.94282	1.0000
O	O67	1.0	0.17179	0.81995	0.92828	1.0000
O	O68	1.0	0.36326	0.81198	0.89026	1.0000
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O	O73	1.0	0.97255	0.47164	0.89904	1.0000
O	O74	1.0	0.37412	0.33035	0.43941	1.0000
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O	O111	1.0	0.51186	0.16874	0.19768	1.0000
O	O112	1.0	0.51800	0.35161	0.14933	1.0000
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O	O116	1.0	0.01695	0.82504	0.99629	1.0000
O	O117	1.0	0.01196	0.48612	0.99830	1.0000
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O	O126	1.0	0.14162	0.53129	0.18863	1.0000
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Al	Al2	1.0	0.86173	0.53788	0.62327	1.0000
Al	Al3	1.0	0.53936	0.86097	0.12632	1.0000
Al	Al4	1.0	0.13979	0.45781	0.12570	1.0000
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Al	Al6	1.0	0.96307	0.22172	0.43745	1.0000
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Si	Si2	1.0	0.72619	0.78540	0.06108	1.0000
Si	Si3	1.0	0.71742	0.52727	0.05294	1.0000
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Si	Si5	1.0	0.96033	0.52572	0.05175	1.0000
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Si	Si20	1.0	0.54332	0.65885	0.80803	1.0000
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Si	Si22	1.0	0.52312	0.28295	0.80265	1.0000
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Si	Si37	1.0	0.54056	0.33967	0.69065	1.0000
Si	Si38	1.0	0.78596	0.72460	0.68917	1.0000

Si	Si39	1.0	0.52889	0.71643	0.69766	1.0000
Si	Si40	1.0	0.78528	0.96850	0.69899	1.0000
Si	Si41	1.0	0.52726	0.95919	0.69865	1.0000
Si	Si42	1.0	0.45976	0.65958	0.19074	1.0000
Si	Si43	1.0	0.20794	0.27171	0.19216	1.0000
Si	Si44	1.0	0.46500	0.28747	0.19594	1.0000
Si	Si45	1.0	0.21668	0.02700	0.20123	1.0000
Si	Si46	1.0	0.47450	0.04381	0.19664	1.0000
Si	Si47	1.0	0.16096	0.83893	0.12511	1.0000
Si	Si48	1.0	0.53365	0.46727	0.12288	1.0000
Si	Si49	1.0	0.84068	0.15992	0.62521	1.0000
Si	Si50	1.0	0.46760	0.53083	0.62745	1.0000
Si	Si51	1.0	0.15072	0.14826	0.37296	1.0000
Si	Si52	1.0	0.53036	0.52921	0.37530	1.0000
Si	Si53	1.0	0.47102	0.46980	0.87513	1.0000
Si	Si54	1.0	0.79181	0.35435	0.70139	1.0000
Si	Si55	1.0	0.35286	0.79373	0.04860	1.0000
Si	Si56	1.0	0.20885	0.64726	0.20167	1.0000
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O	O5	1.0	0.33747	0.50256	0.00151	1.0000
O	O6	1.0	0.21834	0.48406	0.08241	1.0000
O	O7	1.0	0.42757	0.51454	0.08950	1.0000
O	O8	1.0	0.67852	0.65632	0.06306	1.0000
O	O9	1.0	0.82987	0.80760	0.06958	1.0000
O	O10	1.0	0.64138	0.84436	0.10500	1.0000
O	O11	1.0	0.82668	0.50437	0.06840	1.0000
O	O12	1.0	0.63103	0.46193	0.09275	1.0000
O	O13	1.0	0.97597	0.65531	0.06166	1.0000
O	O14	1.0	0.02213	0.84030	0.10413	1.0000
O	O15	1.0	0.01228	0.47177	0.10665	1.0000
O	O16	1.0	0.64010	0.33540	0.55183	1.0000
O	O17	1.0	0.68704	0.17631	0.48936	1.0000
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O	O19	1.0	0.53999	0.14854	0.55959	1.0000
O	O20	1.0	0.67978	0.51184	0.49971	1.0000
O	O21	1.0	0.77360	0.47756	0.58899	1.0000
O	O22	1.0	0.56418	0.52086	0.58077	1.0000
O	O23	1.0	0.28467	0.33175	0.57043	1.0000
O	O24	1.0	0.15532	0.16397	0.55594	1.0000
O	O25	1.0	0.33760	0.14411	0.60596	1.0000
O	O26	1.0	0.17535	0.50452	0.55012	1.0000
O	O27	1.0	0.35634	0.52216	0.60077	1.0000
O	O28	1.0	0.04000	0.33893	0.55276	1.0000
O	O29	1.0	0.95527	0.15973	0.58981	1.0000
O	O30	1.0	0.99937	0.51143	0.60616	1.0000
O	O31	1.0	0.34481	0.38052	0.30942	1.0000
O	O32	1.0	0.16891	0.34549	0.25556	1.0000
O	O33	1.0	0.21044	0.22388	0.33426	1.0000
O	O34	1.0	0.15355	0.42849	0.34568	1.0000
O	O35	1.0	0.50361	0.32750	0.24597	1.0000
O	O36	1.0	0.48411	0.23205	0.33420	1.0000

O	O37	1.0	0.54420	0.43697	0.32799	1.0000
O	O38	1.0	0.33778	0.72905	0.30482	1.0000
O	O39	1.0	0.15633	0.83247	0.31448	1.0000
O	O40	1.0	0.17562	0.64077	0.35237	1.0000
O	O41	1.0	0.49971	0.63673	0.35356	1.0000
O	O42	1.0	0.32367	0.96604	0.31189	1.0000
O	O43	1.0	0.13793	0.02713	0.35003	1.0000
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O	O45	1.0	0.68039	0.62711	0.81011	1.0000
O	O46	1.0	0.83439	0.66235	0.74164	1.0000
O	O47	1.0	0.84241	0.75813	0.83172	1.0000
O	O48	1.0	0.87181	0.54792	0.82042	1.0000
O	O49	1.0	0.51965	0.65062	0.74643	1.0000
O	O50	1.0	0.53233	0.76891	0.83127	1.0000
O	O51	1.0	0.48521	0.56331	0.83295	1.0000
O	O52	1.0	0.65739	0.32217	0.80871	1.0000
O	O53	1.0	0.79661	0.16186	0.82421	1.0000
O	O54	1.0	0.83660	0.35252	0.85554	1.0000
O	O55	1.0	0.51571	0.16635	0.81431	1.0000
O	O56	1.0	0.46540	0.35467	0.84548	1.0000
O	O57	1.0	0.65574	0.00648	0.80958	1.0000
O	O58	1.0	0.84548	0.96644	0.84829	1.0000
O	O59	1.0	0.46077	0.98026	0.84612	1.0000
O	O60	1.0	0.63731	0.66424	0.93990	1.0000
O	O61	1.0	0.66895	0.82567	0.00512	1.0000
O	O62	1.0	0.74015	0.84049	0.91049	1.0000
O	O63	1.0	0.67874	0.49676	0.99699	1.0000
O	O64	1.0	0.78244	0.52409	0.91060	1.0000
O	O65	1.0	0.57482	0.47077	0.91259	1.0000
O	O66	1.0	0.26198	0.65373	0.94140	1.0000
O	O67	1.0	0.15207	0.83340	0.94225	1.0000
O	O68	1.0	0.33341	0.81685	0.88858	1.0000
O	O69	1.0	0.36332	0.48102	0.90345	1.0000
O	O70	1.0	0.02765	0.66229	0.94529	1.0000

O	O71	1.0	0.95399	0.84288	0.90735	1.0000
O	O72	1.0	0.98415	0.46574	0.89642	1.0000
O	O73	1.0	0.31777	0.32207	0.43598	1.0000
O	O74	1.0	0.34500	0.17608	0.50857	1.0000
O	O75	1.0	0.24249	0.12942	0.42264	1.0000
O	O76	1.0	0.45491	0.15884	0.42670	1.0000
O	O77	1.0	0.36225	0.47112	0.50495	1.0000
O	O78	1.0	0.24873	0.51861	0.42431	1.0000
O	O79	1.0	0.45531	0.47702	0.41686	1.0000
O	O80	1.0	0.71045	0.35346	0.43583	1.0000
O	O81	1.0	0.84570	0.19254	0.42283	1.0000
O	O82	1.0	0.65040	0.17630	0.39075	1.0000
O	O83	1.0	0.84250	0.52127	0.43490	1.0000
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O	O85	1.0	0.97479	0.35648	0.44110	1.0000
O	O86	1.0	0.04569	0.18584	0.39525	1.0000
O	O87	1.0	0.04095	0.54475	0.40982	1.0000
O	O88	1.0	0.67231	0.36238	0.69554	1.0000
O	O89	1.0	0.83532	0.31344	0.75634	1.0000
O	O90	1.0	0.84477	0.26116	0.65918	1.0000
O	O91	1.0	0.49351	0.32286	0.74691	1.0000
O	O92	1.0	0.52727	0.23688	0.65577	1.0000
O	O93	1.0	0.48931	0.44527	0.66809	1.0000
O	O94	1.0	0.67164	0.72047	0.68476	1.0000
O	O95	1.0	0.84136	0.85009	0.69284	1.0000
O	O96	1.0	0.85470	0.66642	0.64324	1.0000
O	O97	1.0	0.49759	0.83374	0.69842	1.0000
O	O98	1.0	0.48524	0.65263	0.64865	1.0000
O	O99	1.0	0.66677	0.96520	0.69542	1.0000
O	O100	1.0	0.84277	0.04651	0.65405	1.0000
O	O101	1.0	0.49425	0.00959	0.64517	1.0000
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O	O103	1.0	0.17220	0.66233	0.25346	1.0000
O	O104	1.0	0.20247	0.77880	0.17066	1.0000

O	O105	1.0	0.14701	0.57198	0.16689	1.0000
O	O106	1.0	0.50894	0.66826	0.25339	1.0000
O	O107	1.0	0.48941	0.76692	0.16633	1.0000
O	O108	1.0	0.53606	0.55855	0.17105	1.0000
O	O109	1.0	0.32747	0.28861	0.19577	1.0000
O	O110	1.0	0.15327	0.17193	0.19789	1.0000
O	O111	1.0	0.14800	0.36032	0.15633	1.0000
O	O112	1.0	0.49178	0.16055	0.18284	1.0000
O	O113	1.0	0.49798	0.35508	0.14695	1.0000
O	O114	1.0	0.32057	0.03624	0.18925	1.0000
O	O115	1.0	0.49224	0.97039	0.14177	1.0000
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Al	Al1	1.0	0.46873	0.13399	0.62345	1.0000
Al	Al2	1.0	0.87136	0.53652	0.62502	1.0000
Al	Al3	1.0	0.45887	0.96720	0.30399	1.0000
Al	Al4	1.0	0.15204	0.85548	0.12260	1.0000
Al	Al5	1.0	0.45865	0.85305	0.86827	1.0000
Al	Al6	1.0	0.03225	0.52703	0.94946	1.0000
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Si	Si2	1.0	0.32130	0.54476	0.05928	1.0000
Si	Si3	1.0	0.70610	0.78272	0.06068	1.0000
Si	Si4	1.0	0.70525	0.53074	0.05474	1.0000

Si	Si5	1.0	0.95570	0.78303	0.06027	1.0000
Si	Si6	1.0	0.95258	0.52781	0.05922	1.0000
Si	Si7	1.0	0.51694	0.85131	0.12162	1.0000
Si	Si8	1.0	0.65811	0.20954	0.54675	1.0000
Si	Si9	1.0	0.66756	0.46331	0.55665	1.0000
Si	Si10	1.0	0.27801	0.20384	0.56171	1.0000
Si	Si11	1.0	0.29394	0.45743	0.55729	1.0000
Si	Si12	1.0	0.03618	0.21111	0.54846	1.0000
Si	Si13	1.0	0.05083	0.46839	0.55523	1.0000
Si	Si14	1.0	0.21962	0.34415	0.31190	1.0000
Si	Si15	1.0	0.46921	0.34311	0.30453	1.0000
Si	Si16	1.0	0.20810	0.71603	0.30607	1.0000
Si	Si17	1.0	0.19736	0.95489	0.30756	1.0000
Si	Si18	1.0	0.15523	0.53171	0.38279	1.0000
Si	Si19	1.0	0.80596	0.65184	0.80165	1.0000
Si	Si20	1.0	0.55406	0.65639	0.80524	1.0000
Si	Si21	1.0	0.78071	0.28599	0.81122	1.0000
Si	Si22	1.0	0.53244	0.29012	0.80291	1.0000
Si	Si23	1.0	0.78074	0.03831	0.80816	1.0000
Si	Si24	1.0	0.52987	0.04006	0.80411	1.0000
Si	Si25	1.0	0.86961	0.47292	0.87101	1.0000
Si	Si26	1.0	0.66949	0.53798	0.93937	1.0000
Si	Si27	1.0	0.27062	0.78381	0.93822	1.0000
Si	Si28	1.0	0.02989	0.78906	0.94990	1.0000
Si	Si29	1.0	0.33947	0.19660	0.44788	1.0000
Si	Si30	1.0	0.34549	0.44742	0.44578	1.0000
Si	Si31	1.0	0.72363	0.22548	0.43477	1.0000
Si	Si32	1.0	0.72135	0.48125	0.44380	1.0000
Si	Si33	1.0	0.96558	0.22816	0.43849	1.0000
Si	Si34	1.0	0.96212	0.48402	0.44879	1.0000
Si	Si35	1.0	0.52848	0.14748	0.37567	1.0000
Si	Si36	1.0	0.54364	0.33904	0.69063	1.0000
Si	Si37	1.0	0.80035	0.72697	0.68938	1.0000
Si	Si38	1.0	0.54404	0.71466	0.69443	1.0000

Si	Si39	1.0	0.79441	0.97002	0.69831	1.0000
Si	Si40	1.0	0.53705	0.95708	0.69574	1.0000
Si	Si41	1.0	0.21565	0.66321	0.19529	1.0000
Si	Si42	1.0	0.46745	0.65552	0.19509	1.0000
Si	Si43	1.0	0.19975	0.29354	0.20137	1.0000
Si	Si44	1.0	0.45605	0.28235	0.19302	1.0000
Si	Si45	1.0	0.45198	0.03785	0.19051	1.0000
Si	Si46	1.0	0.13182	0.47368	0.12822	1.0000
Si	Si47	1.0	0.52279	0.47273	0.12521	1.0000
Si	Si48	1.0	0.84641	0.15639	0.62260	1.0000
Si	Si49	1.0	0.47479	0.53446	0.62469	1.0000
Si	Si50	1.0	0.15928	0.14203	0.37586	1.0000
Si	Si51	1.0	0.53741	0.52071	0.37472	1.0000
Si	Si52	1.0	0.84661	0.85046	0.87460	1.0000
Si	Si53	1.0	0.47592	0.46847	0.87322	1.0000
Si	Si54	1.0	0.79803	0.34372	0.70000	1.0000
Si	Si55	1.0	0.46264	0.70788	0.30678	1.0000
Si	Si56	1.0	0.19663	0.05125	0.20114	1.0000
Si	Si57	1.0	0.65103	0.79136	0.94709	1.0000
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T2T7T7T7T7T9

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O	O5	1.0	0.33002	0.48589	0.00323	1.0000
O	O6	1.0	0.21746	0.53750	0.08469	1.0000
O	O7	1.0	0.41728	0.47371	0.09259	1.0000
O	O8	1.0	0.70388	0.65259	0.05928	1.0000
O	O9	1.0	0.83129	0.82296	0.06615	1.0000
O	O10	1.0	0.64185	0.82679	0.10561	1.0000
O	O11	1.0	0.83046	0.48468	0.06853	1.0000
O	O12	1.0	0.63009	0.46706	0.09137	1.0000
O	O13	1.0	0.95945	0.65447	0.06120	1.0000
O	O14	1.0	0.02453	0.83760	0.10172	1.0000
O	O15	1.0	0.02146	0.47543	0.10551	1.0000
O	O16	1.0	0.62878	0.33383	0.55353	1.0000
O	O17	1.0	0.67804	0.17406	0.49152	1.0000
O	O18	1.0	0.73793	0.16134	0.58787	1.0000
O	O19	1.0	0.53523	0.14399	0.56220	1.0000
O	O20	1.0	0.66877	0.51501	0.50332	1.0000
O	O21	1.0	0.77074	0.46830	0.58956	1.0000
O	O22	1.0	0.56386	0.52167	0.58682	1.0000
O	O23	1.0	0.28368	0.33136	0.56187	1.0000
O	O24	1.0	0.14972	0.16482	0.55621	1.0000
O	O25	1.0	0.33183	0.15065	0.60768	1.0000
O	O26	1.0	0.17181	0.50781	0.55367	1.0000
O	O27	1.0	0.35502	0.51597	0.60108	1.0000
O	O28	1.0	0.03542	0.34166	0.55599	1.0000
O	O29	1.0	0.95166	0.15977	0.59146	1.0000
O	O30	1.0	0.99203	0.52119	0.60296	1.0000
O	O31	1.0	0.34063	0.37966	0.30542	1.0000
O	O32	1.0	0.17469	0.34035	0.24404	1.0000
O	O33	1.0	0.17578	0.26158	0.33745	1.0000
O	O34	1.0	0.51101	0.31547	0.25447	1.0000
O	O35	1.0	0.45900	0.22162	0.34050	1.0000
O	O36	1.0	0.53647	0.42236	0.33780	1.0000

O	O37	1.0	0.34962	0.74196	0.30085	1.0000
O	O38	1.0	0.17050	0.84882	0.31047	1.0000
O	O39	1.0	0.19898	0.66564	0.36183	1.0000
O	O40	1.0	0.51406	0.63279	0.34303	1.0000
O	O41	1.0	0.33874	0.97989	0.31095	1.0000
O	O42	1.0	0.15205	0.04981	0.34326	1.0000
O	O43	1.0	0.54492	0.02901	0.34962	1.0000
O	O44	1.0	0.67457	0.61366	0.80905	1.0000
O	O45	1.0	0.82836	0.65300	0.74121	1.0000
O	O46	1.0	0.82684	0.75867	0.82814	1.0000
O	O47	1.0	0.87221	0.54987	0.82399	1.0000
O	O48	1.0	0.50842	0.64825	0.74922	1.0000
O	O49	1.0	0.53806	0.76464	0.83338	1.0000
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O	O52	1.0	0.79290	0.15892	0.82512	1.0000
O	O53	1.0	0.84391	0.34905	0.85619	1.0000
O	O54	1.0	0.52357	0.16408	0.81916	1.0000
O	O55	1.0	0.46216	0.35173	0.84680	1.0000
O	O56	1.0	0.65480	0.99901	0.81208	1.0000
O	O57	1.0	0.84553	0.96345	0.85080	1.0000
O	O58	1.0	0.45703	0.97595	0.84525	1.0000
O	O59	1.0	0.63003	0.66043	0.94174	1.0000
O	O60	1.0	0.66320	0.82393	0.00519	1.0000
O	O61	1.0	0.73990	0.83321	0.91199	1.0000
O	O62	1.0	0.68180	0.48938	0.99668	1.0000
O	O63	1.0	0.76535	0.51739	0.90748	1.0000
O	O64	1.0	0.55827	0.46727	0.91810	1.0000
O	O65	1.0	0.27015	0.64807	0.94622	1.0000
O	O66	1.0	0.15130	0.82154	0.93756	1.0000
O	O67	1.0	0.33329	0.80660	0.88617	1.0000
O	O68	1.0	0.15766	0.47288	0.94530	1.0000
O	O69	1.0	0.34848	0.47173	0.90409	1.0000
O	O70	1.0	0.03116	0.64862	0.94772	1.0000

O	O71	1.0	0.95123	0.82115	0.90405	1.0000
O	O72	1.0	0.97022	0.46937	0.90557	1.0000
O	O73	1.0	0.37517	0.31760	0.44187	1.0000
O	O74	1.0	0.33862	0.16143	0.50895	1.0000
O	O75	1.0	0.23857	0.15888	0.42001	1.0000
O	O76	1.0	0.44836	0.12304	0.42820	1.0000
O	O77	1.0	0.35161	0.48583	0.50256	1.0000
O	O78	1.0	0.23041	0.46208	0.41876	1.0000
O	O79	1.0	0.43445	0.51224	0.41452	1.0000
O	O80	1.0	0.70844	0.35599	0.44219	1.0000
O	O81	1.0	0.83506	0.19013	0.42461	1.0000
O	O82	1.0	0.63709	0.19035	0.39342	1.0000
O	O83	1.0	0.83396	0.52639	0.43982	1.0000
O	O84	1.0	0.64325	0.54085	0.40438	1.0000
O	O85	1.0	0.96426	0.35701	0.43701	1.0000
O	O86	1.0	0.03293	0.17500	0.39730	1.0000
O	O87	1.0	0.02299	0.54727	0.40242	1.0000
O	O88	1.0	0.67035	0.36417	0.69633	1.0000
O	O89	1.0	0.83176	0.31333	0.75770	1.0000
O	O90	1.0	0.84184	0.25882	0.66126	1.0000
O	O91	1.0	0.49668	0.31626	0.74931	1.0000
O	O92	1.0	0.52551	0.23711	0.65690	1.0000
O	O93	1.0	0.48356	0.44495	0.67252	1.0000
O	O94	1.0	0.66161	0.71760	0.68865	1.0000
O	O95	1.0	0.83328	0.84548	0.69464	1.0000
O	O96	1.0	0.83951	0.66435	0.64253	1.0000
O	O97	1.0	0.49165	0.83484	0.70221	1.0000
O	O98	1.0	0.47414	0.65270	0.65153	1.0000
O	O99	1.0	0.66194	0.96531	0.69491	1.0000
O	O100	1.0	0.84019	0.04380	0.65543	1.0000
O	O101	1.0	0.48463	0.00932	0.64702	1.0000
O	O102	1.0	0.33738	0.62803	0.19626	1.0000
O	O103	1.0	0.17850	0.65645	0.26266	1.0000
O	O104	1.0	0.18662	0.77348	0.17764	1.0000

O	O105	1.0	0.14167	0.56210	0.17751	1.0000
O	O106	1.0	0.51371	0.68430	0.24529	1.0000
O	O107	1.0	0.46536	0.77872	0.15835	1.0000
O	O108	1.0	0.52947	0.57592	0.16214	1.0000
O	O109	1.0	0.34661	0.29285	0.19326	1.0000
O	O110	1.0	0.17491	0.17315	0.18215	1.0000
O	O111	1.0	0.17853	0.36652	0.14388	1.0000
O	O112	1.0	0.50979	0.16237	0.18489	1.0000
O	O113	1.0	0.53085	0.36278	0.15864	1.0000
O	O114	1.0	0.33969	0.03398	0.18193	1.0000
O	O115	1.0	0.52055	0.97953	0.13993	1.0000
O	O116	1.0	0.99077	0.82211	0.00194	1.0000
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O	O124	1.0	0.85712	0.46173	0.68749	1.0000
O	O125	1.0	0.52913	0.83263	0.31700	1.0000
O	O126	1.0	0.15036	0.98346	0.14669	1.0000
O	O127	1.0	0.53076	0.84705	0.93076	1.0000
O	O128	1.0	0.15256	0.47132	0.31878	1.0000
Al	Al1	1.0	0.46246	0.13547	0.62535	1.0000
Al	Al2	1.0	0.86525	0.53551	0.62428	1.0000
Al	Al3	1.0	0.47330	0.96885	0.30239	1.0000
Al	Al4	1.0	0.15334	0.84108	0.12310	1.0000
Al	Al5	1.0	0.45749	0.84803	0.86725	1.0000
Al	Al6	1.0	0.15130	0.54350	0.38246	1.0000
Si	Si1	1.0	0.34725	0.79350	0.04573	1.0000
Si	Si2	1.0	0.33445	0.54156	0.05826	1.0000
Si	Si3	1.0	0.71097	0.78139	0.05903	1.0000
Si	Si4	1.0	0.71207	0.52434	0.05358	1.0000

Si	Si5	1.0	0.95375	0.78451	0.05820	1.0000
Si	Si6	1.0	0.95141	0.52552	0.05959	1.0000
Si	Si7	1.0	0.52006	0.85980	0.11744	1.0000
Si	Si8	1.0	0.65123	0.20793	0.54899	1.0000
Si	Si9	1.0	0.66085	0.46106	0.55943	1.0000
Si	Si10	1.0	0.27345	0.20224	0.56030	1.0000
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Si	Si19	1.0	0.78038	0.28459	0.81282	1.0000
Si	Si20	1.0	0.53437	0.28864	0.80627	1.0000
Si	Si21	1.0	0.77869	0.03419	0.80983	1.0000
Si	Si22	1.0	0.53043	0.03822	0.80587	1.0000
Si	Si23	1.0	0.86177	0.47159	0.87324	1.0000
Si	Si24	1.0	0.65855	0.53284	0.94015	1.0000
Si	Si25	1.0	0.27267	0.77606	0.93666	1.0000
Si	Si26	1.0	0.27771	0.51958	0.94895	1.0000
Si	Si27	1.0	0.03120	0.77831	0.94769	1.0000
Si	Si28	1.0	0.03825	0.51950	0.95124	1.0000
Si	Si29	1.0	0.34759	0.19160	0.44917	1.0000
Si	Si30	1.0	0.34422	0.44451	0.44480	1.0000
Si	Si31	1.0	0.71550	0.22800	0.43805	1.0000
Si	Si32	1.0	0.71459	0.48458	0.44831	1.0000
Si	Si33	1.0	0.95533	0.22833	0.43900	1.0000
Si	Si34	1.0	0.95663	0.48667	0.44531	1.0000
Si	Si35	1.0	0.52342	0.13907	0.37823	1.0000
Si	Si36	1.0	0.54209	0.33784	0.69278	1.0000
Si	Si37	1.0	0.79027	0.72280	0.69016	1.0000
Si	Si38	1.0	0.53402	0.71373	0.69752	1.0000

Si	Si39	1.0	0.78943	0.96735	0.69929	1.0000
Si	Si40	1.0	0.53233	0.95815	0.69723	1.0000
Si	Si41	1.0	0.21101	0.65923	0.20211	1.0000
Si	Si42	1.0	0.46016	0.66731	0.18954	1.0000
Si	Si43	1.0	0.21905	0.29468	0.19056	1.0000
Si	Si44	1.0	0.47478	0.28286	0.19783	1.0000
Si	Si45	1.0	0.47047	0.03889	0.18852	1.0000
Si	Si46	1.0	0.14068	0.48620	0.12773	1.0000
Si	Si47	1.0	0.52571	0.47129	0.12588	1.0000
Si	Si48	1.0	0.84340	0.15507	0.62410	1.0000
Si	Si49	1.0	0.46963	0.53308	0.62798	1.0000
Si	Si50	1.0	0.15089	0.16025	0.37504	1.0000
Si	Si51	1.0	0.53150	0.52388	0.37590	1.0000
Si	Si52	1.0	0.84154	0.84344	0.87376	1.0000
Si	Si53	1.0	0.46257	0.46429	0.87619	1.0000
Si	Si54	1.0	0.79585	0.34376	0.70082	1.0000
Si	Si55	1.0	0.47347	0.71393	0.30107	1.0000
Si	Si56	1.0	0.21609	0.05234	0.19274	1.0000
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T2T7T7T7T9T9

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H H3 1.0 0.58137 0.83452 0.34421 1.0000
H H4 1.0 0.08740 0.01975 0.13351 1.0000
H H5 1.0 0.47704 0.85123 0.95828 1.0000
H H6 1.0 0.15036 0.52706 0.29158 1.0000
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O O2 1.0 0.34246 0.82407 0.98525 1.0000

;

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O	O5	1.0	0.33002	0.48589	0.00323	1.0000
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O	O7	1.0	0.41728	0.47371	0.09259	1.0000
O	O8	1.0	0.70388	0.65259	0.05928	1.0000
O	O9	1.0	0.83129	0.82296	0.06615	1.0000
O	O10	1.0	0.64185	0.82679	0.10561	1.0000
O	O11	1.0	0.83046	0.48468	0.06853	1.0000
O	O12	1.0	0.63009	0.46706	0.09137	1.0000
O	O13	1.0	0.95945	0.65447	0.06120	1.0000
O	O14	1.0	0.02453	0.83760	0.10172	1.0000
O	O15	1.0	0.02146	0.47543	0.10551	1.0000
O	O16	1.0	0.62878	0.33383	0.55353	1.0000
O	O17	1.0	0.67804	0.17406	0.49152	1.0000
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O	O19	1.0	0.53523	0.14399	0.56220	1.0000
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O	O22	1.0	0.56386	0.52167	0.58682	1.0000
O	O23	1.0	0.28368	0.33136	0.56187	1.0000
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O	O31	1.0	0.34063	0.37966	0.30542	1.0000
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O	O35	1.0	0.45900	0.22162	0.34050	1.0000
O	O36	1.0	0.53647	0.42236	0.33780	1.0000

O	O37	1.0	0.34962	0.74196	0.30085	1.0000
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O	O39	1.0	0.19898	0.66564	0.36183	1.0000
O	O40	1.0	0.51406	0.63279	0.34303	1.0000
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O	O43	1.0	0.54492	0.02901	0.34962	1.0000
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O	O48	1.0	0.50842	0.64825	0.74922	1.0000
O	O49	1.0	0.53806	0.76464	0.83338	1.0000
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O	O65	1.0	0.27015	0.64807	0.94622	1.0000
O	O66	1.0	0.15130	0.82154	0.93756	1.0000
O	O67	1.0	0.33329	0.80660	0.88617	1.0000
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Al	Al5	1.0	0.45749	0.84803	0.86725	1.0000
Al	Al6	1.0	0.15130	0.54350	0.38246	1.0000
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Si	Si2	1.0	0.33445	0.54156	0.05826	1.0000
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Si	Si6	1.0	0.95141	0.52552	0.05959	1.0000
Si	Si7	1.0	0.52006	0.85980	0.11744	1.0000
Si	Si8	1.0	0.65123	0.20793	0.54899	1.0000
Si	Si9	1.0	0.66085	0.46106	0.55943	1.0000
Si	Si10	1.0	0.27345	0.20224	0.56030	1.0000
Si	Si11	1.0	0.29051	0.46004	0.55544	1.0000
Si	Si12	1.0	0.03077	0.21380	0.55003	1.0000
Si	Si13	1.0	0.04748	0.47189	0.55447	1.0000
Si	Si14	1.0	0.46260	0.33393	0.31026	1.0000
Si	Si15	1.0	0.22160	0.72969	0.31116	1.0000
Si	Si16	1.0	0.21291	0.97186	0.30390	1.0000
Si	Si17	1.0	0.79843	0.64608	0.80120	1.0000
Si	Si18	1.0	0.54906	0.65012	0.80734	1.0000
Si	Si19	1.0	0.78038	0.28459	0.81282	1.0000
Si	Si20	1.0	0.53437	0.28864	0.80627	1.0000
Si	Si21	1.0	0.77869	0.03419	0.80983	1.0000
Si	Si22	1.0	0.53043	0.03822	0.80587	1.0000
Si	Si23	1.0	0.86177	0.47159	0.87324	1.0000
Si	Si24	1.0	0.65855	0.53284	0.94015	1.0000
Si	Si25	1.0	0.27267	0.77606	0.93666	1.0000
Si	Si26	1.0	0.27771	0.51958	0.94895	1.0000
Si	Si27	1.0	0.03120	0.77831	0.94769	1.0000
Si	Si28	1.0	0.03825	0.51950	0.95124	1.0000
Si	Si29	1.0	0.34759	0.19160	0.44917	1.0000
Si	Si30	1.0	0.34422	0.44451	0.44480	1.0000
Si	Si31	1.0	0.71550	0.22800	0.43805	1.0000
Si	Si32	1.0	0.71459	0.48458	0.44831	1.0000
Si	Si33	1.0	0.95533	0.22833	0.43900	1.0000
Si	Si34	1.0	0.95663	0.48667	0.44531	1.0000
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Si	Si36	1.0	0.54209	0.33784	0.69278	1.0000
Si	Si37	1.0	0.79027	0.72280	0.69016	1.0000
Si	Si38	1.0	0.53402	0.71373	0.69752	1.0000

Si	Si39	1.0	0.78943	0.96735	0.69929	1.0000
Si	Si40	1.0	0.53233	0.95815	0.69723	1.0000
Si	Si41	1.0	0.21101	0.65923	0.20211	1.0000
Si	Si42	1.0	0.46016	0.66731	0.18954	1.0000
Si	Si43	1.0	0.21905	0.29468	0.19056	1.0000
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Si	Si45	1.0	0.47047	0.03889	0.18852	1.0000
Si	Si46	1.0	0.14068	0.48620	0.12773	1.0000
Si	Si47	1.0	0.52571	0.47129	0.12588	1.0000
Si	Si48	1.0	0.84340	0.15507	0.62410	1.0000
Si	Si49	1.0	0.46963	0.53308	0.62798	1.0000
Si	Si50	1.0	0.15089	0.16025	0.37504	1.0000
Si	Si51	1.0	0.53150	0.52388	0.37590	1.0000
Si	Si52	1.0	0.84154	0.84344	0.87376	1.0000
Si	Si53	1.0	0.46257	0.46429	0.87619	1.0000
Si	Si54	1.0	0.79585	0.34376	0.70082	1.0000
Si	Si55	1.0	0.47347	0.71393	0.30107	1.0000
Si	Si56	1.0	0.21609	0.05234	0.19274	1.0000
Si	Si57	1.0	0.64678	0.78792	0.94717	1.0000
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T7T7T7T7T9T9

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O	O7	1.0	0.72264	0.65569	0.05622	1.0000
O	O8	1.0	0.85025	0.82665	0.05721	1.0000
O	O9	1.0	0.66865	0.82625	0.10942	1.0000
O	O10	1.0	0.83544	0.48155	0.05477	1.0000
O	O11	1.0	0.64981	0.47763	0.09984	1.0000
O	O12	1.0	0.96768	0.65324	0.05378	1.0000
O	O13	1.0	0.04976	0.83022	0.09366	1.0000
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O	O15	1.0	0.62188	0.33131	0.55141	1.0000
O	O16	1.0	0.66502	0.16906	0.49014	1.0000
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O	O18	1.0	0.53006	0.14023	0.56296	1.0000
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O	O22	1.0	0.27879	0.34310	0.55786	1.0000
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O	O31	1.0	0.17528	0.34555	0.23853	1.0000
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O	O33	1.0	0.14062	0.43659	0.32552	1.0000
O	O34	1.0	0.50633	0.33835	0.25018	1.0000
O	O35	1.0	0.46434	0.22378	0.33361	1.0000
O	O36	1.0	0.53018	0.42509	0.33919	1.0000

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O	O40	1.0	0.50655	0.83628	0.31860	1.0000
O	O41	1.0	0.53254	0.63774	0.34183	1.0000
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O	O43	1.0	0.52953	0.02873	0.35233	1.0000
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O	O45	1.0	0.82494	0.65427	0.73833	1.0000
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O	O47	1.0	0.86139	0.56430	0.82536	1.0000
O	O48	1.0	0.49625	0.65955	0.75017	1.0000
O	O49	1.0	0.53594	0.77630	0.83313	1.0000
O	O50	1.0	0.47123	0.57482	0.83964	1.0000
O	O51	1.0	0.65365	0.29771	0.80798	1.0000
O	O52	1.0	0.81923	0.17238	0.82215	1.0000
O	O53	1.0	0.82068	0.36685	0.85777	1.0000
O	O54	1.0	0.49320	0.16384	0.81893	1.0000
O	O55	1.0	0.46675	0.36231	0.84197	1.0000
O	O56	1.0	0.65756	0.02882	0.81687	1.0000
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O	O61	1.0	0.55258	0.85704	0.92678	1.0000
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O	O63	1.0	0.77907	0.53418	0.91753	1.0000
O	O64	1.0	0.57782	0.47008	0.90995	1.0000
O	O65	1.0	0.29254	0.65053	0.94322	1.0000
O	O66	1.0	0.17153	0.82135	0.92838	1.0000
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O	O68	1.0	0.16625	0.48189	0.93421	1.0000
O	O69	1.0	0.36504	0.46582	0.90903	1.0000
O	O70	1.0	0.04120	0.65398	0.93778	1.0000

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O	O72	1.0	0.97578	0.47349	0.89732	1.0000
O	O73	1.0	0.37390	0.33290	0.44338	1.0000
O	O74	1.0	0.34473	0.17305	0.51078	1.0000
O	O75	1.0	0.23754	0.17115	0.42438	1.0000
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O	O78	1.0	0.22165	0.46666	0.41789	1.0000
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O	O84	1.0	0.63647	0.53462	0.40817	1.0000
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O	O86	1.0	0.02203	0.16451	0.39575	1.0000
O	O87	1.0	0.02471	0.52608	0.39751	1.0000
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O	O89	1.0	0.83223	0.33236	0.75780	1.0000
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O	O91	1.0	0.49139	0.31275	0.74606	1.0000
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O	O93	1.0	0.47844	0.44411	0.67014	1.0000
O	O94	1.0	0.65641	0.72246	0.69143	1.0000
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O	O99	1.0	0.65579	0.96930	0.69428	1.0000
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O	O101	1.0	0.47211	0.02131	0.65299	1.0000
O	O102	1.0	0.33159	0.62094	0.19912	1.0000
O	O103	1.0	0.16727	0.66742	0.25800	1.0000
O	O104	1.0	0.16830	0.73669	0.16271	1.0000

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O	O106	1.0	0.46168	0.75784	0.15420	1.0000
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O	O116	1.0	0.01622	0.82260	0.99587	1.0000
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Al	Al2	1.0	0.85772	0.53997	0.62247	1.0000
Al	Al3	1.0	0.54017	0.85469	0.12605	1.0000
Al	Al4	1.0	0.14350	0.46020	0.12259	1.0000
Al	Al5	1.0	0.84978	0.83979	0.87504	1.0000
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Si	Si3	1.0	0.71668	0.52703	0.05306	1.0000
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Si	Si8	1.0	0.27345	0.21408	0.56039	1.0000
Si	Si9	1.0	0.28441	0.47160	0.55333	1.0000
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Si	Si14	1.0	0.21891	0.70607	0.31149	1.0000
Si	Si15	1.0	0.47393	0.71541	0.30306	1.0000
Si	Si16	1.0	0.47143	0.95800	0.30936	1.0000
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Si	Si18	1.0	0.79113	0.65712	0.79871	1.0000
Si	Si19	1.0	0.54267	0.65847	0.80723	1.0000
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Si	Si21	1.0	0.52569	0.28470	0.80325	1.0000
Si	Si22	1.0	0.52837	0.04224	0.80934	1.0000
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Si	Si25	1.0	0.66104	0.54106	0.94289	1.0000
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Si	Si37	1.0	0.51913	0.14739	0.37576	1.0000
Si	Si38	1.0	0.54265	0.34224	0.69117	1.0000

Si	Si39	1.0	0.78482	0.72615	0.68865	1.0000
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Si	Si41	1.0	0.78350	0.97052	0.69741	1.0000
Si	Si42	1.0	0.52620	0.95950	0.69814	1.0000
Si	Si43	1.0	0.45679	0.65727	0.19114	1.0000
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Si	Si45	1.0	0.47287	0.28270	0.19671	1.0000
Si	Si46	1.0	0.21777	0.02945	0.19666	1.0000
Si	Si47	1.0	0.47481	0.03989	0.19760	1.0000
Si	Si48	1.0	0.16151	0.83769	0.12359	1.0000
Si	Si49	1.0	0.53368	0.46709	0.12569	1.0000
Si	Si50	1.0	0.83866	0.16219	0.62370	1.0000
Si	Si51	1.0	0.46644	0.53292	0.62589	1.0000
Si	Si52	1.0	0.52964	0.53010	0.37506	1.0000
Si	Si53	1.0	0.47126	0.46957	0.87541	1.0000
Si	Si54	1.0	0.79337	0.35534	0.70041	1.0000
Si	Si55	1.0	0.35541	0.79450	0.04759	1.0000
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Si	Si57	1.0	0.78158	0.05237	0.80780	1.0000
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O	O6	1.0	0.44063	0.48480	0.08150	1.0000
O	O7	1.0	0.71563	0.66045	0.05885	1.0000
O	O8	1.0	0.84257	0.83270	0.04963	1.0000
O	O9	1.0	0.66435	0.83975	0.10495	1.0000
O	O10	1.0	0.83203	0.48761	0.05260	1.0000
O	O11	1.0	0.64750	0.47795	0.09950	1.0000
O	O12	1.0	0.96084	0.66037	0.05044	1.0000
O	O13	1.0	0.03603	0.84155	0.09059	1.0000
O	O14	1.0	0.01398	0.48623	0.10065	1.0000
O	O15	1.0	0.63014	0.33240	0.55229	1.0000
O	O16	1.0	0.67578	0.17243	0.49039	1.0000
O	O17	1.0	0.73678	0.16202	0.58745	1.0000
O	O18	1.0	0.53333	0.14185	0.56081	1.0000
O	O19	1.0	0.68217	0.51507	0.50517	1.0000
O	O20	1.0	0.76635	0.46734	0.59443	1.0000
O	O21	1.0	0.55957	0.51776	0.58374	1.0000
O	O22	1.0	0.28090	0.33380	0.56051	1.0000
O	O23	1.0	0.14874	0.16597	0.55312	1.0000
O	O24	1.0	0.32982	0.15218	0.60538	1.0000
O	O25	1.0	0.16945	0.50885	0.55213	1.0000
O	O26	1.0	0.35129	0.51553	0.60189	1.0000
O	O27	1.0	0.03391	0.34110	0.55321	1.0000
O	O28	1.0	0.95028	0.16158	0.59097	1.0000
O	O29	1.0	0.99066	0.51684	0.60409	1.0000
O	O30	1.0	0.33156	0.38139	0.31031	1.0000
O	O31	1.0	0.16987	0.34942	0.24507	1.0000
O	O32	1.0	0.18501	0.22774	0.32722	1.0000
O	O33	1.0	0.13553	0.43566	0.33324	1.0000
O	O34	1.0	0.49772	0.34687	0.24947	1.0000
O	O35	1.0	0.46522	0.22714	0.33176	1.0000
O	O36	1.0	0.53037	0.42911	0.33881	1.0000

O	O37	1.0	0.35286	0.72487	0.30882	1.0000
O	O38	1.0	0.20042	0.62841	0.36373	1.0000
O	O39	1.0	0.52868	0.84033	0.31540	1.0000
O	O40	1.0	0.53067	0.64144	0.34325	1.0000
O	O41	1.0	0.35581	0.96478	0.31737	1.0000
O	O42	1.0	0.15555	0.03116	0.36076	1.0000
O	O43	1.0	0.54556	0.03589	0.34506	1.0000
O	O44	1.0	0.66696	0.61768	0.80961	1.0000
O	O45	1.0	0.82525	0.65689	0.74248	1.0000
O	O46	1.0	0.81672	0.76498	0.82838	1.0000
O	O47	1.0	0.86316	0.55607	0.82641	1.0000
O	O48	1.0	0.50300	0.64977	0.74864	1.0000
O	O49	1.0	0.53371	0.77407	0.82884	1.0000
O	O50	1.0	0.46797	0.57300	0.83979	1.0000
O	O51	1.0	0.65034	0.29530	0.80878	1.0000
O	O52	1.0	0.81181	0.16303	0.82625	1.0000
O	O53	1.0	0.81787	0.35963	0.85860	1.0000
O	O54	1.0	0.48731	0.16179	0.81892	1.0000
O	O55	1.0	0.46256	0.36079	0.84175	1.0000
O	O56	1.0	0.65099	0.02524	0.81301	1.0000
O	O57	1.0	0.83471	0.96586	0.85347	1.0000
O	O58	1.0	0.46127	0.96678	0.84655	1.0000
O	O59	1.0	0.62621	0.66625	0.93767	1.0000
O	O60	1.0	0.65004	0.82410	0.00583	1.0000
O	O61	1.0	0.76900	0.82324	0.92260	1.0000
O	O62	1.0	0.55843	0.86038	0.91959	1.0000
O	O63	1.0	0.65403	0.50161	0.99968	1.0000
O	O64	1.0	0.77856	0.52889	0.91814	1.0000
O	O65	1.0	0.57712	0.46779	0.90901	1.0000
O	O66	1.0	0.28935	0.64831	0.94229	1.0000
O	O67	1.0	0.16677	0.81491	0.92234	1.0000
O	O68	1.0	0.36290	0.80639	0.88778	1.0000
O	O69	1.0	0.16420	0.47989	0.93298	1.0000
O	O70	1.0	0.36527	0.46332	0.91123	1.0000

O	O71	1.0	0.03421	0.64967	0.93535	1.0000
O	O72	1.0	0.96918	0.82835	0.89237	1.0000
O	O73	1.0	0.97313	0.46332	0.90008	1.0000
O	O74	1.0	0.38258	0.32793	0.44045	1.0000
O	O75	1.0	0.34305	0.16916	0.50685	1.0000
O	O76	1.0	0.22863	0.18381	0.42346	1.0000
O	O77	1.0	0.43701	0.13072	0.42017	1.0000
O	O78	1.0	0.35245	0.49185	0.50276	1.0000
O	O79	1.0	0.22380	0.46015	0.42415	1.0000
O	O80	1.0	0.42389	0.52767	0.41101	1.0000
O	O81	1.0	0.71199	0.35542	0.44319	1.0000
O	O82	1.0	0.83187	0.18903	0.42281	1.0000
O	O83	1.0	0.63228	0.19494	0.39232	1.0000
O	O84	1.0	0.83597	0.52715	0.43494	1.0000
O	O85	1.0	0.63701	0.53773	0.40852	1.0000
O	O86	1.0	0.96145	0.35633	0.43863	1.0000
O	O87	1.0	0.02965	0.18326	0.39348	1.0000
O	O88	1.0	0.03336	0.54176	0.40530	1.0000
O	O89	1.0	0.66893	0.36354	0.69741	1.0000
O	O90	1.0	0.83097	0.31950	0.75920	1.0000
O	O91	1.0	0.84031	0.26044	0.66195	1.0000
O	O92	1.0	0.48909	0.30960	0.74611	1.0000
O	O93	1.0	0.52650	0.23809	0.65340	1.0000
O	O94	1.0	0.48412	0.44386	0.67147	1.0000
O	O95	1.0	0.66082	0.71708	0.68862	1.0000
O	O96	1.0	0.83081	0.84839	0.69426	1.0000
O	O97	1.0	0.84246	0.66582	0.64378	1.0000
O	O98	1.0	0.48934	0.83284	0.69922	1.0000
O	O99	1.0	0.47562	0.65018	0.64999	1.0000
O	O100	1.0	0.65880	0.96665	0.69570	1.0000
O	O101	1.0	0.83749	0.04703	0.65626	1.0000
O	O102	1.0	0.48063	0.01142	0.64784	1.0000
O	O103	1.0	0.33131	0.62840	0.20165	1.0000
O	O104	1.0	0.17176	0.66672	0.26479	1.0000

O	O105	1.0	0.16387	0.74766	0.17119	1.0000
O	O106	1.0	0.51193	0.68499	0.24617	1.0000
O	O107	1.0	0.46533	0.76448	0.15538	1.0000
O	O108	1.0	0.51710	0.55942	0.16861	1.0000
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O	O110	1.0	0.16515	0.15922	0.19773	1.0000
O	O111	1.0	0.15733	0.34090	0.14554	1.0000
O	O112	1.0	0.50622	0.16805	0.19644	1.0000
O	O113	1.0	0.51832	0.35247	0.14979	1.0000
O	O114	1.0	0.33697	0.03526	0.19210	1.0000
O	O115	1.0	0.51736	0.98776	0.14656	1.0000
O	O116	1.0	0.01277	0.82427	0.99116	1.0000
O	O117	1.0	0.00889	0.48697	0.99964	1.0000
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O	O120	1.0	0.17378	0.97905	0.25291	1.0000
O	O121	1.0	0.50785	0.98963	0.24735	1.0000
O	O122	1.0	0.82361	0.01551	0.75492	1.0000
O	O123	1.0	0.48827	0.01466	0.74850	1.0000
O	O124	1.0	0.85717	0.46365	0.68923	1.0000
O	O125	1.0	0.46935	0.85955	0.05863	1.0000
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Al	Al1	1.0	0.45982	0.13521	0.62381	1.0000
Al	Al2	1.0	0.86472	0.53627	0.62634	1.0000
Al	Al3	1.0	0.53439	0.86300	0.12259	1.0000
Al	Al4	1.0	0.22040	0.96308	0.31385	1.0000
Al	Al5	1.0	0.13658	0.47085	0.12646	1.0000
Al	Al6	1.0	0.15536	0.83805	0.12204	1.0000
Si	Si1	1.0	0.33813	0.54659	0.05960	1.0000
Si	Si2	1.0	0.72109	0.78946	0.05689	1.0000
Si	Si3	1.0	0.71246	0.53226	0.05295	1.0000
Si	Si4	1.0	0.96449	0.78940	0.04656	1.0000

Si	Si5	1.0	0.95518	0.53079	0.05187	1.0000
Si	Si6	1.0	0.65052	0.20667	0.54814	1.0000
Si	Si7	1.0	0.66214	0.45915	0.56015	1.0000
Si	Si8	1.0	0.27294	0.20479	0.55807	1.0000
Si	Si9	1.0	0.28826	0.46221	0.55504	1.0000
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Si	Si12	1.0	0.20630	0.34621	0.30457	1.0000
Si	Si13	1.0	0.45665	0.34566	0.30748	1.0000
Si	Si14	1.0	0.48291	0.72275	0.30267	1.0000
Si	Si15	1.0	0.48104	0.95887	0.30567	1.0000
Si	Si16	1.0	0.14849	0.51428	0.38183	1.0000
Si	Si17	1.0	0.79238	0.65081	0.80242	1.0000
Si	Si18	1.0	0.54238	0.65369	0.80679	1.0000
Si	Si19	1.0	0.77741	0.28366	0.81348	1.0000
Si	Si20	1.0	0.52229	0.28209	0.80361	1.0000
Si	Si21	1.0	0.77964	0.04114	0.81150	1.0000
Si	Si22	1.0	0.52333	0.04188	0.80584	1.0000
Si	Si23	1.0	0.85680	0.47727	0.87589	1.0000
Si	Si24	1.0	0.65264	0.79271	0.94571	1.0000
Si	Si25	1.0	0.65910	0.54092	0.94139	1.0000
Si	Si26	1.0	0.28620	0.77559	0.93490	1.0000
Si	Si27	1.0	0.28255	0.52020	0.94852	1.0000
Si	Si28	1.0	0.04480	0.77876	0.93602	1.0000
Si	Si29	1.0	0.04465	0.52161	0.94308	1.0000
Si	Si30	1.0	0.47912	0.85063	0.87089	1.0000
Si	Si31	1.0	0.34610	0.20272	0.44688	1.0000
Si	Si32	1.0	0.34604	0.45191	0.44482	1.0000
Si	Si33	1.0	0.71298	0.22795	0.43687	1.0000
Si	Si34	1.0	0.71642	0.48382	0.44828	1.0000
Si	Si35	1.0	0.95249	0.22728	0.43739	1.0000
Si	Si36	1.0	0.95442	0.48409	0.44662	1.0000
Si	Si37	1.0	0.51972	0.14707	0.37237	1.0000
Si	Si38	1.0	0.54081	0.33629	0.69103	1.0000

Si	Si39	1.0	0.78996	0.72454	0.69075	1.0000
Si	Si40	1.0	0.53254	0.71287	0.69626	1.0000
Si	Si41	1.0	0.78681	0.96904	0.70006	1.0000
Si	Si42	1.0	0.52892	0.95689	0.69683	1.0000
Si	Si43	1.0	0.45710	0.66229	0.19125	1.0000
Si	Si44	1.0	0.20713	0.28327	0.19327	1.0000
Si	Si45	1.0	0.46476	0.28854	0.19656	1.0000
Si	Si46	1.0	0.46819	0.04363	0.19486	1.0000
Si	Si47	1.0	0.52990	0.47033	0.12481	1.0000
Si	Si48	1.0	0.84150	0.15727	0.62420	1.0000
Si	Si49	1.0	0.46853	0.53080	0.62677	1.0000
Si	Si50	1.0	0.14974	0.15411	0.37630	1.0000
Si	Si51	1.0	0.52997	0.53273	0.37541	1.0000
Si	Si52	1.0	0.84767	0.84542	0.87440	1.0000
Si	Si53	1.0	0.46884	0.46713	0.87548	1.0000
Si	Si54	1.0	0.79480	0.34510	0.70189	1.0000
Si	Si55	1.0	0.35155	0.79741	0.04503	1.0000
Si	Si56	1.0	0.22880	0.70393	0.31644	1.0000
Si	Si57	1.0	0.20573	0.65335	0.20500	1.0000
Si	Si58	1.0	0.21126	0.03931	0.20261	1.0000

AlSiAl-T7T7T7T9T9

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O	O5	1.0	0.23708	0.54027	0.09725	1.0000
O	O6	1.0	0.44154	0.48851	0.08148	1.0000
O	O7	1.0	0.71629	0.66179	0.05937	1.0000
O	O8	1.0	0.84324	0.83372	0.04950	1.0000
O	O9	1.0	0.66510	0.84213	0.10468	1.0000
O	O10	1.0	0.83184	0.48892	0.05215	1.0000
O	O11	1.0	0.64832	0.47963	0.10066	1.0000
O	O12	1.0	0.96130	0.66120	0.05190	1.0000
O	O13	1.0	0.03695	0.84439	0.09016	1.0000
O	O14	1.0	0.01220	0.48612	0.10196	1.0000
O	O15	1.0	0.63115	0.32778	0.54976	1.0000
O	O16	1.0	0.67364	0.16864	0.48684	1.0000
O	O17	1.0	0.73312	0.15295	0.58437	1.0000
O	O18	1.0	0.53167	0.14070	0.55854	1.0000
O	O19	1.0	0.68540	0.51095	0.50528	1.0000
O	O20	1.0	0.76636	0.46074	0.59490	1.0000
O	O21	1.0	0.56097	0.51238	0.58329	1.0000
O	O22	1.0	0.28530	0.33629	0.56011	1.0000
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O	O24	1.0	0.33500	0.15493	0.60471	1.0000
O	O25	1.0	0.17039	0.50944	0.55189	1.0000
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O	O27	1.0	0.04002	0.33797	0.55202	1.0000
O	O28	1.0	0.96405	0.15483	0.59035	1.0000
O	O29	1.0	0.99071	0.51313	0.60277	1.0000
O	O30	1.0	0.33544	0.38587	0.30899	1.0000
O	O31	1.0	0.17181	0.35330	0.24504	1.0000
O	O32	1.0	0.18750	0.23712	0.32821	1.0000
O	O33	1.0	0.14028	0.44630	0.33142	1.0000
O	O34	1.0	0.50000	0.34863	0.24811	1.0000
O	O35	1.0	0.46836	0.23038	0.33028	1.0000
O	O36	1.0	0.53399	0.43181	0.33777	1.0000

O	O37	1.0	0.35207	0.71357	0.30994	1.0000
O	O38	1.0	0.18445	0.83642	0.32648	1.0000
O	O39	1.0	0.19131	0.64232	0.36376	1.0000
O	O40	1.0	0.51844	0.84100	0.31629	1.0000
O	O41	1.0	0.53722	0.64357	0.34301	1.0000
O	O42	1.0	0.34862	0.97163	0.31464	1.0000
O	O43	1.0	0.16509	0.03595	0.35328	1.0000
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O	O46	1.0	0.82798	0.64638	0.74423	1.0000
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O	O48	1.0	0.86259	0.55423	0.83060	1.0000
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O	O50	1.0	0.53373	0.77111	0.83019	1.0000
O	O51	1.0	0.46839	0.56977	0.83928	1.0000
O	O52	1.0	0.64782	0.28662	0.81031	1.0000
O	O53	1.0	0.81586	0.16408	0.82618	1.0000
O	O54	1.0	0.80943	0.35857	0.86314	1.0000
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O	O59	1.0	0.62286	0.66597	0.93834	1.0000
O	O60	1.0	0.65107	0.82480	0.00568	1.0000
O	O61	1.0	0.76666	0.82044	0.92151	1.0000
O	O62	1.0	0.55687	0.86093	0.92010	1.0000
O	O63	1.0	0.65045	0.50245	0.00130	1.0000
O	O64	1.0	0.77799	0.52997	0.92178	1.0000
O	O65	1.0	0.57713	0.46734	0.90963	1.0000
O	O66	1.0	0.28963	0.64811	0.94191	1.0000
O	O67	1.0	0.16500	0.81231	0.92160	1.0000
O	O68	1.0	0.36153	0.80779	0.88797	1.0000
O	O69	1.0	0.16416	0.47932	0.93316	1.0000
O	O70	1.0	0.36507	0.46303	0.91121	1.0000

O	O71	1.0	0.03231	0.64703	0.93462	1.0000
O	O72	1.0	0.96735	0.82600	0.89231	1.0000
O	O73	1.0	0.97056	0.45727	0.90321	1.0000
O	O74	1.0	0.37724	0.33224	0.43789	1.0000
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O	O80	1.0	0.42649	0.53053	0.40999	1.0000
O	O81	1.0	0.71110	0.35218	0.44114	1.0000
O	O82	1.0	0.83604	0.18723	0.42205	1.0000
O	O83	1.0	0.64008	0.19118	0.38786	1.0000
O	O84	1.0	0.83707	0.52143	0.43461	1.0000
O	O85	1.0	0.63863	0.53754	0.40928	1.0000
O	O86	1.0	0.96738	0.35302	0.43598	1.0000
O	O87	1.0	0.03398	0.17591	0.39248	1.0000
O	O88	1.0	0.03103	0.54196	0.40401	1.0000
O	O89	1.0	0.66790	0.36954	0.70050	1.0000
O	O90	1.0	0.82809	0.33039	0.76381	1.0000
O	O91	1.0	0.83478	0.25190	0.66990	1.0000
O	O92	1.0	0.48817	0.31105	0.74651	1.0000
O	O93	1.0	0.53137	0.23688	0.65456	1.0000
O	O94	1.0	0.48198	0.44167	0.67079	1.0000
O	O95	1.0	0.66400	0.71308	0.69135	1.0000
O	O96	1.0	0.83507	0.83832	0.69915	1.0000
O	O97	1.0	0.84380	0.65947	0.64493	1.0000
O	O98	1.0	0.49509	0.83179	0.69745	1.0000
O	O99	1.0	0.48116	0.64797	0.64952	1.0000
O	O100	1.0	0.66445	0.96504	0.69177	1.0000
O	O101	1.0	0.48435	0.01178	0.64657	1.0000
O	O102	1.0	0.33136	0.62998	0.20104	1.0000
O	O103	1.0	0.17109	0.66987	0.26438	1.0000
O	O104	1.0	0.16506	0.74840	0.17036	1.0000

O	O105	1.0	0.51188	0.68751	0.24620	1.0000
O	O106	1.0	0.46744	0.76267	0.15451	1.0000
O	O107	1.0	0.51687	0.55779	0.16994	1.0000
O	O108	1.0	0.33607	0.28624	0.19246	1.0000
O	O109	1.0	0.16451	0.16158	0.19944	1.0000
O	O110	1.0	0.15702	0.34089	0.14571	1.0000
O	O111	1.0	0.50533	0.16772	0.19614	1.0000
O	O112	1.0	0.51686	0.35174	0.14834	1.0000
O	O113	1.0	0.33533	0.03526	0.19079	1.0000
O	O114	1.0	0.51596	0.98712	0.14595	1.0000
O	O115	1.0	0.01277	0.82176	0.99099	1.0000
O	O116	1.0	0.01188	0.48806	0.00138	1.0000
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O	O120	1.0	0.50281	0.98801	0.24651	1.0000
O	O121	1.0	0.82228	0.01416	0.75577	1.0000
O	O122	1.0	0.49616	0.01219	0.74724	1.0000
O	O123	1.0	0.85968	0.46021	0.68962	1.0000
O	O124	1.0	0.46905	0.85876	0.05820	1.0000
O	O125	1.0	0.13880	0.54027	0.19032	1.0000
O	O126	1.0	0.83385	0.96450	0.85377	1.0000
O	O127	1.0	0.14615	0.97404	0.15594	1.0000
O	O128	1.0	0.85356	0.02599	0.65606	1.0000
Al	Al1	1.0	0.46538	0.13652	0.62246	1.0000
Al	Al2	1.0	0.86566	0.52916	0.62634	1.0000
Al	Al3	1.0	0.53463	0.86208	0.12216	1.0000
Al	Al4	1.0	0.13572	0.47117	0.12706	1.0000
Al	Al5	1.0	0.15573	0.83949	0.12212	1.0000
Al	Al6	1.0	0.84466	0.16026	0.62194	1.0000
Si	Si1	1.0	0.33698	0.54733	0.05982	1.0000
Si	Si2	1.0	0.72196	0.79079	0.05690	1.0000
Si	Si3	1.0	0.71217	0.53337	0.05380	1.0000
Si	Si4	1.0	0.96497	0.78996	0.04675	1.0000

Si	Si5	1.0	0.95510	0.53152	0.05294	1.0000
Si	Si6	1.0	0.65066	0.20098	0.54540	1.0000
Si	Si7	1.0	0.66341	0.45322	0.55954	1.0000
Si	Si8	1.0	0.27916	0.20732	0.55702	1.0000
Si	Si9	1.0	0.28987	0.46465	0.55405	1.0000
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Si	Si13	1.0	0.45985	0.34922	0.30630	1.0000
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Si	Si15	1.0	0.48001	0.72044	0.30320	1.0000
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Si	Si17	1.0	0.47618	0.95939	0.30469	1.0000
Si	Si18	1.0	0.14787	0.52560	0.38048	1.0000
Si	Si19	1.0	0.79272	0.64612	0.80404	1.0000
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Si	Si21	1.0	0.77517	0.28461	0.81590	1.0000
Si	Si22	1.0	0.51989	0.27978	0.80364	1.0000
Si	Si23	1.0	0.52371	0.04120	0.80529	1.0000
Si	Si24	1.0	0.85412	0.47489	0.87966	1.0000
Si	Si25	1.0	0.65109	0.79221	0.94575	1.0000
Si	Si26	1.0	0.65697	0.54097	0.94302	1.0000
Si	Si27	1.0	0.28488	0.77536	0.93476	1.0000
Si	Si28	1.0	0.28249	0.52005	0.94852	1.0000
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Si	Si31	1.0	0.47823	0.84978	0.87112	1.0000
Si	Si32	1.0	0.35002	0.20589	0.44573	1.0000
Si	Si33	1.0	0.34553	0.45774	0.44323	1.0000
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Si	Si37	1.0	0.95652	0.48066	0.44521	1.0000
Si	Si38	1.0	0.52329	0.15034	0.37067	1.0000

Si	Si39	1.0	0.54203	0.33684	0.69166	1.0000
Si	Si40	1.0	0.79243	0.71429	0.69304	1.0000
Si	Si41	1.0	0.53524	0.71035	0.69640	1.0000
Si	Si42	1.0	0.53312	0.95587	0.69476	1.0000
Si	Si43	1.0	0.45719	0.66240	0.19151	1.0000
Si	Si44	1.0	0.20764	0.28564	0.19378	1.0000
Si	Si45	1.0	0.46502	0.28912	0.19579	1.0000
Si	Si46	1.0	0.46669	0.04380	0.19388	1.0000
Si	Si47	1.0	0.52993	0.47114	0.12501	1.0000
Si	Si48	1.0	0.47027	0.52860	0.62595	1.0000
Si	Si49	1.0	0.15499	0.15678	0.37436	1.0000
Si	Si50	1.0	0.53324	0.53487	0.37514	1.0000
Si	Si51	1.0	0.46899	0.46545	0.87590	1.0000
Si	Si52	1.0	0.79343	0.34489	0.70498	1.0000
Si	Si53	1.0	0.34970	0.79931	0.04516	1.0000
Si	Si54	1.0	0.20589	0.65530	0.20548	1.0000
Si	Si55	1.0	0.77982	0.04276	0.81289	1.0000
Si	Si56	1.0	0.84625	0.84325	0.87404	1.0000
Si	Si57	1.0	0.21145	0.04260	0.20310	1.0000
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T2T2T7T7T7T9

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O	O4	1.0	0.45287	0.85660	0.06483	1.0000
O	O5	1.0	0.32116	0.48378	0.00706	1.0000
O	O6	1.0	0.21476	0.54106	0.08913	1.0000
O	O7	1.0	0.41445	0.47415	0.09460	1.0000
O	O8	1.0	0.70480	0.65254	0.05846	1.0000
O	O9	1.0	0.83230	0.82406	0.06531	1.0000
O	O10	1.0	0.64227	0.82665	0.10480	1.0000
O	O11	1.0	0.83121	0.48487	0.06942	1.0000
O	O12	1.0	0.62688	0.46819	0.08870	1.0000
O	O13	1.0	0.95816	0.65513	0.06082	1.0000
O	O14	1.0	0.02401	0.83593	0.10293	1.0000
O	O15	1.0	0.01674	0.48265	0.11129	1.0000
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O	O19	1.0	0.53333	0.14489	0.56265	1.0000
O	O20	1.0	0.66977	0.51577	0.50267	1.0000
O	O21	1.0	0.76898	0.46976	0.58936	1.0000
O	O22	1.0	0.56203	0.52321	0.58519	1.0000
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O	O26	1.0	0.17060	0.50968	0.55175	1.0000
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O	O28	1.0	0.03614	0.34250	0.55424	1.0000
O	O29	1.0	0.95062	0.16342	0.59193	1.0000
O	O30	1.0	0.99134	0.51928	0.60265	1.0000
O	O31	1.0	0.34115	0.38090	0.30480	1.0000
O	O32	1.0	0.17469	0.33805	0.24476	1.0000
O	O33	1.0	0.17709	0.26268	0.33839	1.0000
O	O34	1.0	0.51040	0.31349	0.25366	1.0000
O	O35	1.0	0.45951	0.22451	0.34076	1.0000

O	O36	1.0	0.53725	0.42533	0.33562	1.0000
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O	O38	1.0	0.17350	0.84990	0.31292	1.0000
O	O39	1.0	0.20308	0.66538	0.36334	1.0000
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O	O41	1.0	0.34105	0.98201	0.31021	1.0000
O	O42	1.0	0.15524	0.05097	0.34455	1.0000
O	O43	1.0	0.54580	0.03172	0.34862	1.0000
O	O44	1.0	0.68098	0.61583	0.80880	1.0000
O	O45	1.0	0.83194	0.65740	0.74011	1.0000
O	O46	1.0	0.83801	0.75528	0.82942	1.0000
O	O47	1.0	0.87695	0.54633	0.82029	1.0000
O	O48	1.0	0.51390	0.64560	0.74890	1.0000
O	O49	1.0	0.54306	0.76713	0.83141	1.0000
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O	O59	1.0	0.62914	0.65846	0.94196	1.0000
O	O60	1.0	0.66443	0.82323	0.00461	1.0000
O	O61	1.0	0.74029	0.82932	0.91084	1.0000
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O	O63	1.0	0.78152	0.53130	0.90846	1.0000
O	O64	1.0	0.57825	0.46217	0.91330	1.0000
O	O65	1.0	0.26168	0.64576	0.94965	1.0000
O	O66	1.0	0.15330	0.82463	0.93685	1.0000
O	O67	1.0	0.33741	0.79398	0.88691	1.0000
O	O68	1.0	0.36726	0.47787	0.90924	1.0000
O	O69	1.0	0.02552	0.65577	0.94408	1.0000

O	O70	1.0	0.95248	0.83673	0.90545	1.0000
O	O71	1.0	0.97840	0.45680	0.89935	1.0000
O	O72	1.0	0.37774	0.31826	0.44217	1.0000
O	O73	1.0	0.33992	0.16297	0.50941	1.0000
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O	O78	1.0	0.43407	0.51276	0.41281	1.0000
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O	O81	1.0	0.63696	0.19149	0.39319	1.0000
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O	O90	1.0	0.48782	0.32052	0.74829	1.0000
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O	O103	1.0	0.18694	0.77067	0.17790	1.0000

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O	O105	1.0	0.51639	0.68592	0.24486	1.0000
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O	O123	1.0	0.85378	0.46316	0.68681	1.0000
O	O124	1.0	0.53259	0.83506	0.31599	1.0000
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Al	Al2	1.0	0.86435	0.53627	0.62368	1.0000
Al	Al3	1.0	0.47571	0.97072	0.30144	1.0000
Al	Al4	1.0	0.15280	0.83917	0.12390	1.0000
Al	Al5	1.0	0.45907	0.84352	0.86726	1.0000
Al	Al6	1.0	0.03157	0.52040	0.95068	1.0000
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Si	Si4	1.0	0.71440	0.52442	0.05285	1.0000
Si	Si5	1.0	0.95529	0.78479	0.05814	1.0000
Si	Si6	1.0	0.95380	0.52538	0.06132	1.0000
Si	Si7	1.0	0.52054	0.85965	0.11685	1.0000
Si	Si8	1.0	0.64901	0.20937	0.54866	1.0000
Si	Si9	1.0	0.66005	0.46223	0.55871	1.0000
Si	Si10	1.0	0.27304	0.20447	0.56041	1.0000
Si	Si11	1.0	0.28934	0.46215	0.55421	1.0000
Si	Si12	1.0	0.03043	0.21470	0.54975	1.0000
Si	Si13	1.0	0.04648	0.47253	0.55345	1.0000
Si	Si14	1.0	0.46312	0.33538	0.30946	1.0000
Si	Si15	1.0	0.22487	0.73106	0.31297	1.0000
Si	Si16	1.0	0.21491	0.97284	0.30485	1.0000
Si	Si17	1.0	0.80573	0.64648	0.80038	1.0000
Si	Si18	1.0	0.55579	0.65179	0.80652	1.0000
Si	Si19	1.0	0.77579	0.28303	0.81206	1.0000
Si	Si20	1.0	0.52313	0.28518	0.80446	1.0000
Si	Si21	1.0	0.77467	0.03754	0.80895	1.0000
Si	Si22	1.0	0.52002	0.03896	0.80549	1.0000
Si	Si23	1.0	0.86732	0.47173	0.87118	1.0000
Si	Si24	1.0	0.67027	0.53455	0.93902	1.0000
Si	Si25	1.0	0.27171	0.77406	0.93738	1.0000
Si	Si26	1.0	0.03093	0.78296	0.94728	1.0000
Si	Si27	1.0	0.34795	0.19274	0.44947	1.0000
Si	Si28	1.0	0.34519	0.44465	0.44417	1.0000
Si	Si29	1.0	0.71463	0.22840	0.43796	1.0000
Si	Si30	1.0	0.71467	0.48466	0.44756	1.0000
Si	Si31	1.0	0.95486	0.22822	0.43935	1.0000
Si	Si32	1.0	0.95633	0.48664	0.44494	1.0000
Si	Si33	1.0	0.52325	0.14074	0.37777	1.0000
Si	Si34	1.0	0.53839	0.33714	0.69217	1.0000
Si	Si35	1.0	0.79222	0.72454	0.68888	1.0000
Si	Si36	1.0	0.53592	0.71128	0.69679	1.0000

Si	Si37	1.0	0.78520	0.96844	0.69787	1.0000
Si	Si38	1.0	0.52811	0.95511	0.69656	1.0000
Si	Si39	1.0	0.21255	0.65875	0.20412	1.0000
Si	Si40	1.0	0.46183	0.66793	0.18962	1.0000
Si	Si41	1.0	0.21834	0.29413	0.19079	1.0000
Si	Si42	1.0	0.47423	0.28357	0.19685	1.0000
Si	Si43	1.0	0.47063	0.03893	0.18772	1.0000
Si	Si44	1.0	0.13699	0.48719	0.13167	1.0000
Si	Si45	1.0	0.52587	0.47224	0.12563	1.0000
Si	Si46	1.0	0.84077	0.15761	0.62373	1.0000
Si	Si47	1.0	0.46746	0.53253	0.62645	1.0000
Si	Si48	1.0	0.15158	0.16150	0.37594	1.0000
Si	Si49	1.0	0.53243	0.52519	0.37464	1.0000
Si	Si50	1.0	0.84353	0.84437	0.87357	1.0000
Si	Si51	1.0	0.47578	0.46589	0.87598	1.0000
Si	Si52	1.0	0.79175	0.34581	0.70084	1.0000
Si	Si53	1.0	0.47675	0.71616	0.30070	1.0000
Si	Si54	1.0	0.21610	0.05072	0.19361	1.0000
Si	Si55	1.0	0.64788	0.78593	0.94699	1.0000
Si	Si56	1.0	0.28790	0.52131	0.95105	1.0000
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AlSiAl-T1T7T7T7T7T9T9

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O	O4	1.0	0.31078	0.48435	0.00619	1.0000
O	O5	1.0	0.23532	0.53782	0.09653	1.0000
O	O6	1.0	0.44009	0.48508	0.08208	1.0000
O	O7	1.0	0.71545	0.66314	0.05849	1.0000
O	O8	1.0	0.84495	0.83341	0.04837	1.0000
O	O9	1.0	0.66744	0.84403	0.10449	1.0000
O	O10	1.0	0.83074	0.48913	0.05176	1.0000
O	O11	1.0	0.64789	0.48061	0.10033	1.0000
O	O12	1.0	0.96256	0.66002	0.05109	1.0000
O	O13	1.0	0.03720	0.84326	0.09050	1.0000
O	O14	1.0	0.01001	0.48626	0.10308	1.0000
O	O15	1.0	0.62780	0.32974	0.54823	1.0000
O	O16	1.0	0.67275	0.17054	0.48560	1.0000
O	O17	1.0	0.73401	0.15852	0.58298	1.0000
O	O18	1.0	0.53195	0.13999	0.55773	1.0000
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O	O20	1.0	0.76655	0.45845	0.59507	1.0000
O	O21	1.0	0.56237	0.51465	0.58330	1.0000
O	O22	1.0	0.28552	0.33680	0.55926	1.0000
O	O23	1.0	0.15812	0.16517	0.54738	1.0000
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O	O26	1.0	0.35357	0.51903	0.60075	1.0000
O	O27	1.0	0.04182	0.33887	0.55076	1.0000
O	O28	1.0	0.96488	0.15625	0.58926	1.0000
O	O29	1.0	0.99146	0.51215	0.60295	1.0000
O	O30	1.0	0.33598	0.38885	0.30907	1.0000
O	O31	1.0	0.17238	0.35392	0.24499	1.0000
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O	O33	1.0	0.13995	0.44656	0.33155	1.0000
O	O34	1.0	0.50010	0.35139	0.24797	1.0000
O	O35	1.0	0.46725	0.23190	0.32935	1.0000

O	O36	1.0	0.53538	0.43326	0.33812	1.0000
O	O37	1.0	0.35415	0.71605	0.30929	1.0000
O	O38	1.0	0.18570	0.83663	0.32709	1.0000
O	O39	1.0	0.19557	0.64229	0.36393	1.0000
O	O40	1.0	0.52155	0.84275	0.31620	1.0000
O	O41	1.0	0.53916	0.64521	0.34278	1.0000
O	O42	1.0	0.35038	0.97246	0.31482	1.0000
O	O43	1.0	0.16642	0.03671	0.35351	1.0000
O	O44	1.0	0.54186	0.03931	0.34243	1.0000
O	O45	1.0	0.66925	0.61396	0.80939	1.0000
O	O46	1.0	0.83021	0.64981	0.74394	1.0000
O	O47	1.0	0.81430	0.76968	0.82681	1.0000
O	O48	1.0	0.86652	0.56211	0.83132	1.0000
O	O49	1.0	0.50318	0.64939	0.74922	1.0000
O	O50	1.0	0.53854	0.77102	0.83018	1.0000
O	O51	1.0	0.46957	0.56981	0.83929	1.0000
O	O52	1.0	0.64551	0.27524	0.80941	1.0000
O	O53	1.0	0.80078	0.36992	0.86270	1.0000
O	O54	1.0	0.47044	0.15773	0.81661	1.0000
O	O55	1.0	0.46550	0.35772	0.84263	1.0000
O	O56	1.0	0.64343	0.03355	0.81627	1.0000
O	O57	1.0	0.45319	0.96026	0.84347	1.0000
O	O58	1.0	0.61525	0.66847	0.93963	1.0000
O	O59	1.0	0.65075	0.82787	0.00569	1.0000
O	O60	1.0	0.76939	0.81424	0.92292	1.0000
O	O61	1.0	0.56072	0.86605	0.91871	1.0000
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O	O63	1.0	0.77645	0.54034	0.92206	1.0000
O	O64	1.0	0.57768	0.46808	0.90958	1.0000
O	O65	1.0	0.28526	0.64330	0.94308	1.0000
O	O66	1.0	0.16836	0.81061	0.92145	1.0000
O	O67	1.0	0.36702	0.79825	0.88901	1.0000
O	O68	1.0	0.16336	0.47045	0.93368	1.0000
O	O69	1.0	0.36480	0.46106	0.91051	1.0000

O	O70	1.0	0.03890	0.64283	0.93752	1.0000
O	O71	1.0	0.96953	0.81498	0.89242	1.0000
O	O72	1.0	0.96659	0.45711	0.90445	1.0000
O	O73	1.0	0.38044	0.33382	0.43753	1.0000
O	O74	1.0	0.35243	0.17482	0.50488	1.0000
O	O75	1.0	0.23422	0.17966	0.42195	1.0000
O	O76	1.0	0.44387	0.13825	0.41823	1.0000
O	O77	1.0	0.35441	0.49606	0.50156	1.0000
O	O78	1.0	0.22593	0.47082	0.42234	1.0000
O	O79	1.0	0.42733	0.53331	0.40988	1.0000
O	O80	1.0	0.71263	0.35527	0.44134	1.0000
O	O81	1.0	0.83559	0.18971	0.42083	1.0000
O	O82	1.0	0.63946	0.19663	0.38684	1.0000
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O	O85	1.0	0.96837	0.35525	0.43531	1.0000
O	O86	1.0	0.03406	0.17739	0.39162	1.0000
O	O87	1.0	0.03353	0.54464	0.40452	1.0000
O	O88	1.0	0.66769	0.36793	0.70058	1.0000
O	O89	1.0	0.82658	0.33061	0.76369	1.0000
O	O90	1.0	0.83694	0.25194	0.66978	1.0000
O	O91	1.0	0.48744	0.31051	0.74613	1.0000
O	O92	1.0	0.53097	0.23484	0.65422	1.0000
O	O93	1.0	0.48260	0.44021	0.67002	1.0000
O	O94	1.0	0.66439	0.71271	0.69175	1.0000
O	O95	1.0	0.83525	0.84058	0.69681	1.0000
O	O96	1.0	0.84333	0.65901	0.64454	1.0000
O	O97	1.0	0.49416	0.83124	0.69801	1.0000
O	O98	1.0	0.48086	0.64759	0.65009	1.0000
O	O99	1.0	0.66330	0.96469	0.69162	1.0000
O	O100	1.0	0.48358	0.00974	0.64580	1.0000
O	O101	1.0	0.33214	0.63088	0.20106	1.0000
O	O102	1.0	0.17211	0.66999	0.26474	1.0000
O	O103	1.0	0.16483	0.74714	0.17057	1.0000

O	O104	1.0	0.51411	0.68808	0.24605	1.0000
O	O105	1.0	0.46963	0.76313	0.15464	1.0000
O	O106	1.0	0.51680	0.55762	0.16986	1.0000
O	O107	1.0	0.33630	0.28687	0.19196	1.0000
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O	O109	1.0	0.15560	0.33948	0.14597	1.0000
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O	O111	1.0	0.51887	0.35089	0.14853	1.0000
O	O112	1.0	0.33559	0.03506	0.19040	1.0000
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O	O116	1.0	0.98734	0.17838	0.49007	1.0000
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O	O124	1.0	0.13941	0.53913	0.19078	1.0000
O	O125	1.0	0.84320	0.96672	0.85984	1.0000
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Al	Al3	1.0	0.53649	0.86296	0.12212	1.0000
Al	Al4	1.0	0.13425	0.46993	0.12754	1.0000
Al	Al5	1.0	0.15629	0.83789	0.12230	1.0000
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Si	Si2	1.0	0.72269	0.79244	0.05628	1.0000

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Si	Si4	1.0	0.96656	0.78914	0.04633	1.0000
Si	Si5	1.0	0.95484	0.53034	0.05340	1.0000
Si	Si6	1.0	0.64994	0.20311	0.54420	1.0000
Si	Si7	1.0	0.66375	0.45422	0.55928	1.0000
Si	Si8	1.0	0.27969	0.20761	0.55594	1.0000
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Si	Si10	1.0	0.03671	0.20995	0.54552	1.0000
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Si	Si12	1.0	0.21005	0.35554	0.30437	1.0000
Si	Si13	1.0	0.46026	0.35152	0.30620	1.0000
Si	Si14	1.0	0.22684	0.71643	0.31633	1.0000
Si	Si15	1.0	0.48246	0.72196	0.30297	1.0000
Si	Si16	1.0	0.22171	0.95795	0.31313	1.0000
Si	Si17	1.0	0.47803	0.96036	0.30418	1.0000
Si	Si18	1.0	0.14980	0.52608	0.38063	1.0000
Si	Si19	1.0	0.79430	0.65144	0.80363	1.0000
Si	Si20	1.0	0.54458	0.65120	0.80701	1.0000
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Si	Si23	1.0	0.85251	0.48462	0.88040	1.0000
Si	Si24	1.0	0.65092	0.79437	0.94569	1.0000
Si	Si25	1.0	0.65418	0.54510	0.94342	1.0000
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Si	Si28	1.0	0.04728	0.77229	0.93628	1.0000
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Si	Si32	1.0	0.34722	0.45895	0.44312	1.0000
Si	Si33	1.0	0.71580	0.22786	0.43388	1.0000
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Si	Si35	1.0	0.95717	0.22589	0.43529	1.0000
Si	Si36	1.0	0.95772	0.48294	0.44519	1.0000

Si	Si37	1.0	0.52338	0.15276	0.36953	1.0000
Si	Si38	1.0	0.54128	0.33527	0.69113	1.0000
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Si	Si41	1.0	0.53199	0.95603	0.69469	1.0000
Si	Si42	1.0	0.45848	0.66289	0.19153	1.0000
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Si	Si44	1.0	0.46555	0.28972	0.19604	1.0000
Si	Si45	1.0	0.46718	0.04404	0.19361	1.0000
Si	Si46	1.0	0.52981	0.47040	0.12514	1.0000
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Si	Si49	1.0	0.53469	0.53709	0.37529	1.0000
Si	Si50	1.0	0.46965	0.46549	0.87562	1.0000
Si	Si51	1.0	0.79343	0.34485	0.70411	1.0000
Si	Si52	1.0	0.35108	0.79645	0.04546	1.0000
Si	Si53	1.0	0.20636	0.65499	0.20583	1.0000
Si	Si54	1.0	0.84934	0.84374	0.87576	1.0000
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Si	Si56	1.0	0.78896	0.96035	0.70191	1.0000
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AlSiAl-T2T7T7T7T9T9

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O	O5	1.0	0.23468	0.54089	0.09638	1.0000
O	O6	1.0	0.43955	0.48900	0.08305	1.0000
O	O7	1.0	0.71563	0.66285	0.05973	1.0000
O	O8	1.0	0.84337	0.83431	0.04780	1.0000
O	O9	1.0	0.66544	0.84612	0.10299	1.0000
O	O10	1.0	0.83020	0.48909	0.05261	1.0000
O	O11	1.0	0.64720	0.48096	0.10149	1.0000
O	O12	1.0	0.96064	0.66131	0.05163	1.0000
O	O13	1.0	0.03645	0.84501	0.08932	1.0000
O	O14	1.0	0.00988	0.48732	0.10344	1.0000
O	O15	1.0	0.62944	0.33088	0.54895	1.0000
O	O16	1.0	0.67450	0.17089	0.48751	1.0000
O	O17	1.0	0.73022	0.15644	0.58556	1.0000
O	O18	1.0	0.52990	0.14269	0.55842	1.0000
O	O19	1.0	0.68569	0.51726	0.50581	1.0000
O	O20	1.0	0.76648	0.46124	0.59486	1.0000
O	O21	1.0	0.56146	0.51483	0.58364	1.0000
O	O22	1.0	0.28445	0.33554	0.56084	1.0000
O	O23	1.0	0.15501	0.16536	0.55044	1.0000
O	O24	1.0	0.33315	0.15339	0.60535	1.0000
O	O25	1.0	0.17142	0.51055	0.55259	1.0000
O	O26	1.0	0.35340	0.51865	0.60131	1.0000
O	O27	1.0	0.03922	0.34013	0.55274	1.0000
O	O28	1.0	0.96123	0.15615	0.59044	1.0000
O	O29	1.0	0.99041	0.51584	0.60257	1.0000
O	O30	1.0	0.33704	0.38554	0.30970	1.0000
O	O31	1.0	0.17265	0.35452	0.24540	1.0000
O	O32	1.0	0.18826	0.23674	0.32837	1.0000
O	O33	1.0	0.14200	0.44622	0.33190	1.0000
O	O34	1.0	0.50111	0.34440	0.24954	1.0000
O	O35	1.0	0.46499	0.22491	0.33185	1.0000

O	O36	1.0	0.53572	0.42554	0.33932	1.0000
O	O37	1.0	0.35397	0.72712	0.30910	1.0000
O	O38	1.0	0.17881	0.83650	0.32652	1.0000
O	O39	1.0	0.19960	0.64130	0.36314	1.0000
O	O40	1.0	0.53440	0.63685	0.34193	1.0000
O	O41	1.0	0.34170	0.97566	0.31681	1.0000
O	O42	1.0	0.15224	0.03522	0.35163	1.0000
O	O43	1.0	0.54985	0.03578	0.34850	1.0000
O	O44	1.0	0.66616	0.61205	0.80987	1.0000
O	O45	1.0	0.82776	0.64457	0.74444	1.0000
O	O46	1.0	0.81441	0.76328	0.82640	1.0000
O	O47	1.0	0.86205	0.55410	0.83176	1.0000
O	O48	1.0	0.50143	0.64781	0.74905	1.0000
O	O49	1.0	0.53456	0.76898	0.82963	1.0000
O	O50	1.0	0.46748	0.56776	0.83986	1.0000
O	O51	1.0	0.64638	0.28593	0.81029	1.0000
O	O52	1.0	0.81430	0.16362	0.82655	1.0000
O	O53	1.0	0.80691	0.35763	0.86381	1.0000
O	O54	1.0	0.48018	0.15751	0.81767	1.0000
O	O55	1.0	0.46081	0.35576	0.84309	1.0000
O	O56	1.0	0.65042	0.02749	0.81449	1.0000
O	O57	1.0	0.45968	0.96106	0.84360	1.0000
O	O58	1.0	0.61973	0.66402	0.93799	1.0000
O	O59	1.0	0.65011	0.82380	0.00459	1.0000
O	O60	1.0	0.76558	0.81748	0.92084	1.0000
O	O61	1.0	0.55597	0.85978	0.91912	1.0000
O	O62	1.0	0.64803	0.50254	0.00227	1.0000
O	O63	1.0	0.77513	0.52820	0.92246	1.0000
O	O64	1.0	0.57396	0.46418	0.91094	1.0000
O	O65	1.0	0.28720	0.64507	0.94188	1.0000
O	O66	1.0	0.16416	0.80984	0.91979	1.0000
O	O67	1.0	0.36128	0.80271	0.88697	1.0000
O	O68	1.0	0.16200	0.47543	0.93437	1.0000
O	O69	1.0	0.36184	0.45963	0.91100	1.0000

O	O70	1.0	0.03156	0.64467	0.93530	1.0000
O	O71	1.0	0.96603	0.82288	0.89167	1.0000
O	O72	1.0	0.96778	0.45506	0.90475	1.0000
O	O73	1.0	0.37320	0.32970	0.43851	1.0000
O	O74	1.0	0.34723	0.17195	0.50650	1.0000
O	O75	1.0	0.23574	0.16848	0.42102	1.0000
O	O76	1.0	0.44788	0.13732	0.42271	1.0000
O	O77	1.0	0.35379	0.49337	0.50232	1.0000
O	O78	1.0	0.22415	0.47217	0.42353	1.0000
O	O79	1.0	0.42771	0.52711	0.41087	1.0000
O	O80	1.0	0.71870	0.35707	0.44468	1.0000
O	O81	1.0	0.83581	0.19001	0.42212	1.0000
O	O82	1.0	0.63837	0.20472	0.38932	1.0000
O	O83	1.0	0.83920	0.53003	0.43519	1.0000
O	O84	1.0	0.64041	0.53844	0.40908	1.0000
O	O85	1.0	0.96579	0.35785	0.43588	1.0000
O	O86	1.0	0.03438	0.18163	0.39320	1.0000
O	O87	1.0	0.03328	0.54603	0.40331	1.0000
O	O88	1.0	0.66775	0.36828	0.70079	1.0000
O	O89	1.0	0.82750	0.33126	0.76455	1.0000
O	O90	1.0	0.83549	0.25185	0.67099	1.0000
O	O91	1.0	0.48698	0.30958	0.74658	1.0000
O	O92	1.0	0.52979	0.23723	0.65447	1.0000
O	O93	1.0	0.48301	0.44241	0.67127	1.0000
O	O94	1.0	0.66356	0.71331	0.69219	1.0000
O	O95	1.0	0.83560	0.83821	0.69995	1.0000
O	O96	1.0	0.84265	0.66020	0.64520	1.0000
O	O97	1.0	0.49428	0.83155	0.69844	1.0000
O	O98	1.0	0.48081	0.64910	0.64965	1.0000
O	O99	1.0	0.66452	0.96412	0.69183	1.0000
O	O100	1.0	0.48508	0.01088	0.64599	1.0000
O	O101	1.0	0.33271	0.63483	0.20042	1.0000
O	O102	1.0	0.17436	0.67025	0.26427	1.0000
O	O103	1.0	0.16399	0.74998	0.17002	1.0000

O	O104	1.0	0.51285	0.69324	0.24514	1.0000
O	O105	1.0	0.47014	0.76632	0.15281	1.0000
O	O106	1.0	0.51730	0.56047	0.17046	1.0000
O	O107	1.0	0.33603	0.28757	0.19317	1.0000
O	O108	1.0	0.16359	0.16196	0.20004	1.0000
O	O109	1.0	0.15674	0.34164	0.14625	1.0000
O	O110	1.0	0.50406	0.16612	0.19585	1.0000
O	O111	1.0	0.51734	0.35333	0.15008	1.0000
O	O112	1.0	0.33319	0.03545	0.18916	1.0000
O	O113	1.0	0.51003	0.99344	0.13974	1.0000
O	O114	1.0	0.01396	0.82137	0.99012	1.0000
O	O115	1.0	0.01114	0.48631	0.00284	1.0000
O	O116	1.0	0.98715	0.18119	0.49148	1.0000
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O	O120	1.0	0.82175	0.01455	0.75596	1.0000
O	O121	1.0	0.49623	0.01397	0.74647	1.0000
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O	O124	1.0	0.14080	0.54104	0.19058	1.0000
O	O125	1.0	0.83353	0.96365	0.85377	1.0000
O	O126	1.0	0.14441	0.97521	0.15489	1.0000
O	O127	1.0	0.85305	0.02649	0.65628	1.0000
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Al	Al1	1.0	0.46424	0.13625	0.62244	1.0000
Al	Al2	1.0	0.86548	0.53010	0.62656	1.0000
Al	Al3	1.0	0.53432	0.86718	0.11921	1.0000
Al	Al4	1.0	0.13445	0.47181	0.12750	1.0000
Al	Al5	1.0	0.15540	0.84131	0.12135	1.0000
Al	Al6	1.0	0.84267	0.16149	0.62259	1.0000
Al	Al7	1.0	0.47552	0.96975	0.30344	1.0000
Si	Si1	1.0	0.33594	0.54675	0.05973	1.0000
Si	Si2	1.0	0.72174	0.79207	0.05594	1.0000

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Si	Si3	1.0	0.71089	0.53418	0.05435	1.0000
Si	Si4	1.0	0.96501	0.79026	0.04586	1.0000
Si	Si5	1.0	0.95383	0.53146	0.05378	1.0000
Si	Si6	1.0	0.64916	0.20369	0.54565	1.0000
Si	Si7	1.0	0.66327	0.45591	0.55955	1.0000
Si	Si8	1.0	0.27709	0.20630	0.55774	1.0000
Si	Si9	1.0	0.29010	0.46409	0.55475	1.0000
Si	Si10	1.0	0.03432	0.21119	0.54735	1.0000
Si	Si11	1.0	0.04727	0.46995	0.55362	1.0000
Si	Si12	1.0	0.21070	0.35431	0.30475	1.0000
Si	Si13	1.0	0.45997	0.34382	0.30747	1.0000
Si	Si14	1.0	0.22519	0.71936	0.31586	1.0000
Si	Si15	1.0	0.21568	0.95912	0.31258	1.0000
Si	Si16	1.0	0.15027	0.52633	0.38038	1.0000
Si	Si17	1.0	0.79189	0.64459	0.80420	1.0000
Si	Si18	1.0	0.54183	0.64884	0.80713	1.0000
Si	Si19	1.0	0.77366	0.28431	0.81635	1.0000
Si	Si20	1.0	0.51839	0.27831	0.80381	1.0000
Si	Si21	1.0	0.52276	0.03985	0.80488	1.0000
Si	Si22	1.0	0.85200	0.47380	0.88068	1.0000
Si	Si23	1.0	0.64954	0.79034	0.94496	1.0000
Si	Si24	1.0	0.65412	0.53909	0.94367	1.0000
Si	Si25	1.0	0.28348	0.77236	0.93374	1.0000
Si	Si26	1.0	0.28090	0.51679	0.94889	1.0000
Si	Si27	1.0	0.04298	0.77404	0.93509	1.0000
Si	Si28	1.0	0.04293	0.51700	0.94537	1.0000
Si	Si29	1.0	0.47752	0.84684	0.87017	1.0000
Si	Si30	1.0	0.34901	0.20211	0.44617	1.0000
Si	Si31	1.0	0.34459	0.45543	0.44422	1.0000
Si	Si32	1.0	0.71711	0.22986	0.43586	1.0000
Si	Si33	1.0	0.72080	0.48543	0.44918	1.0000
Si	Si34	1.0	0.95673	0.22830	0.43643	1.0000
Si	Si35	1.0	0.95807	0.48573	0.44505	1.0000
Si	Si36	1.0	0.52607	0.14906	0.37306	1.0000

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Si	Si37	1.0	0.54151	0.33630	0.69191	1.0000
Si	Si38	1.0	0.79210	0.71413	0.69355	1.0000
Si	Si39	1.0	0.53458	0.71013	0.69694	1.0000
Si	Si40	1.0	0.53307	0.95578	0.69466	1.0000
Si	Si41	1.0	0.45823	0.66664	0.18994	1.0000
Si	Si42	1.0	0.20755	0.28591	0.19427	1.0000
Si	Si43	1.0	0.46507	0.28743	0.19667	1.0000
Si	Si44	1.0	0.46572	0.04123	0.19112	1.0000
Si	Si45	1.0	0.52908	0.47234	0.12609	1.0000
Si	Si46	1.0	0.47074	0.52945	0.62634	1.0000
Si	Si47	1.0	0.15304	0.15527	0.37397	1.0000
Si	Si48	1.0	0.53379	0.52868	0.37593	1.0000
Si	Si49	1.0	0.46686	0.46271	0.87639	1.0000
Si	Si50	1.0	0.79344	0.34485	0.70561	1.0000
Si	Si51	1.0	0.34853	0.79885	0.04388	1.0000
Si	Si52	1.0	0.20659	0.65740	0.20504	1.0000
Si	Si53	1.0	0.77888	0.04206	0.81301	1.0000
Si	Si54	1.0	0.84517	0.84159	0.87350	1.0000
Si	Si55	1.0	0.21008	0.04226	0.20265	1.0000
Si	Si56	1.0	0.78855	0.95714	0.70374	1.0000
Si	Si57	1.0	0.47972	0.71503	0.30233	1.0000

AlSiAl-T7T7T7T7T9T9T9

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H H4 1.0 0.13291 0.48512 0.21799 1.0000
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H H6 1.0 0.08465 0.00719 0.14443 1.0000
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O	O2	1.0	0.33797	0.83102	0.98771	1.0000
O	O3	1.0	0.26669	0.84417	0.08386	1.0000
O	O4	1.0	0.30681	0.48833	0.00630	1.0000
O	O5	1.0	0.23944	0.53716	0.09843	1.0000
O	O6	1.0	0.44196	0.48383	0.07994	1.0000
O	O7	1.0	0.71745	0.65774	0.05625	1.0000
O	O8	1.0	0.84257	0.83175	0.05155	1.0000
O	O9	1.0	0.66541	0.83184	0.10781	1.0000
O	O10	1.0	0.83380	0.48520	0.05218	1.0000
O	O11	1.0	0.64849	0.47728	0.09907	1.0000
O	O12	1.0	0.96154	0.65972	0.05233	1.0000
O	O13	1.0	0.03537	0.84151	0.09300	1.0000
O	O14	1.0	0.01489	0.48301	0.10022	1.0000
O	O15	1.0	0.62522	0.32790	0.54857	1.0000
O	O16	1.0	0.67202	0.16856	0.48614	1.0000
O	O17	1.0	0.73089	0.15605	0.58357	1.0000
O	O18	1.0	0.52991	0.13817	0.55786	1.0000
O	O19	1.0	0.67717	0.51245	0.50482	1.0000
O	O20	1.0	0.76888	0.45683	0.59087	1.0000
O	O21	1.0	0.56387	0.51230	0.58713	1.0000
O	O22	1.0	0.28426	0.33490	0.55985	1.0000
O	O23	1.0	0.15572	0.16426	0.54853	1.0000
O	O24	1.0	0.33231	0.15280	0.60378	1.0000
O	O25	1.0	0.17204	0.50989	0.55301	1.0000
O	O26	1.0	0.35406	0.51627	0.60155	1.0000
O	O27	1.0	0.04043	0.33888	0.55209	1.0000
O	O28	1.0	0.96211	0.15614	0.58975	1.0000
O	O29	1.0	0.99074	0.51570	0.60239	1.0000
O	O30	1.0	0.33610	0.38555	0.30932	1.0000
O	O31	1.0	0.17235	0.35217	0.24555	1.0000
O	O32	1.0	0.18856	0.23621	0.32840	1.0000
O	O33	1.0	0.14130	0.44504	0.33236	1.0000
O	O34	1.0	0.50042	0.35044	0.24793	1.0000
O	O35	1.0	0.46921	0.23013	0.32951	1.0000

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O	O36	1.0	0.53422	0.43227	0.33780	1.0000
O	O37	1.0	0.35211	0.71394	0.30992	1.0000
O	O38	1.0	0.18409	0.83557	0.32626	1.0000
O	O39	1.0	0.19174	0.64244	0.36405	1.0000
O	O40	1.0	0.51935	0.84064	0.31506	1.0000
O	O41	1.0	0.53640	0.64491	0.34415	1.0000
O	O42	1.0	0.34936	0.97112	0.31634	1.0000
O	O43	1.0	0.16341	0.03509	0.35283	1.0000
O	O44	1.0	0.54038	0.03604	0.34409	1.0000
O	O45	1.0	0.66581	0.61377	0.80671	1.0000
O	O46	1.0	0.82507	0.64340	0.73976	1.0000
O	O47	1.0	0.81234	0.77040	0.81982	1.0000
O	O48	1.0	0.86246	0.56155	0.82806	1.0000
O	O49	1.0	0.49836	0.65567	0.74992	1.0000
O	O50	1.0	0.53858	0.77248	0.83194	1.0000
O	O51	1.0	0.46826	0.57234	0.83980	1.0000
O	O52	1.0	0.64913	0.29211	0.80970	1.0000
O	O53	1.0	0.81862	0.17239	0.82242	1.0000
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O	O56	1.0	0.46154	0.36083	0.84113	1.0000
O	O57	1.0	0.65624	0.02823	0.81656	1.0000
O	O58	1.0	0.46648	0.96483	0.84742	1.0000
O	O59	1.0	0.61633	0.66476	0.94224	1.0000
O	O60	1.0	0.64797	0.82530	0.00884	1.0000
O	O61	1.0	0.76133	0.81982	0.92368	1.0000
O	O62	1.0	0.55325	0.86023	0.92357	1.0000
O	O63	1.0	0.65517	0.49460	0.99949	1.0000
O	O64	1.0	0.77691	0.53836	0.91932	1.0000
O	O65	1.0	0.57866	0.46722	0.90815	1.0000
O	O66	1.0	0.29173	0.64844	0.94265	1.0000
O	O67	1.0	0.17160	0.81896	0.92700	1.0000
O	O68	1.0	0.36227	0.80697	0.88775	1.0000
O	O69	1.0	0.16477	0.48067	0.93181	1.0000

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O	O70	1.0	0.36674	0.46278	0.91176	1.0000
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O	O72	1.0	0.97818	0.83458	0.89416	1.0000
O	O73	1.0	0.97119	0.46776	0.90097	1.0000
O	O74	1.0	0.37479	0.33193	0.43793	1.0000
O	O75	1.0	0.34936	0.17231	0.50513	1.0000
O	O76	1.0	0.23295	0.17461	0.42215	1.0000
O	O77	1.0	0.44360	0.13849	0.41894	1.0000
O	O78	1.0	0.35413	0.49415	0.50239	1.0000
O	O79	1.0	0.22502	0.47404	0.42338	1.0000
O	O80	1.0	0.42860	0.53000	0.41115	1.0000
O	O81	1.0	0.71326	0.35312	0.44188	1.0000
O	O82	1.0	0.83517	0.18658	0.42172	1.0000
O	O83	1.0	0.63931	0.19407	0.38757	1.0000
O	O84	1.0	0.83730	0.52431	0.43758	1.0000
O	O85	1.0	0.64138	0.53754	0.40812	1.0000
O	O86	1.0	0.96514	0.35381	0.43613	1.0000
O	O87	1.0	0.03355	0.17670	0.39231	1.0000
O	O88	1.0	0.03070	0.54197	0.40401	1.0000
O	O89	1.0	0.66583	0.37106	0.69935	1.0000
O	O90	1.0	0.82776	0.33939	0.76186	1.0000
O	O91	1.0	0.83305	0.25318	0.66965	1.0000
O	O92	1.0	0.48909	0.30347	0.74578	1.0000
O	O93	1.0	0.52811	0.24201	0.65162	1.0000
O	O94	1.0	0.47891	0.44459	0.67401	1.0000
O	O95	1.0	0.65984	0.71675	0.69110	1.0000
O	O96	1.0	0.83360	0.83831	0.69643	1.0000
O	O97	1.0	0.83488	0.66051	0.64054	1.0000
O	O98	1.0	0.49177	0.83534	0.69761	1.0000
O	O99	1.0	0.47685	0.64982	0.65058	1.0000
O	O100	1.0	0.66362	0.96699	0.69141	1.0000
O	O101	1.0	0.48248	0.01672	0.64888	1.0000
O	O102	1.0	0.33117	0.62484	0.20170	1.0000
O	O103	1.0	0.17130	0.66746	0.26469	1.0000

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O	O104	1.0	0.16779	0.74598	0.17073	1.0000
O	O105	1.0	0.51187	0.68129	0.24692	1.0000
O	O106	1.0	0.46347	0.76554	0.15801	1.0000
O	O107	1.0	0.51708	0.55977	0.16734	1.0000
O	O108	1.0	0.33677	0.28714	0.19236	1.0000
O	O109	1.0	0.16706	0.15964	0.20005	1.0000
O	O110	1.0	0.15640	0.33823	0.14634	1.0000
O	O111	1.0	0.50628	0.16882	0.19644	1.0000
O	O112	1.0	0.51754	0.35185	0.14820	1.0000
O	O113	1.0	0.33813	0.03416	0.18926	1.0000
O	O114	1.0	0.52283	0.98734	0.14699	1.0000
O	O115	1.0	0.01429	0.82493	0.99380	1.0000
O	O116	1.0	0.01150	0.48830	0.99963	1.0000
O	O117	1.0	0.98663	0.17820	0.49082	1.0000
O	O118	1.0	0.99355	0.51354	0.50225	1.0000
O	O119	1.0	0.18321	0.98346	0.25532	1.0000
O	O120	1.0	0.50201	0.98970	0.24701	1.0000
O	O121	1.0	0.82311	0.01446	0.75393	1.0000
O	O122	1.0	0.50048	0.01372	0.74950	1.0000
O	O123	1.0	0.85634	0.46432	0.68679	1.0000
O	O124	1.0	0.47145	0.85713	0.06110	1.0000
O	O125	1.0	0.13691	0.53821	0.19037	1.0000
O	O126	1.0	0.84631	0.98050	0.85312	1.0000
O	O127	1.0	0.14828	0.97168	0.15634	1.0000
O	O128	1.0	0.85176	0.02743	0.65439	1.0000
Al	Al1	1.0	0.46273	0.13802	0.62161	1.0000
Al	Al2	1.0	0.86345	0.53019	0.62343	1.0000
Al	Al3	1.0	0.53612	0.85979	0.12451	1.0000
Al	Al4	1.0	0.13621	0.46833	0.12704	1.0000
Al	Al5	1.0	0.84894	0.83565	0.87464	1.0000
Al	Al6	1.0	0.15642	0.83649	0.12257	1.0000
Al	Al7	1.0	0.84220	0.16286	0.62086	1.0000
Si	Si1	1.0	0.33765	0.54489	0.05992	1.0000
Si	Si2	1.0	0.72148	0.78706	0.05812	1.0000

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Si	Si3	1.0	0.71407	0.52896	0.05221	1.0000
Si	Si4	1.0	0.96468	0.78913	0.04845	1.0000
Si	Si5	1.0	0.95650	0.52983	0.05216	1.0000
Si	Si6	1.0	0.64783	0.20137	0.54452	1.0000
Si	Si7	1.0	0.66112	0.45265	0.55896	1.0000
Si	Si8	1.0	0.27733	0.20575	0.55628	1.0000
Si	Si9	1.0	0.29066	0.46353	0.55455	1.0000
Si	Si10	1.0	0.03496	0.20996	0.54626	1.0000
Si	Si11	1.0	0.04834	0.46886	0.55352	1.0000
Si	Si12	1.0	0.21043	0.35368	0.30470	1.0000
Si	Si13	1.0	0.46042	0.34950	0.30612	1.0000
Si	Si14	1.0	0.22489	0.71492	0.31613	1.0000
Si	Si15	1.0	0.48011	0.71927	0.30330	1.0000
Si	Si16	1.0	0.22126	0.95671	0.31290	1.0000
Si	Si17	1.0	0.47652	0.95933	0.30492	1.0000
Si	Si18	1.0	0.14827	0.52577	0.38103	1.0000
Si	Si19	1.0	0.79082	0.65072	0.80023	1.0000
Si	Si20	1.0	0.54269	0.65341	0.80725	1.0000
Si	Si21	1.0	0.77623	0.29451	0.81402	1.0000
Si	Si22	1.0	0.52122	0.28081	0.80352	1.0000
Si	Si23	1.0	0.52708	0.04119	0.80760	1.0000
Si	Si24	1.0	0.85499	0.48449	0.87761	1.0000
Si	Si25	1.0	0.64866	0.79176	0.94852	1.0000
Si	Si26	1.0	0.65656	0.54160	0.94266	1.0000
Si	Si27	1.0	0.28984	0.77624	0.93652	1.0000
Si	Si28	1.0	0.28275	0.52030	0.94852	1.0000
Si	Si29	1.0	0.04834	0.78286	0.93790	1.0000
Si	Si30	1.0	0.04636	0.52457	0.94334	1.0000
Si	Si31	1.0	0.48042	0.84907	0.87323	1.0000
Si	Si32	1.0	0.34853	0.20514	0.44533	1.0000
Si	Si33	1.0	0.34560	0.45812	0.44379	1.0000
Si	Si34	1.0	0.71554	0.22547	0.43437	1.0000
Si	Si35	1.0	0.71710	0.48169	0.44847	1.0000
Si	Si36	1.0	0.95593	0.22442	0.43593	1.0000

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Si	Si37	1.0	0.95668	0.48181	0.44583	1.0000
Si	Si38	1.0	0.52334	0.15106	0.37020	1.0000
Si	Si39	1.0	0.53997	0.33765	0.69126	1.0000
Si	Si40	1.0	0.78807	0.71435	0.69012	1.0000
Si	Si41	1.0	0.53127	0.71344	0.69705	1.0000
Si	Si42	1.0	0.53226	0.95880	0.69576	1.0000
Si	Si43	1.0	0.45620	0.66068	0.19208	1.0000
Si	Si44	1.0	0.20843	0.28447	0.19412	1.0000
Si	Si45	1.0	0.46559	0.29004	0.19573	1.0000
Si	Si46	1.0	0.46915	0.04420	0.19393	1.0000
Si	Si47	1.0	0.53015	0.47010	0.12356	1.0000
Si	Si48	1.0	0.46931	0.52897	0.62795	1.0000
Si	Si49	1.0	0.15438	0.15610	0.37421	1.0000
Si	Si50	1.0	0.53423	0.53528	0.37544	1.0000
Si	Si51	1.0	0.46948	0.46713	0.87560	1.0000
Si	Si52	1.0	0.79176	0.34936	0.70312	1.0000
Si	Si53	1.0	0.35354	0.79750	0.04639	1.0000
Si	Si54	1.0	0.20623	0.65237	0.20576	1.0000
Si	Si55	1.0	0.78078	0.05199	0.80912	1.0000
Si	Si56	1.0	0.21468	0.04084	0.20281	1.0000
Si	Si57	1.0	0.78771	0.95719	0.70121	1.0000

AlSiAl-T1T1T7T7T7T9T9

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H H6 1.0 0.90957 0.98818 0.63770 1.0000
H H7 1.0 0.87118 0.17656 0.86050 1.0000
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O	O1	1.0	0.37354	0.66784	0.04856	1.0000
O	O2	1.0	0.32973	0.82738	0.98671	1.0000
O	O3	1.0	0.26856	0.83914	0.08418	1.0000
O	O4	1.0	0.31013	0.48310	0.00612	1.0000
O	O5	1.0	0.23407	0.53999	0.09581	1.0000
O	O6	1.0	0.43786	0.48282	0.08274	1.0000
O	O7	1.0	0.71586	0.66461	0.05798	1.0000
O	O8	1.0	0.84512	0.83496	0.04714	1.0000
O	O9	1.0	0.66809	0.84596	0.10365	1.0000
O	O10	1.0	0.82932	0.48937	0.05122	1.0000
O	O11	1.0	0.64689	0.48290	0.10010	1.0000
O	O12	1.0	0.96103	0.66024	0.05048	1.0000
O	O13	1.0	0.03738	0.84286	0.08942	1.0000
O	O14	1.0	0.00875	0.48726	0.10312	1.0000
O	O15	1.0	0.62655	0.33168	0.54856	1.0000
O	O16	1.0	0.67028	0.17309	0.48592	1.0000
O	O17	1.0	0.73183	0.16007	0.58332	1.0000
O	O18	1.0	0.52981	0.14095	0.55772	1.0000
O	O19	1.0	0.68761	0.51688	0.50605	1.0000
O	O20	1.0	0.76753	0.45960	0.59480	1.0000
O	O21	1.0	0.56346	0.51659	0.58413	1.0000
O	O22	1.0	0.28541	0.33479	0.55810	1.0000
O	O23	1.0	0.15575	0.16469	0.54659	1.0000
O	O24	1.0	0.33218	0.15252	0.60301	1.0000
O	O25	1.0	0.17199	0.51023	0.55163	1.0000
O	O26	1.0	0.35391	0.51635	0.60064	1.0000
O	O27	1.0	0.04033	0.33954	0.54955	1.0000
O	O28	1.0	0.96317	0.15726	0.58888	1.0000
O	O29	1.0	0.99239	0.51120	0.60366	1.0000
O	O30	1.0	0.33325	0.38874	0.30913	1.0000
O	O31	1.0	0.17168	0.35107	0.24437	1.0000
O	O32	1.0	0.18978	0.23079	0.32651	1.0000
O	O33	1.0	0.13566	0.43768	0.33226	1.0000
O	O34	1.0	0.49846	0.35310	0.24817	1.0000

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O	O35	1.0	0.46401	0.23192	0.32909	1.0000
O	O36	1.0	0.53340	0.43369	0.33814	1.0000
O	O37	1.0	0.35608	0.72607	0.30908	1.0000
O	O38	1.0	0.20247	0.63044	0.36318	1.0000
O	O39	1.0	0.53152	0.84412	0.31539	1.0000
O	O40	1.0	0.53616	0.64576	0.34333	1.0000
O	O41	1.0	0.35792	0.96759	0.31595	1.0000
O	O42	1.0	0.15668	0.03408	0.35934	1.0000
O	O43	1.0	0.54913	0.04259	0.34119	1.0000
O	O44	1.0	0.66854	0.61300	0.80959	1.0000
O	O45	1.0	0.82889	0.64984	0.74394	1.0000
O	O46	1.0	0.81359	0.76986	0.82656	1.0000
O	O47	1.0	0.86623	0.56254	0.83146	1.0000
O	O48	1.0	0.50306	0.64879	0.74903	1.0000
O	O49	1.0	0.53872	0.77063	0.82969	1.0000
O	O50	1.0	0.46823	0.56931	0.83909	1.0000
O	O51	1.0	0.64414	0.27501	0.80899	1.0000
O	O52	1.0	0.79838	0.37048	0.86259	1.0000
O	O53	1.0	0.46907	0.15678	0.81655	1.0000
O	O54	1.0	0.46411	0.35710	0.84231	1.0000
O	O55	1.0	0.64256	0.03302	0.81577	1.0000
O	O56	1.0	0.45188	0.95894	0.84246	1.0000
O	O57	1.0	0.61409	0.66909	0.93901	1.0000
O	O58	1.0	0.65012	0.82855	0.00502	1.0000
O	O59	1.0	0.77005	0.81394	0.92278	1.0000
O	O60	1.0	0.56196	0.86719	0.91762	1.0000
O	O61	1.0	0.64737	0.50446	0.00089	1.0000
O	O62	1.0	0.77518	0.54073	0.92199	1.0000
O	O63	1.0	0.57632	0.46804	0.90941	1.0000
O	O64	1.0	0.28513	0.64217	0.94306	1.0000
O	O65	1.0	0.16902	0.80957	0.92093	1.0000
O	O66	1.0	0.36789	0.79671	0.88890	1.0000
O	O67	1.0	0.16200	0.46970	0.93366	1.0000
O	O68	1.0	0.36334	0.45973	0.91031	1.0000

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O	O69	1.0	0.03772	0.64230	0.93686	1.0000
O	O70	1.0	0.97011	0.81520	0.89162	1.0000
O	O71	1.0	0.96464	0.45618	0.90479	1.0000
O	O72	1.0	0.38662	0.33144	0.43892	1.0000
O	O73	1.0	0.35119	0.17127	0.50446	1.0000
O	O74	1.0	0.23122	0.18612	0.42261	1.0000
O	O75	1.0	0.43985	0.13422	0.41671	1.0000
O	O76	1.0	0.35432	0.49550	0.50142	1.0000
O	O77	1.0	0.22612	0.46079	0.42271	1.0000
O	O78	1.0	0.42550	0.53230	0.40988	1.0000
O	O79	1.0	0.71576	0.35852	0.44272	1.0000
O	O80	1.0	0.83228	0.19095	0.42069	1.0000
O	O81	1.0	0.63429	0.20421	0.38798	1.0000
O	O82	1.0	0.83883	0.53149	0.43477	1.0000
O	O83	1.0	0.63853	0.54108	0.40989	1.0000
O	O84	1.0	0.96213	0.35854	0.43789	1.0000
O	O85	1.0	0.03154	0.18793	0.39113	1.0000
O	O86	1.0	0.03626	0.54414	0.40541	1.0000
O	O87	1.0	0.66682	0.36613	0.70062	1.0000
O	O88	1.0	0.82617	0.32985	0.76379	1.0000
O	O89	1.0	0.83736	0.25331	0.66960	1.0000
O	O90	1.0	0.48554	0.30920	0.74592	1.0000
O	O91	1.0	0.52811	0.23499	0.65384	1.0000
O	O92	1.0	0.48276	0.44065	0.67048	1.0000
O	O93	1.0	0.66375	0.71174	0.69068	1.0000
O	O94	1.0	0.83419	0.84126	0.69701	1.0000
O	O95	1.0	0.84484	0.65970	0.64490	1.0000
O	O96	1.0	0.49427	0.83116	0.69821	1.0000
O	O97	1.0	0.47840	0.64786	0.65019	1.0000
O	O98	1.0	0.66282	0.96597	0.69109	1.0000
O	O99	1.0	0.48218	0.00900	0.64538	1.0000
O	O100	1.0	0.33270	0.63357	0.20080	1.0000
O	O101	1.0	0.17380	0.66973	0.26440	1.0000
O	O102	1.0	0.16221	0.74702	0.17044	1.0000

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O	O103	1.0	0.51437	0.68737	0.24632	1.0000
O	O104	1.0	0.47185	0.76617	0.15517	1.0000
O	O105	1.0	0.51631	0.55955	0.16937	1.0000
O	O106	1.0	0.33665	0.28819	0.19106	1.0000
O	O107	1.0	0.16566	0.15927	0.19764	1.0000
O	O108	1.0	0.15559	0.34023	0.14539	1.0000
O	O109	1.0	0.50662	0.16957	0.19792	1.0000
O	O110	1.0	0.52101	0.35202	0.14923	1.0000
O	O111	1.0	0.33728	0.03557	0.19057	1.0000
O	O112	1.0	0.51812	0.99184	0.14472	1.0000
O	O113	1.0	0.01653	0.82079	0.99013	1.0000
O	O114	1.0	0.01182	0.48304	0.00277	1.0000
O	O115	1.0	0.98456	0.17843	0.48960	1.0000
O	O116	1.0	0.98964	0.51830	0.50343	1.0000
O	O117	1.0	0.17487	0.97867	0.25202	1.0000
O	O118	1.0	0.50831	0.98650	0.24493	1.0000
O	O119	1.0	0.82621	0.02119	0.75203	1.0000
O	O120	1.0	0.49101	0.01400	0.74570	1.0000
O	O121	1.0	0.85846	0.46190	0.69031	1.0000
O	O122	1.0	0.47073	0.85784	0.05829	1.0000
O	O123	1.0	0.14055	0.53828	0.19069	1.0000
O	O124	1.0	0.84295	0.96684	0.85961	1.0000
O	O125	1.0	0.15034	0.97373	0.15216	1.0000
O	O126	1.0	0.84966	0.02673	0.65189	1.0000
O	O127	1.0	0.82054	0.17464	0.83258	1.0000
O	O128	1.0	0.17948	0.82596	0.33273	1.0000
Al	Al1	1.0	0.46267	0.13354	0.62132	1.0000
Al	Al2	1.0	0.86677	0.52937	0.62663	1.0000
Al	Al3	1.0	0.53757	0.86613	0.12180	1.0000
Al	Al4	1.0	0.13364	0.47030	0.12696	1.0000
Al	Al5	1.0	0.15611	0.83751	0.12155	1.0000
Al	Al6	1.0	0.84392	0.16237	0.62080	1.0000
Al	Al7	1.0	0.77846	0.03495	0.81293	1.0000
Al	Al8	1.0	0.22201	0.96539	0.31293	1.0000

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Si	Si1	1.0	0.33635	0.54350	0.05944	1.0000
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Si	Si3	1.0	0.71046	0.53592	0.05306	1.0000
Si	Si4	1.0	0.96619	0.78930	0.04539	1.0000
Si	Si5	1.0	0.95378	0.53063	0.05322	1.0000
Si	Si6	1.0	0.64786	0.20488	0.54451	1.0000
Si	Si7	1.0	0.66382	0.45602	0.55949	1.0000
Si	Si8	1.0	0.27818	0.20539	0.55512	1.0000
Si	Si9	1.0	0.29076	0.46353	0.55346	1.0000
Si	Si10	1.0	0.03472	0.21038	0.54480	1.0000
Si	Si11	1.0	0.04749	0.46905	0.55340	1.0000
Si	Si12	1.0	0.20832	0.34961	0.30385	1.0000
Si	Si13	1.0	0.45797	0.35165	0.30615	1.0000
Si	Si14	1.0	0.48639	0.72547	0.30286	1.0000
Si	Si15	1.0	0.48319	0.96139	0.30386	1.0000
Si	Si16	1.0	0.15025	0.51590	0.38118	1.0000
Si	Si17	1.0	0.79365	0.65133	0.80368	1.0000
Si	Si18	1.0	0.54398	0.65060	0.80686	1.0000
Si	Si19	1.0	0.51388	0.27491	0.80283	1.0000
Si	Si20	1.0	0.51707	0.03948	0.80454	1.0000
Si	Si21	1.0	0.85107	0.48487	0.88049	1.0000
Si	Si22	1.0	0.65085	0.79491	0.94514	1.0000
Si	Si23	1.0	0.65268	0.54573	0.94319	1.0000
Si	Si24	1.0	0.28760	0.76959	0.93493	1.0000
Si	Si25	1.0	0.28091	0.51383	0.94865	1.0000
Si	Si26	1.0	0.04735	0.77183	0.93557	1.0000
Si	Si27	1.0	0.04425	0.51455	0.94560	1.0000
Si	Si28	1.0	0.48021	0.84860	0.86990	1.0000
Si	Si29	1.0	0.35050	0.20549	0.44470	1.0000
Si	Si30	1.0	0.34866	0.45490	0.44357	1.0000
Si	Si31	1.0	0.71349	0.23111	0.43437	1.0000
Si	Si32	1.0	0.71946	0.48683	0.44874	1.0000
Si	Si33	1.0	0.95362	0.22906	0.43551	1.0000
Si	Si34	1.0	0.95650	0.48641	0.44641	1.0000

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Si	Si35	1.0	0.52174	0.15308	0.36894	1.0000
Si	Si36	1.0	0.53989	0.33452	0.69112	1.0000
Si	Si37	1.0	0.79274	0.71657	0.69229	1.0000
Si	Si38	1.0	0.53467	0.71034	0.69667	1.0000
Si	Si39	1.0	0.53134	0.95630	0.69434	1.0000
Si	Si40	1.0	0.45976	0.66496	0.19132	1.0000
Si	Si41	1.0	0.20762	0.28378	0.19273	1.0000
Si	Si42	1.0	0.46589	0.29027	0.19623	1.0000
Si	Si43	1.0	0.46872	0.04468	0.19376	1.0000
Si	Si44	1.0	0.52927	0.47108	0.12528	1.0000
Si	Si45	1.0	0.47089	0.52863	0.62622	1.0000
Si	Si46	1.0	0.15195	0.15737	0.37521	1.0000
Si	Si47	1.0	0.53316	0.53690	0.37540	1.0000
Si	Si48	1.0	0.46821	0.46476	0.87538	1.0000
Si	Si49	1.0	0.79294	0.34479	0.70431	1.0000
Si	Si50	1.0	0.35239	0.79468	0.04506	1.0000
Si	Si51	1.0	0.20663	0.65514	0.20476	1.0000
Si	Si52	1.0	0.84946	0.84378	0.87545	1.0000
Si	Si53	1.0	0.21172	0.03944	0.20195	1.0000
Si	Si54	1.0	0.78849	0.96123	0.70185	1.0000
Si	Si55	1.0	0.76892	0.29437	0.81586	1.0000
Si	Si56	1.0	0.23135	0.70607	0.31623	1.0000

AlSiAl-T1T2T7T7T7T7T9T9

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O	O2	1.0	0.32602	0.82822	0.98640	1.0000
O	O3	1.0	0.26904	0.84332	0.08441	1.0000
O	O4	1.0	0.31195	0.48300	0.00618	1.0000
O	O5	1.0	0.23284	0.53853	0.09551	1.0000
O	O6	1.0	0.43777	0.48559	0.08361	1.0000
O	O7	1.0	0.71550	0.66550	0.05920	1.0000
O	O8	1.0	0.84555	0.83537	0.04740	1.0000
O	O9	1.0	0.66786	0.84867	0.10317	1.0000
O	O10	1.0	0.82923	0.49060	0.05221	1.0000
O	O11	1.0	0.64643	0.48301	0.10089	1.0000
O	O12	1.0	0.96171	0.66098	0.05102	1.0000
O	O13	1.0	0.03789	0.84421	0.08945	1.0000
O	O14	1.0	0.00814	0.48767	0.10395	1.0000
O	O15	1.0	0.62657	0.33170	0.54813	1.0000
O	O16	1.0	0.67335	0.17155	0.48662	1.0000
O	O17	1.0	0.73050	0.16004	0.58430	1.0000
O	O18	1.0	0.52973	0.14154	0.55789	1.0000
O	O19	1.0	0.68605	0.51831	0.50611	1.0000
O	O20	1.0	0.76646	0.45972	0.59470	1.0000
O	O21	1.0	0.56234	0.51586	0.58419	1.0000
O	O22	1.0	0.28485	0.33490	0.55991	1.0000
O	O23	1.0	0.15518	0.16466	0.54869	1.0000
O	O24	1.0	0.33267	0.15230	0.60414	1.0000
O	O25	1.0	0.17248	0.51076	0.55250	1.0000
O	O26	1.0	0.35376	0.51722	0.60136	1.0000
O	O27	1.0	0.04082	0.34006	0.55109	1.0000
O	O28	1.0	0.96138	0.15729	0.58905	1.0000
O	O29	1.0	0.99092	0.51380	0.60264	1.0000
O	O30	1.0	0.33739	0.38738	0.30956	1.0000
O	O31	1.0	0.17322	0.35476	0.24530	1.0000
O	O32	1.0	0.18996	0.23642	0.32770	1.0000
O	O33	1.0	0.14174	0.44552	0.33220	1.0000
O	O34	1.0	0.50065	0.34587	0.24903	1.0000

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O	O35	1.0	0.46497	0.22672	0.33115	1.0000
O	O36	1.0	0.53670	0.42741	0.33881	1.0000
O	O37	1.0	0.35544	0.72750	0.30937	1.0000
O	O38	1.0	0.17974	0.83623	0.32657	1.0000
O	O39	1.0	0.20141	0.64098	0.36317	1.0000
O	O40	1.0	0.53634	0.63870	0.34250	1.0000
O	O41	1.0	0.34272	0.97606	0.31656	1.0000
O	O42	1.0	0.15307	0.03536	0.35160	1.0000
O	O43	1.0	0.55180	0.03836	0.34691	1.0000
O	O44	1.0	0.66890	0.61306	0.81006	1.0000
O	O45	1.0	0.82897	0.64875	0.74412	1.0000
O	O46	1.0	0.81381	0.76997	0.82618	1.0000
O	O47	1.0	0.86623	0.56250	0.83213	1.0000
O	O48	1.0	0.50350	0.64844	0.74948	1.0000
O	O49	1.0	0.53863	0.77067	0.82998	1.0000
O	O50	1.0	0.46904	0.56944	0.83979	1.0000
O	O51	1.0	0.64490	0.27517	0.80962	1.0000
O	O52	1.0	0.79956	0.36971	0.86306	1.0000
O	O53	1.0	0.47002	0.15696	0.81717	1.0000
O	O54	1.0	0.46517	0.35730	0.84284	1.0000
O	O55	1.0	0.64290	0.03287	0.81597	1.0000
O	O56	1.0	0.45217	0.95914	0.84284	1.0000
O	O57	1.0	0.61410	0.66843	0.93920	1.0000
O	O58	1.0	0.65117	0.82809	0.00479	1.0000
O	O59	1.0	0.76921	0.81322	0.92225	1.0000
O	O60	1.0	0.56077	0.86626	0.91810	1.0000
O	O61	1.0	0.64764	0.50517	0.00187	1.0000
O	O62	1.0	0.77460	0.53918	0.92255	1.0000
O	O63	1.0	0.57521	0.46724	0.91075	1.0000
O	O64	1.0	0.28448	0.64206	0.94300	1.0000
O	O65	1.0	0.16784	0.80915	0.92010	1.0000
O	O66	1.0	0.36720	0.79661	0.88882	1.0000
O	O67	1.0	0.16178	0.46944	0.93466	1.0000
O	O68	1.0	0.36230	0.45934	0.91018	1.0000

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O	O69	1.0	0.03738	0.64215	0.93743	1.0000
O	O70	1.0	0.96923	0.81444	0.89166	1.0000
O	O71	1.0	0.96466	0.45611	0.90559	1.0000
O	O72	1.0	0.37499	0.33021	0.43819	1.0000
O	O73	1.0	0.34845	0.17163	0.50554	1.0000
O	O74	1.0	0.23528	0.17023	0.42076	1.0000
O	O75	1.0	0.44723	0.13732	0.42113	1.0000
O	O76	1.0	0.35488	0.49381	0.50220	1.0000
O	O77	1.0	0.22528	0.47195	0.42337	1.0000
O	O78	1.0	0.42875	0.52814	0.41082	1.0000
O	O79	1.0	0.72022	0.35803	0.44517	1.0000
O	O80	1.0	0.83543	0.19073	0.42118	1.0000
O	O81	1.0	0.63791	0.20809	0.38875	1.0000
O	O82	1.0	0.84019	0.53165	0.43559	1.0000
O	O83	1.0	0.64163	0.53861	0.40922	1.0000
O	O84	1.0	0.96590	0.35883	0.43561	1.0000
O	O85	1.0	0.03438	0.18312	0.39197	1.0000
O	O86	1.0	0.03466	0.54719	0.40377	1.0000
O	O87	1.0	0.66697	0.36692	0.70090	1.0000
O	O88	1.0	0.82612	0.33091	0.76406	1.0000
O	O89	1.0	0.83646	0.25233	0.67032	1.0000
O	O90	1.0	0.48660	0.30918	0.74645	1.0000
O	O91	1.0	0.52865	0.23573	0.65415	1.0000
O	O92	1.0	0.48275	0.44112	0.67111	1.0000
O	O93	1.0	0.66381	0.71242	0.69143	1.0000
O	O94	1.0	0.83469	0.84060	0.69756	1.0000
O	O95	1.0	0.84345	0.65968	0.64492	1.0000
O	O96	1.0	0.49402	0.83125	0.69870	1.0000
O	O97	1.0	0.47952	0.64813	0.65050	1.0000
O	O98	1.0	0.66314	0.96489	0.69185	1.0000
O	O99	1.0	0.48385	0.00943	0.64573	1.0000
O	O100	1.0	0.33320	0.63530	0.20026	1.0000
O	O101	1.0	0.17543	0.66930	0.26457	1.0000
O	O102	1.0	0.16356	0.74882	0.17044	1.0000

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O	O103	1.0	0.51404	0.69161	0.24550	1.0000
O	O104	1.0	0.47318	0.76598	0.15351	1.0000
O	O105	1.0	0.51699	0.55948	0.17049	1.0000
O	O106	1.0	0.33605	0.28811	0.19200	1.0000
O	O107	1.0	0.16368	0.16138	0.20040	1.0000
O	O108	1.0	0.15486	0.34055	0.14647	1.0000
O	O109	1.0	0.50392	0.16611	0.19633	1.0000
O	O110	1.0	0.51939	0.35228	0.14989	1.0000
O	O111	1.0	0.33313	0.03516	0.18904	1.0000
O	O112	1.0	0.51019	0.99385	0.13938	1.0000
O	O113	1.0	0.01674	0.82123	0.99017	1.0000
O	O114	1.0	0.01123	0.48311	0.00355	1.0000
O	O115	1.0	0.98690	0.18096	0.49010	1.0000
O	O116	1.0	0.99322	0.51675	0.50224	1.0000
O	O117	1.0	0.17520	0.98253	0.25461	1.0000
O	O118	1.0	0.50435	0.97658	0.23984	1.0000
O	O119	1.0	0.82653	0.02115	0.75209	1.0000
O	O120	1.0	0.49132	0.01426	0.74610	1.0000
O	O121	1.0	0.85856	0.46155	0.68988	1.0000
O	O122	1.0	0.47037	0.85609	0.05630	1.0000
O	O123	1.0	0.14134	0.53992	0.19071	1.0000
O	O124	1.0	0.84301	0.96677	0.85959	1.0000
O	O125	1.0	0.14449	0.97392	0.15519	1.0000
O	O126	1.0	0.84912	0.02592	0.65201	1.0000
O	O127	1.0	0.82117	0.17438	0.83248	1.0000
O	O128	1.0	0.53207	0.83691	0.31907	1.0000
Al	Al1	1.0	0.46339	0.13411	0.62185	1.0000
Al	Al2	1.0	0.86567	0.52973	0.62618	1.0000
Al	Al3	1.0	0.53611	0.86723	0.11962	1.0000
Al	Al4	1.0	0.13299	0.47061	0.12761	1.0000
Al	Al5	1.0	0.15637	0.83975	0.12178	1.0000
Al	Al6	1.0	0.84281	0.16195	0.62136	1.0000
Al	Al7	1.0	0.77857	0.03505	0.81292	1.0000
Al	Al8	1.0	0.47658	0.97009	0.30279	1.0000

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Si	Si3	1.0	0.71033	0.53674	0.05402	1.0000
Si	Si4	1.0	0.96674	0.79010	0.04561	1.0000
Si	Si5	1.0	0.95363	0.53126	0.05398	1.0000
Si	Si6	1.0	0.64808	0.20473	0.54478	1.0000
Si	Si7	1.0	0.66293	0.45610	0.55945	1.0000
Si	Si8	1.0	0.27742	0.20554	0.55664	1.0000
Si	Si9	1.0	0.29086	0.46356	0.55443	1.0000
Si	Si10	1.0	0.03471	0.21105	0.54583	1.0000
Si	Si11	1.0	0.04816	0.46977	0.55332	1.0000
Si	Si12	1.0	0.21113	0.35461	0.30462	1.0000
Si	Si13	1.0	0.46029	0.34558	0.30705	1.0000
Si	Si14	1.0	0.22643	0.71914	0.31603	1.0000
Si	Si15	1.0	0.21648	0.95900	0.31260	1.0000
Si	Si16	1.0	0.15130	0.52630	0.38056	1.0000
Si	Si17	1.0	0.79386	0.65099	0.80389	1.0000
Si	Si18	1.0	0.54442	0.65058	0.80729	1.0000
Si	Si19	1.0	0.51486	0.27506	0.80341	1.0000
Si	Si20	1.0	0.51758	0.03954	0.80491	1.0000
Si	Si21	1.0	0.85126	0.48429	0.88108	1.0000
Si	Si22	1.0	0.65065	0.79422	0.94506	1.0000
Si	Si23	1.0	0.65242	0.54497	0.94390	1.0000
Si	Si24	1.0	0.28614	0.76952	0.93458	1.0000
Si	Si25	1.0	0.28079	0.51366	0.94890	1.0000
Si	Si26	1.0	0.04677	0.77169	0.93559	1.0000
Si	Si27	1.0	0.04402	0.51438	0.94636	1.0000
Si	Si28	1.0	0.47969	0.84832	0.87019	1.0000
Si	Si29	1.0	0.34961	0.20261	0.44546	1.0000
Si	Si30	1.0	0.34583	0.45579	0.44409	1.0000
Si	Si31	1.0	0.71703	0.23103	0.43540	1.0000
Si	Si32	1.0	0.72161	0.48644	0.44951	1.0000
Si	Si33	1.0	0.95669	0.22916	0.43546	1.0000
Si	Si34	1.0	0.95883	0.48676	0.44526	1.0000

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Si	Si35	1.0	0.52636	0.15097	0.37192	1.0000
Si	Si36	1.0	0.54034	0.33494	0.69155	1.0000
Si	Si37	1.0	0.79258	0.71623	0.69265	1.0000
Si	Si38	1.0	0.53490	0.71044	0.69714	1.0000
Si	Si39	1.0	0.53184	0.95624	0.69486	1.0000
Si	Si40	1.0	0.45930	0.66614	0.19023	1.0000
Si	Si41	1.0	0.20730	0.28557	0.19411	1.0000
Si	Si42	1.0	0.46530	0.28749	0.19636	1.0000
Si	Si43	1.0	0.46581	0.04099	0.19093	1.0000
Si	Si44	1.0	0.52882	0.47145	0.12602	1.0000
Si	Si45	1.0	0.47075	0.52889	0.62666	1.0000
Si	Si46	1.0	0.15353	0.15604	0.37346	1.0000
Si	Si47	1.0	0.53509	0.52997	0.37596	1.0000
Si	Si48	1.0	0.46829	0.46462	0.87603	1.0000
Si	Si49	1.0	0.79282	0.34496	0.70453	1.0000
Si	Si50	1.0	0.35033	0.79606	0.04466	1.0000
Si	Si51	1.0	0.20689	0.65675	0.20526	1.0000
Si	Si52	1.0	0.84910	0.84344	0.87519	1.0000
Si	Si53	1.0	0.21002	0.04174	0.20290	1.0000
Si	Si54	1.0	0.78872	0.96053	0.70222	1.0000
Si	Si55	1.0	0.76952	0.29450	0.81619	1.0000
Si	Si56	1.0	0.48133	0.71529	0.30257	1.0000

AlSiAl-T1T7T7T7T9T9T9

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H	H3	1.0	0.52669	0.85550	0.03146	1.0000
H	H4	1.0	0.14287	0.47965	0.21532	1.0000
H	H5	1.0	0.08228	0.00640	0.14142	1.0000
H	H6	1.0	0.90943	0.98806	0.63816	1.0000
H	H7	1.0	0.87197	0.17618	0.86012	1.0000
H	H8	1.0	0.09283	0.98271	0.36746	1.0000

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O	O1	1.0	0.37384	0.66939	0.04884	1.0000
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O	O3	1.0	0.26910	0.84126	0.08483	1.0000
O	O4	1.0	0.31589	0.48372	0.00554	1.0000
O	O5	1.0	0.23253	0.54105	0.09347	1.0000
O	O6	1.0	0.43724	0.48486	0.08445	1.0000
O	O7	1.0	0.71611	0.66399	0.05827	1.0000
O	O8	1.0	0.84574	0.83395	0.04780	1.0000
O	O9	1.0	0.66879	0.84507	0.10386	1.0000
O	O10	1.0	0.82919	0.48873	0.05237	1.0000
O	O11	1.0	0.64635	0.48289	0.10063	1.0000
O	O12	1.0	0.96156	0.65932	0.05179	1.0000
O	O13	1.0	0.03760	0.84249	0.09021	1.0000
O	O14	1.0	0.00930	0.48345	0.10255	1.0000
O	O15	1.0	0.62573	0.33118	0.54974	1.0000
O	O16	1.0	0.66085	0.17287	0.48582	1.0000
O	O17	1.0	0.73447	0.15930	0.58146	1.0000
O	O18	1.0	0.52945	0.14088	0.55987	1.0000
O	O19	1.0	0.68811	0.51414	0.50559	1.0000
O	O20	1.0	0.76488	0.46091	0.59547	1.0000
O	O21	1.0	0.56166	0.51773	0.58271	1.0000
O	O22	1.0	0.28534	0.33786	0.55850	1.0000
O	O23	1.0	0.15861	0.16513	0.54818	1.0000
O	O24	1.0	0.33350	0.15827	0.60564	1.0000
O	O25	1.0	0.17019	0.51156	0.55208	1.0000
O	O26	1.0	0.35307	0.52001	0.60022	1.0000
O	O27	1.0	0.04160	0.33798	0.55082	1.0000
O	O28	1.0	0.96566	0.15617	0.59037	1.0000
O	O29	1.0	0.99011	0.51140	0.60255	1.0000
O	O30	1.0	0.33649	0.39394	0.30620	1.0000
O	O31	1.0	0.17425	0.35825	0.24131	1.0000
O	O32	1.0	0.19540	0.23213	0.32036	1.0000
O	O33	1.0	0.13928	0.43938	0.33045	1.0000
O	O34	1.0	0.50266	0.34914	0.24842	1.0000

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O	O35	1.0	0.46284	0.23543	0.33121	1.0000
O	O36	1.0	0.53545	0.43604	0.33734	1.0000
O	O37	1.0	0.35190	0.71530	0.30901	1.0000
O	O38	1.0	0.18025	0.82910	0.32318	1.0000
O	O39	1.0	0.19322	0.63588	0.36284	1.0000
O	O40	1.0	0.51635	0.84432	0.31749	1.0000
O	O41	1.0	0.53770	0.64722	0.34330	1.0000
O	O42	1.0	0.34484	0.97273	0.31776	1.0000
O	O43	1.0	0.53729	0.04291	0.34170	1.0000
O	O44	1.0	0.66941	0.61462	0.81040	1.0000
O	O45	1.0	0.82899	0.65017	0.74433	1.0000
O	O46	1.0	0.81481	0.77037	0.82697	1.0000
O	O47	1.0	0.86653	0.56301	0.83183	1.0000
O	O48	1.0	0.50492	0.64832	0.74920	1.0000
O	O49	1.0	0.53736	0.77102	0.83002	1.0000
O	O50	1.0	0.46969	0.56938	0.83915	1.0000
O	O51	1.0	0.64536	0.27552	0.80915	1.0000
O	O52	1.0	0.80046	0.36993	0.86226	1.0000
O	O53	1.0	0.47050	0.15787	0.81592	1.0000
O	O54	1.0	0.46580	0.35665	0.84337	1.0000
O	O55	1.0	0.64326	0.03348	0.81658	1.0000
O	O56	1.0	0.45296	0.96056	0.84355	1.0000
O	O57	1.0	0.61640	0.66877	0.93955	1.0000
O	O58	1.0	0.65115	0.82862	0.00531	1.0000
O	O59	1.0	0.76983	0.81523	0.92285	1.0000
O	O60	1.0	0.56119	0.86612	0.91832	1.0000
O	O61	1.0	0.64846	0.50354	0.00137	1.0000
O	O62	1.0	0.77552	0.53833	0.92226	1.0000
O	O63	1.0	0.57535	0.46843	0.91047	1.0000
O	O64	1.0	0.28420	0.64343	0.94372	1.0000
O	O65	1.0	0.16857	0.81098	0.92149	1.0000
O	O66	1.0	0.36727	0.79799	0.88943	1.0000
O	O67	1.0	0.16270	0.46990	0.93514	1.0000
O	O68	1.0	0.36214	0.46166	0.90926	1.0000

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O	O69	1.0	0.03889	0.64272	0.93699	1.0000
O	O70	1.0	0.96980	0.81617	0.89265	1.0000
O	O71	1.0	0.96613	0.45676	0.90449	1.0000
O	O72	1.0	0.38610	0.33335	0.44035	1.0000
O	O73	1.0	0.35537	0.17379	0.50723	1.0000
O	O74	1.0	0.23787	0.17894	0.42420	1.0000
O	O75	1.0	0.44596	0.13779	0.42008	1.0000
O	O76	1.0	0.35117	0.49917	0.50101	1.0000
O	O77	1.0	0.22791	0.46418	0.42069	1.0000
O	O78	1.0	0.42775	0.53260	0.41003	1.0000
O	O79	1.0	0.71014	0.35603	0.44120	1.0000
O	O80	1.0	0.82861	0.18502	0.42531	1.0000
O	O81	1.0	0.63818	0.19815	0.38619	1.0000
O	O82	1.0	0.83892	0.52454	0.43424	1.0000
O	O83	1.0	0.64021	0.54241	0.40963	1.0000
O	O84	1.0	0.96218	0.35081	0.43736	1.0000
O	O85	1.0	0.02216	0.17175	0.39159	1.0000
O	O86	1.0	0.03398	0.53643	0.40405	1.0000
O	O87	1.0	0.66733	0.36993	0.70104	1.0000
O	O88	1.0	0.82652	0.32954	0.76328	1.0000
O	O89	1.0	0.83417	0.25257	0.66905	1.0000
O	O90	1.0	0.48690	0.31415	0.74662	1.0000
O	O91	1.0	0.53210	0.23293	0.65630	1.0000
O	O92	1.0	0.48253	0.43925	0.66875	1.0000
O	O93	1.0	0.66447	0.71150	0.69074	1.0000
O	O94	1.0	0.83382	0.84130	0.69730	1.0000
O	O95	1.0	0.84542	0.65983	0.64525	1.0000
O	O96	1.0	0.49485	0.83042	0.69845	1.0000
O	O97	1.0	0.47962	0.64741	0.65038	1.0000
O	O98	1.0	0.66230	0.96575	0.69101	1.0000
O	O99	1.0	0.48022	0.00882	0.64640	1.0000
O	O100	1.0	0.33272	0.63102	0.19966	1.0000
O	O101	1.0	0.17202	0.66086	0.26331	1.0000
O	O102	1.0	0.16396	0.74673	0.17098	1.0000

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O	O103	1.0	0.51224	0.69123	0.24636	1.0000
O	O104	1.0	0.47194	0.76226	0.15392	1.0000
O	O105	1.0	0.51812	0.55717	0.17144	1.0000
O	O106	1.0	0.33866	0.28459	0.19170	1.0000
O	O107	1.0	0.16449	0.16171	0.19834	1.0000
O	O108	1.0	0.16194	0.33840	0.14237	1.0000
O	O109	1.0	0.50719	0.16684	0.19758	1.0000
O	O110	1.0	0.52108	0.35056	0.14921	1.0000
O	O111	1.0	0.33492	0.03635	0.18689	1.0000
O	O112	1.0	0.51945	0.98756	0.14624	1.0000
O	O113	1.0	0.01730	0.81976	0.99110	1.0000
O	O114	1.0	0.00960	0.48310	0.00243	1.0000
O	O115	1.0	0.98659	0.17473	0.49125	1.0000
O	O116	1.0	0.98980	0.51296	0.50220	1.0000
O	O117	1.0	0.18175	0.98378	0.25336	1.0000
O	O118	1.0	0.49288	0.98468	0.24610	1.0000
O	O119	1.0	0.82523	0.02124	0.75187	1.0000
O	O120	1.0	0.49194	0.01217	0.74658	1.0000
O	O121	1.0	0.85978	0.46110	0.68985	1.0000
O	O122	1.0	0.47076	0.85867	0.05838	1.0000
O	O123	1.0	0.14146	0.53577	0.18830	1.0000
O	O124	1.0	0.84365	0.96757	0.85968	1.0000
O	O125	1.0	0.14545	0.97210	0.15479	1.0000
O	O126	1.0	0.84862	0.02614	0.65168	1.0000
O	O127	1.0	0.82174	0.17455	0.83209	1.0000
O	O128	1.0	0.15243	0.02214	0.35191	1.0000
Al	Al1	1.0	0.46323	0.13471	0.62318	1.0000
Al	Al2	1.0	0.86576	0.52964	0.62623	1.0000
Al	Al3	1.0	0.53821	0.86295	0.12168	1.0000
Al	Al4	1.0	0.13524	0.46873	0.12510	1.0000
Al	Al5	1.0	0.15655	0.83581	0.12182	1.0000
Al	Al6	1.0	0.84438	0.16183	0.62025	1.0000
Al	Al7	1.0	0.77872	0.03512	0.81285	1.0000
Al	Al8	1.0	0.15292	0.16660	0.37414	1.0000

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Si	Si1	1.0	0.33747	0.54464	0.05913	1.0000
Si	Si2	1.0	0.72341	0.79330	0.05569	1.0000
Si	Si3	1.0	0.71054	0.53519	0.05365	1.0000
Si	Si4	1.0	0.96660	0.78835	0.04615	1.0000
Si	Si5	1.0	0.95341	0.52944	0.05345	1.0000
Si	Si6	1.0	0.64606	0.20423	0.54496	1.0000
Si	Si7	1.0	0.66263	0.45591	0.55943	1.0000
Si	Si8	1.0	0.27992	0.20833	0.55688	1.0000
Si	Si9	1.0	0.28940	0.46654	0.55334	1.0000
Si	Si10	1.0	0.03688	0.20870	0.54596	1.0000
Si	Si11	1.0	0.04689	0.46768	0.55309	1.0000
Si	Si12	1.0	0.21202	0.35271	0.30120	1.0000
Si	Si13	1.0	0.45957	0.35361	0.30608	1.0000
Si	Si14	1.0	0.22489	0.70776	0.31481	1.0000
Si	Si15	1.0	0.48047	0.72274	0.30339	1.0000
Si	Si16	1.0	0.47335	0.96176	0.30514	1.0000
Si	Si17	1.0	0.14938	0.51774	0.37967	1.0000
Si	Si18	1.0	0.79424	0.65202	0.80397	1.0000
Si	Si19	1.0	0.54485	0.65111	0.80710	1.0000
Si	Si20	1.0	0.51543	0.27628	0.80298	1.0000
Si	Si21	1.0	0.51818	0.03987	0.80506	1.0000
Si	Si22	1.0	0.85204	0.48436	0.88047	1.0000
Si	Si23	1.0	0.65145	0.79491	0.94538	1.0000
Si	Si24	1.0	0.65364	0.54491	0.94364	1.0000
Si	Si25	1.0	0.28699	0.77088	0.93534	1.0000
Si	Si26	1.0	0.28174	0.51480	0.94869	1.0000
Si	Si27	1.0	0.04760	0.77230	0.93614	1.0000
Si	Si28	1.0	0.04464	0.51485	0.94570	1.0000
Si	Si29	1.0	0.47972	0.84908	0.87043	1.0000
Si	Si30	1.0	0.35263	0.20654	0.44703	1.0000
Si	Si31	1.0	0.34835	0.45699	0.44335	1.0000
Si	Si32	1.0	0.71034	0.22810	0.43499	1.0000
Si	Si33	1.0	0.71904	0.48406	0.44820	1.0000
Si	Si34	1.0	0.95214	0.22061	0.43641	1.0000

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Si	Si35	1.0	0.95640	0.47883	0.44548	1.0000
Si	Si36	1.0	0.52077	0.15547	0.37046	1.0000
Si	Si37	1.0	0.54130	0.33602	0.69148	1.0000
Si	Si38	1.0	0.79308	0.71651	0.69252	1.0000
Si	Si39	1.0	0.53583	0.70977	0.69673	1.0000
Si	Si40	1.0	0.53122	0.95567	0.69479	1.0000
Si	Si41	1.0	0.45926	0.66329	0.19153	1.0000
Si	Si42	1.0	0.21007	0.28594	0.19164	1.0000
Si	Si43	1.0	0.46770	0.28861	0.19651	1.0000
Si	Si44	1.0	0.46609	0.04354	0.19311	1.0000
Si	Si45	1.0	0.52958	0.47082	0.12625	1.0000
Si	Si46	1.0	0.47039	0.52928	0.62534	1.0000
Si	Si47	1.0	0.53468	0.53803	0.37549	1.0000
Si	Si48	1.0	0.46863	0.46524	0.87564	1.0000
Si	Si49	1.0	0.79263	0.34512	0.70386	1.0000
Si	Si50	1.0	0.35217	0.79611	0.04539	1.0000
Si	Si51	1.0	0.20650	0.65138	0.20418	1.0000
Si	Si52	1.0	0.84977	0.84457	0.87575	1.0000
Si	Si53	1.0	0.21181	0.04329	0.20055	1.0000
Si	Si54	1.0	0.78770	0.96124	0.70170	1.0000
Si	Si55	1.0	0.77003	0.29435	0.81545	1.0000
Si	Si56	1.0	0.22029	0.94873	0.30920	1.0000

AlSiAl-T2T7T7T7T9T9T9

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H H3 1.0 0.52452 0.85384 0.02848 1.0000
H H4 1.0 0.14414 0.48167 0.21563 1.0000
H H5 1.0 0.08039 0.01013 0.13961 1.0000
H H6 1.0 0.91629 0.99295 0.64420 1.0000
H H7 1.0 0.57565 0.83939 0.34803 1.0000
H H8 1.0 0.07507 0.98914 0.36094 1.0000

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O	O1	1.0	0.37194	0.67127	0.04734	1.0000
O	O2	1.0	0.32400	0.83068	0.98494	1.0000
O	O3	1.0	0.26760	0.84340	0.08296	1.0000
O	O4	1.0	0.31516	0.48504	0.00606	1.0000
O	O5	1.0	0.23232	0.54393	0.09368	1.0000
O	O6	1.0	0.43680	0.48754	0.08510	1.0000
O	O7	1.0	0.71505	0.66244	0.05942	1.0000
O	O8	1.0	0.84335	0.83362	0.04684	1.0000
O	O9	1.0	0.66582	0.84647	0.10178	1.0000
O	O10	1.0	0.82906	0.48811	0.05342	1.0000
O	O11	1.0	0.64569	0.48065	0.10146	1.0000
O	O12	1.0	0.95987	0.66005	0.05186	1.0000
O	O13	1.0	0.03631	0.84374	0.08866	1.0000
O	O14	1.0	0.00948	0.48450	0.10323	1.0000
O	O15	1.0	0.62761	0.33347	0.55053	1.0000
O	O16	1.0	0.66582	0.17341	0.48848	1.0000
O	O17	1.0	0.73168	0.15890	0.58503	1.0000
O	O18	1.0	0.52865	0.14462	0.56090	1.0000
O	O19	1.0	0.68677	0.51868	0.50554	1.0000
O	O20	1.0	0.76568	0.46404	0.59513	1.0000
O	O21	1.0	0.56192	0.51998	0.58279	1.0000
O	O22	1.0	0.28505	0.33771	0.56096	1.0000
O	O23	1.0	0.15659	0.16665	0.55113	1.0000
O	O24	1.0	0.33241	0.15698	0.60793	1.0000
O	O25	1.0	0.17058	0.51204	0.55285	1.0000
O	O26	1.0	0.35367	0.52171	0.60026	1.0000
O	O27	1.0	0.03951	0.34029	0.55310	1.0000
O	O28	1.0	0.96317	0.15655	0.59184	1.0000
O	O29	1.0	0.98961	0.51666	0.60197	1.0000
O	O30	1.0	0.33771	0.39150	0.30684	1.0000
O	O31	1.0	0.17388	0.35937	0.24204	1.0000
O	O32	1.0	0.19425	0.23343	0.32192	1.0000
O	O33	1.0	0.14131	0.44187	0.33054	1.0000
O	O34	1.0	0.50380	0.34109	0.25056	1.0000

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O	O35	1.0	0.46065	0.22873	0.33446	1.0000
O	O36	1.0	0.53586	0.42838	0.33884	1.0000
O	O37	1.0	0.35187	0.72771	0.30802	1.0000
O	O38	1.0	0.17440	0.83023	0.32289	1.0000
O	O39	1.0	0.19903	0.63645	0.36218	1.0000
O	O40	1.0	0.53289	0.63942	0.34236	1.0000
O	O41	1.0	0.33596	0.97783	0.31870	1.0000
O	O42	1.0	0.54551	0.03909	0.34784	1.0000
O	O43	1.0	0.66659	0.61204	0.81052	1.0000
O	O44	1.0	0.82730	0.64448	0.74463	1.0000
O	O45	1.0	0.81468	0.76350	0.82614	1.0000
O	O46	1.0	0.86249	0.55438	0.83214	1.0000
O	O47	1.0	0.50297	0.64515	0.74895	1.0000
O	O48	1.0	0.53318	0.76819	0.82896	1.0000
O	O49	1.0	0.46802	0.56632	0.83980	1.0000
O	O50	1.0	0.64621	0.28624	0.81045	1.0000
O	O51	1.0	0.81371	0.16336	0.82649	1.0000
O	O52	1.0	0.80715	0.35707	0.86367	1.0000
O	O53	1.0	0.47997	0.15762	0.81667	1.0000
O	O54	1.0	0.46084	0.35371	0.84433	1.0000
O	O55	1.0	0.64973	0.02694	0.81472	1.0000
O	O56	1.0	0.45850	0.96059	0.84307	1.0000
O	O57	1.0	0.61941	0.66305	0.93786	1.0000
O	O58	1.0	0.64967	0.82355	0.00378	1.0000
O	O59	1.0	0.76545	0.81641	0.92050	1.0000
O	O60	1.0	0.55592	0.85872	0.91812	1.0000
O	O61	1.0	0.64798	0.50159	0.00241	1.0000
O	O62	1.0	0.77402	0.52656	0.92231	1.0000
O	O63	1.0	0.57204	0.46302	0.91194	1.0000
O	O64	1.0	0.28477	0.64438	0.94234	1.0000
O	O65	1.0	0.16399	0.81020	0.91961	1.0000
O	O66	1.0	0.36106	0.80107	0.88678	1.0000
O	O67	1.0	0.16125	0.47327	0.93613	1.0000
O	O68	1.0	0.35961	0.45979	0.91017	1.0000

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O	O69	1.0	0.03231	0.64372	0.93530	1.0000
O	O70	1.0	0.96577	0.82221	0.89159	1.0000
O	O71	1.0	0.96723	0.45433	0.90521	1.0000
O	O72	1.0	0.38075	0.32940	0.44108	1.0000
O	O73	1.0	0.35237	0.17270	0.50953	1.0000
O	O74	1.0	0.24063	0.16820	0.42431	1.0000
O	O75	1.0	0.45116	0.13612	0.42508	1.0000
O	O76	1.0	0.35086	0.49654	0.50154	1.0000
O	O77	1.0	0.22644	0.46504	0.42160	1.0000
O	O78	1.0	0.42822	0.52756	0.41096	1.0000
O	O79	1.0	0.71603	0.35800	0.44486	1.0000
O	O80	1.0	0.83036	0.18668	0.42625	1.0000
O	O81	1.0	0.63792	0.20518	0.38927	1.0000
O	O82	1.0	0.83988	0.52949	0.43472	1.0000
O	O83	1.0	0.64108	0.54056	0.40877	1.0000
O	O84	1.0	0.96212	0.35450	0.43709	1.0000
O	O85	1.0	0.02368	0.17475	0.39347	1.0000
O	O86	1.0	0.03470	0.54048	0.40300	1.0000
O	O87	1.0	0.66779	0.37016	0.70099	1.0000
O	O88	1.0	0.82723	0.33148	0.76452	1.0000
O	O89	1.0	0.83447	0.25268	0.67105	1.0000
O	O90	1.0	0.48684	0.31546	0.74740	1.0000
O	O91	1.0	0.53102	0.23370	0.65768	1.0000
O	O92	1.0	0.48314	0.44068	0.66903	1.0000
O	O93	1.0	0.66377	0.71263	0.69170	1.0000
O	O94	1.0	0.83495	0.83875	0.70030	1.0000
O	O95	1.0	0.84398	0.66145	0.64561	1.0000
O	O96	1.0	0.49472	0.83050	0.69976	1.0000
O	O97	1.0	0.48016	0.64947	0.64997	1.0000
O	O98	1.0	0.66395	0.96427	0.69168	1.0000
O	O99	1.0	0.48327	0.00887	0.64615	1.0000
O	O100	1.0	0.33329	0.63376	0.19921	1.0000
O	O101	1.0	0.17463	0.66291	0.26284	1.0000
O	O102	1.0	0.16398	0.74972	0.17003	1.0000

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O	O103	1.0	0.51176	0.69424	0.24513	1.0000
O	O104	1.0	0.47140	0.76546	0.15221	1.0000
O	O105	1.0	0.51901	0.55993	0.17122	1.0000
O	O106	1.0	0.33793	0.28404	0.19446	1.0000
O	O107	1.0	0.16254	0.16277	0.19868	1.0000
O	O108	1.0	0.16390	0.34082	0.14317	1.0000
O	O109	1.0	0.50559	0.16374	0.19652	1.0000
O	O110	1.0	0.51833	0.35236	0.15130	1.0000
O	O111	1.0	0.33190	0.03677	0.18601	1.0000
O	O112	1.0	0.51193	0.99207	0.14029	1.0000
O	O113	1.0	0.01413	0.82005	0.98979	1.0000
O	O114	1.0	0.00873	0.48521	0.00301	1.0000
O	O115	1.0	0.98672	0.17930	0.49293	1.0000
O	O116	1.0	0.99279	0.51517	0.50154	1.0000
O	O117	1.0	0.17550	0.98122	0.25157	1.0000
O	O118	1.0	0.49447	0.97442	0.24090	1.0000
O	O119	1.0	0.82048	0.01476	0.75600	1.0000
O	O120	1.0	0.49634	0.01393	0.74629	1.0000
O	O121	1.0	0.86025	0.46119	0.68979	1.0000
O	O122	1.0	0.46850	0.85959	0.05507	1.0000
O	O123	1.0	0.14225	0.53827	0.18848	1.0000
O	O124	1.0	0.83331	0.96355	0.85372	1.0000
O	O125	1.0	0.14349	0.97508	0.15280	1.0000
O	O126	1.0	0.85241	0.02755	0.65653	1.0000
O	O127	1.0	0.52609	0.83773	0.31980	1.0000
O	O128	1.0	0.14136	0.02356	0.34958	1.0000
Al	Al1	1.0	0.46335	0.13629	0.62426	1.0000
Al	Al2	1.0	0.86570	0.53143	0.62656	1.0000
Al	Al3	1.0	0.53514	0.86672	0.11847	1.0000
Al	Al4	1.0	0.13566	0.47087	0.12553	1.0000
Al	Al5	1.0	0.15545	0.83926	0.12034	1.0000
Al	Al6	1.0	0.84324	0.16309	0.62257	1.0000
Al	Al7	1.0	0.47073	0.97174	0.30409	1.0000
Al	Al8	1.0	0.15314	0.16381	0.37498	1.0000

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Si	Si1	1.0	0.33674	0.54656	0.05912	1.0000
Si	Si2	1.0	0.72159	0.79178	0.05498	1.0000
Si	Si3	1.0	0.71006	0.53354	0.05445	1.0000
Si	Si4	1.0	0.96465	0.78906	0.04530	1.0000
Si	Si5	1.0	0.95269	0.53002	0.05398	1.0000
Si	Si6	1.0	0.64659	0.20590	0.54692	1.0000
Si	Si7	1.0	0.66300	0.45870	0.55958	1.0000
Si	Si8	1.0	0.27833	0.20805	0.55918	1.0000
Si	Si9	1.0	0.28942	0.46631	0.55435	1.0000
Si	Si10	1.0	0.03526	0.21099	0.54798	1.0000
Si	Si11	1.0	0.04691	0.47019	0.55350	1.0000
Si	Si12	1.0	0.21234	0.35325	0.30186	1.0000
Si	Si13	1.0	0.45912	0.34609	0.30783	1.0000
Si	Si14	1.0	0.22392	0.71217	0.31421	1.0000
Si	Si15	1.0	0.15059	0.51969	0.37942	1.0000
Si	Si16	1.0	0.79209	0.64458	0.80427	1.0000
Si	Si17	1.0	0.54219	0.64775	0.80704	1.0000
Si	Si18	1.0	0.77342	0.28431	0.81625	1.0000
Si	Si19	1.0	0.51829	0.27923	0.80395	1.0000
Si	Si20	1.0	0.52237	0.03971	0.80453	1.0000
Si	Si21	1.0	0.85174	0.47317	0.88082	1.0000
Si	Si22	1.0	0.64923	0.78957	0.94432	1.0000
Si	Si23	1.0	0.65349	0.53793	0.94376	1.0000
Si	Si24	1.0	0.28302	0.77185	0.93351	1.0000
Si	Si25	1.0	0.28058	0.51568	0.94903	1.0000
Si	Si26	1.0	0.04311	0.77332	0.93483	1.0000
Si	Si27	1.0	0.04227	0.51583	0.94583	1.0000
Si	Si28	1.0	0.47680	0.84588	0.86946	1.0000
Si	Si29	1.0	0.35225	0.20134	0.44863	1.0000
Si	Si30	1.0	0.34630	0.45363	0.44427	1.0000
Si	Si31	1.0	0.71285	0.23027	0.43726	1.0000
Si	Si32	1.0	0.72100	0.48637	0.44902	1.0000
Si	Si33	1.0	0.95315	0.22402	0.43749	1.0000
Si	Si34	1.0	0.95780	0.48256	0.44505	1.0000

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Si	Si35	1.0	0.52415	0.15127	0.37430	1.0000
Si	Si36	1.0	0.54179	0.33698	0.69234	1.0000
Si	Si37	1.0	0.79218	0.71440	0.69362	1.0000
Si	Si38	1.0	0.53506	0.70918	0.69709	1.0000
Si	Si39	1.0	0.53268	0.95502	0.69485	1.0000
Si	Si40	1.0	0.45894	0.66611	0.18971	1.0000
Si	Si41	1.0	0.20979	0.28642	0.19277	1.0000
Si	Si42	1.0	0.46687	0.28545	0.19786	1.0000
Si	Si43	1.0	0.46426	0.04001	0.19063	1.0000
Si	Si44	1.0	0.52879	0.47150	0.12696	1.0000
Si	Si45	1.0	0.47081	0.53101	0.62540	1.0000
Si	Si46	1.0	0.53393	0.53005	0.37610	1.0000
Si	Si47	1.0	0.46603	0.46158	0.87671	1.0000
Si	Si48	1.0	0.79319	0.34559	0.70561	1.0000
Si	Si49	1.0	0.34941	0.79804	0.04321	1.0000
Si	Si50	1.0	0.20690	0.65410	0.20345	1.0000
Si	Si51	1.0	0.77808	0.04186	0.81293	1.0000
Si	Si52	1.0	0.84507	0.84115	0.87329	1.0000
Si	Si53	1.0	0.20929	0.04339	0.19969	1.0000
Si	Si54	1.0	0.78782	0.95774	0.70377	1.0000
Si	Si55	1.0	0.47811	0.71590	0.30209	1.0000
Si	Si56	1.0	0.21444	0.95113	0.30849	1.0000

RAI-T1-T1T2T9T3

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H H4 1.0 0.70117 0.99681 0.66242 1.0000
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O O2 1.0 0.35230 0.82114 0.00310 1.0000
O O3 1.0 0.22842 0.84708 0.08241 1.0000
O O4 1.0 0.43754 0.81083 0.09250 1.0000

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O	O5	1.0	0.34126	0.50393	0.99364	1.0000
O	O6	1.0	0.23575	0.45934	0.07720	1.0000
O	O7	1.0	0.44437	0.50037	0.07999	1.0000
O	O8	1.0	0.70334	0.66813	0.06733	1.0000
O	O9	1.0	0.83177	0.83776	0.06260	1.0000
O	O10	1.0	0.64213	0.85771	0.10165	1.0000
O	O11	1.0	0.83414	0.49980	0.06036	1.0000
O	O12	1.0	0.64818	0.47949	0.10200	1.0000
O	O13	1.0	0.96151	0.66923	0.05544	1.0000
O	O14	1.0	0.02106	0.84410	0.10414	1.0000
O	O15	1.0	0.02849	0.48766	0.09443	1.0000
O	O16	1.0	0.62951	0.33633	0.56073	1.0000
O	O17	1.0	0.65552	0.17653	0.49419	1.0000
O	O18	1.0	0.77997	0.19116	0.57435	1.0000
O	O19	1.0	0.57495	0.13775	0.58398	1.0000
O	O20	1.0	0.66314	0.49165	0.49450	1.0000
O	O21	1.0	0.77256	0.49107	0.57989	1.0000
O	O22	1.0	0.56412	0.53373	0.57821	1.0000
O	O23	1.0	0.30580	0.32656	0.56214	1.0000
O	O24	1.0	0.16905	0.16147	0.55819	1.0000
O	O25	1.0	0.36183	0.13365	0.59096	1.0000
O	O26	1.0	0.16936	0.48720	0.56579	1.0000
O	O27	1.0	0.36141	0.50900	0.60532	1.0000
O	O28	1.0	0.03080	0.32258	0.55971	1.0000
O	O29	1.0	0.97762	0.13097	0.59468	1.0000
O	O30	1.0	0.97789	0.50753	0.60172	1.0000
O	O31	1.0	0.33784	0.31636	0.31573	1.0000
O	O32	1.0	0.18475	0.34970	0.24738	1.0000
O	O33	1.0	0.14980	0.22049	0.32371	1.0000
O	O34	1.0	0.16674	0.43021	0.33868	1.0000
O	O35	1.0	0.48109	0.34665	0.24288	1.0000
O	O36	1.0	0.52936	0.23221	0.32310	1.0000
O	O37	1.0	0.50726	0.44445	0.32942	1.0000
O	O38	1.0	0.32738	0.70250	0.31847	1.0000

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O	O39	1.0	0.15638	0.82537	0.30498	1.0000
O	O40	1.0	0.13582	0.63886	0.34644	1.0000
O	O41	1.0	0.49322	0.83524	0.31307	1.0000
O	O42	1.0	0.51224	0.64846	0.35723	1.0000
O	O43	1.0	0.32197	0.95981	0.30601	1.0000
O	O44	1.0	0.13757	0.01456	0.34727	1.0000
O	O45	1.0	0.49732	0.02980	0.35064	1.0000
O	O46	1.0	0.67219	0.70072	0.81761	1.0000
O	O47	1.0	0.82320	0.67338	0.74731	1.0000
O	O48	1.0	0.86874	0.76710	0.83473	1.0000
O	O49	1.0	0.82670	0.55778	0.82814	1.0000
O	O50	1.0	0.52340	0.66861	0.74766	1.0000
O	O51	1.0	0.47982	0.77946	0.83113	1.0000
O	O52	1.0	0.50607	0.56964	0.83333	1.0000
O	O53	1.0	0.66879	0.31732	0.81429	1.0000
O	O54	1.0	0.81729	0.16252	0.81818	1.0000
O	O55	1.0	0.85985	0.35697	0.85055	1.0000
O	O56	1.0	0.51365	0.17172	0.81351	1.0000
O	O57	1.0	0.47234	0.36294	0.84408	1.0000
O	O58	1.0	0.66172	0.01773	0.81589	1.0000
O	O59	1.0	0.84974	0.97482	0.85664	1.0000
O	O60	1.0	0.47120	0.98690	0.85275	1.0000
O	O61	1.0	0.65233	0.66382	0.93546	1.0000
O	O62	1.0	0.66026	0.82348	0.00311	1.0000
O	O63	1.0	0.78360	0.82785	0.92255	1.0000
O	O64	1.0	0.57329	0.85495	0.91473	1.0000
O	O65	1.0	0.66040	0.50834	0.00333	1.0000
O	O66	1.0	0.76995	0.48948	0.91885	1.0000
O	O67	1.0	0.55763	0.47676	0.91916	1.0000
O	O68	1.0	0.29311	0.67149	0.93726	1.0000
O	O69	1.0	0.17478	0.84549	0.94879	1.0000
O	O70	1.0	0.36117	0.85802	0.90566	1.0000
O	O71	1.0	0.16454	0.50255	0.93695	1.0000
O	O72	1.0	0.35302	0.49293	0.89396	1.0000

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O	O73	1.0	0.04343	0.67671	0.94550	1.0000
O	O74	1.0	0.98842	0.86092	0.90478	1.0000
O	O75	1.0	0.97438	0.50490	0.89593	1.0000
O	O76	1.0	0.30434	0.34242	0.43807	1.0000
O	O77	1.0	0.33496	0.17123	0.49513	1.0000
O	O78	1.0	0.23283	0.15201	0.40944	1.0000
O	O79	1.0	0.44295	0.19172	0.41173	1.0000
O	O80	1.0	0.33856	0.49802	0.50571	1.0000
O	O81	1.0	0.24096	0.53787	0.41867	1.0000
O	O82	1.0	0.44909	0.49751	0.42223	1.0000
O	O83	1.0	0.70909	0.33163	0.43143	1.0000
O	O84	1.0	0.83244	0.16030	0.43871	1.0000
O	O85	1.0	0.64488	0.14344	0.39566	1.0000
O	O86	1.0	0.83877	0.50071	0.44005	1.0000
O	O87	1.0	0.65107	0.51861	0.39602	1.0000
O	O88	1.0	0.96362	0.32941	0.44220	1.0000
O	O89	1.0	0.02144	0.15090	0.39660	1.0000
O	O90	1.0	0.03125	0.51250	0.40464	1.0000
O	O91	1.0	0.67183	0.30411	0.68431	1.0000
O	O92	1.0	0.83239	0.31843	0.75189	1.0000
O	O93	1.0	0.85367	0.20592	0.66786	1.0000
O	O94	1.0	0.84554	0.42113	0.66743	1.0000
O	O95	1.0	0.51032	0.33089	0.74768	1.0000
O	O96	1.0	0.47640	0.24370	0.65790	1.0000
O	O97	1.0	0.52125	0.44985	0.66720	1.0000
O	O98	1.0	0.67296	0.72357	0.68099	1.0000
O	O99	1.0	0.86163	0.83050	0.68224	1.0000
O	O100	1.0	0.84626	0.63040	0.64950	1.0000
O	O101	1.0	0.50158	0.84198	0.69104	1.0000
O	O102	1.0	0.48131	0.65274	0.65074	1.0000
O	O103	1.0	0.66202	0.99135	0.69489	1.0000
O	O104	1.0	0.80950	0.01363	0.62500	1.0000
O	O105	1.0	0.47173	0.02996	0.65440	1.0000
O	O106	1.0	0.34437	0.67840	0.18565	1.0000

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O	O107	1.0	0.18272	0.64867	0.24940	1.0000
O	O108	1.0	0.16234	0.77729	0.17170	1.0000
O	O109	1.0	0.17235	0.56568	0.15874	1.0000
O	O110	1.0	0.48997	0.65488	0.25817	1.0000
O	O111	1.0	0.53560	0.76816	0.17764	1.0000
O	O112	1.0	0.51447	0.55576	0.17140	1.0000
O	O113	1.0	0.32679	0.29335	0.17810	1.0000
O	O114	1.0	0.15677	0.17044	0.19310	1.0000
O	O115	1.0	0.13484	0.35728	0.15059	1.0000
O	O116	1.0	0.49546	0.16599	0.18931	1.0000
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O	O118	1.0	0.32507	0.03958	0.19392	1.0000
O	O119	1.0	0.14533	0.98278	0.14855	1.0000
O	O120	1.0	0.50406	0.97111	0.15220	1.0000
O	O121	1.0	0.00114	0.84495	0.00415	1.0000
O	O122	1.0	0.99473	0.50124	0.99576	1.0000
O	O123	1.0	0.00460	0.15751	0.49624	1.0000
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O	O125	1.0	0.15327	0.99671	0.24818	1.0000
O	O126	1.0	0.49369	0.00057	0.25126	1.0000
O	O127	1.0	0.82704	0.98700	0.75669	1.0000
O	O128	1.0	0.49506	0.00500	0.75363	1.0000
Si	Si1	1.0	0.33125	0.78397	0.06056	1.0000
Si	Si2	1.0	0.33228	0.52992	0.05351	1.0000
Si	Si3	1.0	0.70935	0.79630	0.05828	1.0000
Si	Si4	1.0	0.71181	0.53991	0.05775	1.0000
Si	Si5	1.0	0.95383	0.79855	0.05638	1.0000
Si	Si6	1.0	0.95532	0.54000	0.05127	1.0000
Si	Si7	1.0	0.52954	0.85202	0.13118	1.0000
Si	Si8	1.0	0.65964	0.21046	0.55332	1.0000
Si	Si9	1.0	0.65855	0.46293	0.55363	1.0000
Si	Si10	1.0	0.29173	0.19948	0.55123	1.0000
Si	Si11	1.0	0.29367	0.45534	0.55943	1.0000
Si	Si12	1.0	0.04529	0.19425	0.55199	1.0000

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Si	Si13	1.0	0.04602	0.45186	0.55719	1.0000
Si	Si14	1.0	0.47267	0.13793	0.62182	1.0000
Si	Si15	1.0	0.20987	0.32966	0.30647	1.0000
Si	Si16	1.0	0.46384	0.33535	0.30297	1.0000
Si	Si17	1.0	0.20130	0.70431	0.30448	1.0000
Si	Si18	1.0	0.45561	0.71080	0.31132	1.0000
Si	Si19	1.0	0.19321	0.94922	0.30150	1.0000
Si	Si20	1.0	0.45113	0.95626	0.30495	1.0000
Si	Si21	1.0	0.14471	0.52861	0.37736	1.0000
Si	Si22	1.0	0.79739	0.67484	0.80697	1.0000
Si	Si23	1.0	0.54536	0.67929	0.80763	1.0000
Si	Si24	1.0	0.79448	0.28772	0.80846	1.0000
Si	Si25	1.0	0.54250	0.29553	0.80432	1.0000
Si	Si26	1.0	0.78997	0.03613	0.81138	1.0000
Si	Si27	1.0	0.53660	0.04571	0.80857	1.0000
Si	Si28	1.0	0.85676	0.47780	0.87372	1.0000
Si	Si29	1.0	0.66740	0.79237	0.94366	1.0000
Si	Si30	1.0	0.66104	0.53526	0.94388	1.0000
Si	Si31	1.0	0.29485	0.79869	0.94890	1.0000
Si	Si32	1.0	0.28764	0.54254	0.94090	1.0000
Si	Si33	1.0	0.05171	0.80600	0.95085	1.0000
Si	Si34	1.0	0.04405	0.54701	0.94365	1.0000
Si	Si35	1.0	0.47307	0.86823	0.87638	1.0000
Si	Si36	1.0	0.32924	0.21459	0.43798	1.0000
Si	Si37	1.0	0.33376	0.46894	0.44597	1.0000
Si	Si38	1.0	0.71083	0.20344	0.44034	1.0000
Si	Si39	1.0	0.71583	0.46007	0.44067	1.0000
Si	Si40	1.0	0.95545	0.20006	0.44355	1.0000
Si	Si41	1.0	0.95956	0.45855	0.44780	1.0000
Si	Si42	1.0	0.52761	0.14930	0.37002	1.0000
Si	Si43	1.0	0.80057	0.31281	0.69276	1.0000
Si	Si44	1.0	0.54558	0.33227	0.68916	1.0000
Si	Si45	1.0	0.80077	0.71500	0.69047	1.0000
Si	Si46	1.0	0.54613	0.72125	0.69303	1.0000

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Si	Si47	1.0	0.53328	0.96666	0.69823	1.0000
Si	Si48	1.0	0.85878	0.51226	0.62491	1.0000
Si	Si49	1.0	0.21548	0.66692	0.19106	1.0000
Si	Si50	1.0	0.47090	0.66390	0.19796	1.0000
Si	Si51	1.0	0.20107	0.29238	0.19253	1.0000
Si	Si52	1.0	0.45409	0.28866	0.18909	1.0000
Si	Si53	1.0	0.19600	0.04752	0.19608	1.0000
Si	Si54	1.0	0.45416	0.04403	0.19686	1.0000
Si	Si55	1.0	0.14346	0.46843	0.12005	1.0000
Si	Si56	1.0	0.13998	0.86143	0.12659	1.0000
Si	Si57	1.0	0.52869	0.47270	0.12445	1.0000
Si	Si58	1.0	0.85637	0.13490	0.61601	1.0000
Si	Si59	1.0	0.48143	0.53463	0.62526	1.0000
Si	Si60	1.0	0.13571	0.13580	0.36946	1.0000
Si	Si61	1.0	0.52887	0.52677	0.37618	1.0000
Si	Si62	1.0	0.87075	0.85737	0.87951	1.0000
Si	Si63	1.0	0.47286	0.47737	0.87279	1.0000

RAI-T2-T1T2T4T7

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O O2 1.0 0.34601 0.82680 0.99992 1.0000
O O3 1.0 0.23084 0.85746 0.08221 1.0000
O O4 1.0 0.43950 0.81098 0.08851 1.0000

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O	O7	1.0	0.44527	0.51508	0.08174	1.0000
O	O8	1.0	0.70797	0.66991	0.07062	1.0000
O	O9	1.0	0.83075	0.84215	0.05805	1.0000
O	O10	1.0	0.64283	0.86094	0.09937	1.0000
O	O11	1.0	0.83468	0.49999	0.06123	1.0000
O	O12	1.0	0.64807	0.48258	0.10576	1.0000
O	O13	1.0	0.95551	0.67199	0.05158	1.0000
O	O14	1.0	0.02109	0.84155	0.10050	1.0000
O	O15	1.0	0.02948	0.50014	0.09795	1.0000
O	O16	1.0	0.69662	0.34252	0.56212	1.0000
O	O17	1.0	0.66074	0.18646	0.49701	1.0000
O	O18	1.0	0.75226	0.14576	0.58648	1.0000
O	O19	1.0	0.54704	0.19388	0.58044	1.0000
O	O20	1.0	0.67089	0.50307	0.49580	1.0000
O	O21	1.0	0.77975	0.53121	0.58018	1.0000
O	O22	1.0	0.56703	0.50624	0.58069	1.0000
O	O23	1.0	0.29868	0.31997	0.56854	1.0000
O	O24	1.0	0.16045	0.15967	0.56457	1.0000
O	O25	1.0	0.35203	0.13133	0.60397	1.0000
O	O26	1.0	0.17249	0.49002	0.55760	1.0000
O	O27	1.0	0.35973	0.51029	0.60080	1.0000
O	O28	1.0	0.03231	0.33059	0.55862	1.0000
O	O29	1.0	0.96361	0.14531	0.59324	1.0000
O	O30	1.0	0.98698	0.51126	0.60429	1.0000
O	O31	1.0	0.34105	0.35584	0.31336	1.0000
O	O32	1.0	0.17467	0.34007	0.24984	1.0000
O	O33	1.0	0.18234	0.22026	0.33224	1.0000
O	O34	1.0	0.15026	0.42987	0.33795	1.0000
O	O35	1.0	0.49034	0.32830	0.24242	1.0000
O	O36	1.0	0.49795	0.21626	0.32757	1.0000
O	O37	1.0	0.54029	0.42374	0.32706	1.0000
O	O38	1.0	0.33763	0.74698	0.31459	1.0000

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O	O39	1.0	0.14833	0.83149	0.30948	1.0000
O	O40	1.0	0.16601	0.64144	0.35021	1.0000
O	O41	1.0	0.46899	0.61318	0.35659	1.0000
O	O42	1.0	0.30887	0.98078	0.30938	1.0000
O	O43	1.0	0.11540	0.02142	0.34649	1.0000
O	O44	1.0	0.51583	0.01461	0.35285	1.0000
O	O45	1.0	0.65842	0.69713	0.81397	1.0000
O	O46	1.0	0.81863	0.65585	0.75084	1.0000
O	O47	1.0	0.85200	0.76794	0.83409	1.0000
O	O48	1.0	0.81117	0.55877	0.83794	1.0000
O	O49	1.0	0.50983	0.66535	0.74324	1.0000
O	O50	1.0	0.46220	0.76315	0.82908	1.0000
O	O51	1.0	0.50092	0.55433	0.82754	1.0000
O	O52	1.0	0.67139	0.29373	0.82112	1.0000
O	O53	1.0	0.84216	0.16850	0.81224	1.0000
O	O54	1.0	0.86248	0.35755	0.85116	1.0000
O	O55	1.0	0.50274	0.16450	0.81114	1.0000
O	O56	1.0	0.48147	0.35168	0.85382	1.0000
O	O57	1.0	0.67351	0.04002	0.80324	1.0000
O	O58	1.0	0.84936	0.97709	0.85055	1.0000
O	O59	1.0	0.49623	0.96981	0.84591	1.0000
O	O60	1.0	0.68771	0.65885	0.93475	1.0000
O	O61	1.0	0.65515	0.81507	0.00161	1.0000
O	O62	1.0	0.77718	0.84587	0.92130	1.0000
O	O63	1.0	0.56591	0.82555	0.91200	1.0000
O	O64	1.0	0.65578	0.51351	0.00696	1.0000
O	O65	1.0	0.77137	0.46699	0.92610	1.0000
O	O66	1.0	0.55971	0.49178	0.91983	1.0000
O	O67	1.0	0.30174	0.67484	0.93331	1.0000
O	O68	1.0	0.17219	0.84212	0.94175	1.0000
O	O69	1.0	0.36012	0.86664	0.90158	1.0000
O	O70	1.0	0.16691	0.50963	0.93678	1.0000
O	O71	1.0	0.35503	0.48954	0.89542	1.0000
O	O72	1.0	0.03775	0.67671	0.94407	1.0000

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O	O73	1.0	0.98375	0.85839	0.89993	1.0000
O	O74	1.0	0.97358	0.50189	0.89829	1.0000
O	O75	1.0	0.29972	0.31276	0.43833	1.0000
O	O76	1.0	0.33081	0.15683	0.50495	1.0000
O	O77	1.0	0.22442	0.12073	0.41901	1.0000
O	O78	1.0	0.43483	0.15042	0.41942	1.0000
O	O79	1.0	0.35084	0.46990	0.50292	1.0000
O	O80	1.0	0.25227	0.51264	0.41728	1.0000
O	O81	1.0	0.45709	0.44769	0.41847	1.0000
O	O82	1.0	0.70755	0.34500	0.43246	1.0000
O	O83	1.0	0.83306	0.17644	0.43820	1.0000
O	O84	1.0	0.64069	0.15864	0.39831	1.0000
O	O85	1.0	0.83946	0.51393	0.43460	1.0000
O	O86	1.0	0.64584	0.53252	0.39712	1.0000
O	O87	1.0	0.96484	0.34493	0.44261	1.0000
O	O88	1.0	0.02216	0.17233	0.39539	1.0000
O	O89	1.0	0.04022	0.52986	0.40781	1.0000
O	O90	1.0	0.66446	0.31589	0.68401	1.0000
O	O91	1.0	0.82073	0.33793	0.75265	1.0000
O	O92	1.0	0.84983	0.22483	0.66889	1.0000
O	O93	1.0	0.83648	0.43615	0.66607	1.0000
O	O94	1.0	0.51647	0.34124	0.75563	1.0000
O	O95	1.0	0.47165	0.23372	0.67220	1.0000
O	O96	1.0	0.49826	0.44539	0.67101	1.0000
O	O97	1.0	0.67330	0.70702	0.68130	1.0000
O	O98	1.0	0.84636	0.83019	0.69459	1.0000
O	O99	1.0	0.86721	0.64330	0.65407	1.0000
O	O100	1.0	0.50543	0.83824	0.68387	1.0000
O	O101	1.0	0.48580	0.64836	0.64427	1.0000
O	O102	1.0	0.67814	0.95762	0.69645	1.0000
O	O103	1.0	0.85536	0.01746	0.65014	1.0000
O	O104	1.0	0.51322	0.03321	0.64624	1.0000
O	O105	1.0	0.34672	0.68344	0.18437	1.0000
O	O106	1.0	0.19165	0.66087	0.25227	1.0000

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O	O107	1.0	0.16146	0.77874	0.17019	1.0000
O	O108	1.0	0.17414	0.56688	0.16441	1.0000
O	O109	1.0	0.49032	0.65742	0.25910	1.0000
O	O110	1.0	0.54016	0.76311	0.17434	1.0000
O	O111	1.0	0.51195	0.55193	0.17559	1.0000
O	O112	1.0	0.32312	0.29261	0.18244	1.0000
O	O113	1.0	0.15013	0.17040	0.19065	1.0000
O	O114	1.0	0.13317	0.36172	0.15222	1.0000
O	O115	1.0	0.49016	0.16102	0.18161	1.0000
O	O116	1.0	0.50526	0.35357	0.14276	1.0000
O	O117	1.0	0.31699	0.03753	0.18780	1.0000
O	O118	1.0	0.13228	0.98337	0.14757	1.0000
O	O119	1.0	0.50009	0.96647	0.15025	1.0000
O	O120	1.0	0.00231	0.84753	0.00021	1.0000
O	O121	1.0	0.00040	0.50125	0.99820	1.0000
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O	O123	1.0	0.99275	0.50646	0.50473	1.0000
O	O124	1.0	0.14897	0.99701	0.24702	1.0000
O	O125	1.0	0.47731	0.99996	0.24996	1.0000
O	O126	1.0	0.84999	0.00379	0.75070	1.0000
O	O127	1.0	0.50189	0.00367	0.74636	1.0000
O	O128	1.0	0.54566	0.80249	0.32501	1.0000
Si	Si1	1.0	0.32917	0.79045	0.05841	1.0000
Si	Si2	1.0	0.33132	0.53929	0.05490	1.0000
Si	Si3	1.0	0.70930	0.79644	0.05715	1.0000
Si	Si4	1.0	0.71222	0.54236	0.06081	1.0000
Si	Si5	1.0	0.95261	0.80070	0.05248	1.0000
Si	Si6	1.0	0.95544	0.54330	0.05219	1.0000
Si	Si7	1.0	0.52965	0.85033	0.12867	1.0000
Si	Si8	1.0	0.66419	0.21718	0.55665	1.0000
Si	Si9	1.0	0.67799	0.47039	0.55504	1.0000
Si	Si10	1.0	0.28523	0.19257	0.55995	1.0000
Si	Si11	1.0	0.29468	0.44708	0.55733	1.0000
Si	Si12	1.0	0.04083	0.20235	0.55279	1.0000

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Si	Si13	1.0	0.04661	0.45908	0.55616	1.0000
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Si	Si16	1.0	0.46688	0.33040	0.30247	1.0000
Si	Si17	1.0	0.21169	0.71877	0.30644	1.0000
Si	Si18	1.0	0.17921	0.95640	0.30329	1.0000
Si	Si19	1.0	0.15287	0.52749	0.37805	1.0000
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Si	Si21	1.0	0.53265	0.66912	0.80363	1.0000
Si	Si22	1.0	0.79850	0.28951	0.80889	1.0000
Si	Si23	1.0	0.54366	0.28713	0.81015	1.0000
Si	Si24	1.0	0.80305	0.04685	0.80404	1.0000
Si	Si25	1.0	0.54405	0.04411	0.80150	1.0000
Si	Si26	1.0	0.85454	0.47208	0.87876	1.0000
Si	Si27	1.0	0.67079	0.78635	0.94234	1.0000
Si	Si28	1.0	0.66840	0.53274	0.94670	1.0000
Si	Si29	1.0	0.29470	0.80172	0.94449	1.0000
Si	Si30	1.0	0.29090	0.54680	0.94068	1.0000
Si	Si31	1.0	0.04875	0.80533	0.94664	1.0000
Si	Si32	1.0	0.04461	0.54788	0.94463	1.0000
Si	Si33	1.0	0.47239	0.85573	0.87189	1.0000
Si	Si34	1.0	0.32320	0.18552	0.44520	1.0000
Si	Si35	1.0	0.34010	0.43617	0.44397	1.0000
Si	Si36	1.0	0.71028	0.21731	0.44185	1.0000
Si	Si37	1.0	0.71680	0.47304	0.44031	1.0000
Si	Si38	1.0	0.95618	0.21631	0.44325	1.0000
Si	Si39	1.0	0.95966	0.47341	0.44735	1.0000
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Si	Si41	1.0	0.79290	0.32897	0.69289	1.0000
Si	Si42	1.0	0.53788	0.33407	0.69550	1.0000
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Si	Si44	1.0	0.54446	0.71526	0.68870	1.0000
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Si	Si46	1.0	0.54913	0.95841	0.69336	1.0000

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Si	Si47	1.0	0.86722	0.52923	0.62597	1.0000
Si	Si48	1.0	0.21840	0.67223	0.19239	1.0000
Si	Si49	1.0	0.47241	0.66449	0.19853	1.0000
Si	Si50	1.0	0.19597	0.29096	0.19400	1.0000
Si	Si51	1.0	0.45205	0.28348	0.18763	1.0000
Si	Si52	1.0	0.18846	0.04753	0.19351	1.0000
Si	Si53	1.0	0.44678	0.04107	0.19282	1.0000
Si	Si54	1.0	0.14423	0.47546	0.12352	1.0000
Si	Si55	1.0	0.13759	0.86389	0.12487	1.0000
Si	Si56	1.0	0.52640	0.47640	0.12645	1.0000
Si	Si57	1.0	0.85410	0.13504	0.62471	1.0000
Si	Si58	1.0	0.47856	0.52690	0.62410	1.0000
Si	Si59	1.0	0.13640	0.13554	0.37357	1.0000
Si	Si60	1.0	0.52795	0.50528	0.37434	1.0000
Si	Si61	1.0	0.86421	0.86120	0.87629	1.0000
Si	Si62	1.0	0.47492	0.47307	0.87412	1.0000
Si	Si63	1.0	0.46172	0.70720	0.31410	1.0000

RAI-T7-T2T3T6T5

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O O4 1.0 0.42755 0.84803 0.08838 1.0000

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O	O7	1.0	0.44702	0.48947	0.07766	1.0000
O	O8	1.0	0.70755	0.67906	0.06899	1.0000
O	O9	1.0	0.82753	0.84955	0.05305	1.0000
O	O10	1.0	0.63847	0.87017	0.09445	1.0000
O	O11	1.0	0.83593	0.50964	0.06462	1.0000
O	O12	1.0	0.64809	0.49666	0.10920	1.0000
O	O13	1.0	0.95943	0.68046	0.05552	1.0000
O	O14	1.0	0.01360	0.86355	0.09782	1.0000
O	O15	1.0	0.03201	0.50472	0.10036	1.0000
O	O16	1.0	0.63527	0.32031	0.56128	1.0000
O	O17	1.0	0.69893	0.18077	0.49126	1.0000
O	O18	1.0	0.75142	0.14961	0.58766	1.0000
O	O19	1.0	0.66460	0.48655	0.50075	1.0000
O	O20	1.0	0.77861	0.46908	0.58562	1.0000
O	O21	1.0	0.57035	0.51426	0.58825	1.0000
O	O22	1.0	0.28918	0.33030	0.57030	1.0000
O	O23	1.0	0.15654	0.16574	0.55966	1.0000
O	O24	1.0	0.16990	0.50411	0.56092	1.0000
O	O25	1.0	0.35864	0.51737	0.60194	1.0000
O	O26	1.0	0.03500	0.33991	0.55543	1.0000
O	O27	1.0	0.96261	0.16413	0.59833	1.0000
O	O28	1.0	0.98140	0.51874	0.60236	1.0000
O	O29	1.0	0.33921	0.37577	0.30898	1.0000
O	O30	1.0	0.17312	0.33095	0.24807	1.0000
O	O31	1.0	0.20480	0.22218	0.33421	1.0000
O	O32	1.0	0.14232	0.42665	0.33543	1.0000
O	O33	1.0	0.50003	0.32943	0.24641	1.0000
O	O34	1.0	0.48623	0.23308	0.33595	1.0000
O	O35	1.0	0.53575	0.44082	0.32887	1.0000
O	O36	1.0	0.32978	0.71674	0.30895	1.0000
O	O37	1.0	0.15416	0.83281	0.30977	1.0000
O	O38	1.0	0.15337	0.63908	0.34796	1.0000

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O	O39	1.0	0.50020	0.83912	0.31614	1.0000
O	O40	1.0	0.50036	0.64437	0.35480	1.0000
O	O41	1.0	0.32519	0.96088	0.31108	1.0000
O	O42	1.0	0.14225	0.02339	0.35056	1.0000
O	O43	1.0	0.49947	0.02768	0.35900	1.0000
O	O44	1.0	0.66629	0.68574	0.81195	1.0000
O	O45	1.0	0.82242	0.65027	0.74469	1.0000
O	O46	1.0	0.86317	0.75090	0.83037	1.0000
O	O47	1.0	0.81997	0.54243	0.83051	1.0000
O	O48	1.0	0.50332	0.65444	0.74836	1.0000
O	O49	1.0	0.46899	0.73861	0.83913	1.0000
O	O50	1.0	0.51926	0.53588	0.83095	1.0000
O	O51	1.0	0.66267	0.28484	0.82048	1.0000
O	O52	1.0	0.82837	0.15320	0.81683	1.0000
O	O53	1.0	0.84699	0.34386	0.86113	1.0000
O	O54	1.0	0.49258	0.15471	0.81442	1.0000
O	O55	1.0	0.47167	0.33910	0.85470	1.0000
O	O56	1.0	0.65842	0.02696	0.80212	1.0000
O	O57	1.0	0.83047	0.95719	0.84914	1.0000
O	O58	1.0	0.47155	0.94815	0.82676	1.0000
O	O59	1.0	0.63818	0.65908	0.93208	1.0000
O	O60	1.0	0.65120	0.82024	0.99729	1.0000
O	O61	1.0	0.78416	0.81039	0.91971	1.0000
O	O62	1.0	0.57881	0.85654	0.90430	1.0000
O	O63	1.0	0.65723	0.51768	0.00878	1.0000
O	O64	1.0	0.76821	0.49020	0.92535	1.0000
O	O65	1.0	0.55592	0.46603	0.92511	1.0000
O	O66	1.0	0.29058	0.67520	0.92518	1.0000
O	O67	1.0	0.17231	0.84612	0.93984	1.0000
O	O68	1.0	0.36515	0.86666	0.90154	1.0000
O	O69	1.0	0.16563	0.50512	0.93730	1.0000
O	O70	1.0	0.35442	0.48842	0.89350	1.0000
O	O71	1.0	0.04103	0.67601	0.94130	1.0000
O	O72	1.0	0.98392	0.85626	0.89618	1.0000

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O	O73	1.0	0.97094	0.49512	0.89969	1.0000
O	O74	1.0	0.31153	0.32071	0.44187	1.0000
O	O75	1.0	0.34474	0.16638	0.51305	1.0000
O	O76	1.0	0.25112	0.12461	0.42262	1.0000
O	O77	1.0	0.45965	0.16867	0.43188	1.0000
O	O78	1.0	0.34404	0.48273	0.50395	1.0000
O	O79	1.0	0.22963	0.50896	0.41941	1.0000
O	O80	1.0	0.44011	0.48235	0.41569	1.0000
O	O81	1.0	0.70820	0.34424	0.42792	1.0000
O	O82	1.0	0.84788	0.18192	0.42102	1.0000
O	O83	1.0	0.65025	0.15670	0.39204	1.0000
O	O84	1.0	0.83312	0.51391	0.44125	1.0000
O	O85	1.0	0.64245	0.53737	0.40372	1.0000
O	O86	1.0	0.96875	0.34860	0.44372	1.0000
O	O87	1.0	0.05088	0.17861	0.40053	1.0000
O	O88	1.0	0.02174	0.53122	0.40119	1.0000
O	O89	1.0	0.67377	0.35977	0.69317	1.0000
O	O90	1.0	0.82966	0.32915	0.76094	1.0000
O	O91	1.0	0.83402	0.22521	0.67351	1.0000
O	O92	1.0	0.86706	0.43502	0.67657	1.0000
O	O93	1.0	0.50706	0.32667	0.75469	1.0000
O	O94	1.0	0.48587	0.44907	0.67580	1.0000
O	O95	1.0	0.66039	0.70779	0.68555	1.0000
O	O96	1.0	0.83430	0.82701	0.68694	1.0000
O	O97	1.0	0.83602	0.63563	0.64443	1.0000
O	O98	1.0	0.49613	0.83783	0.69729	1.0000
O	O99	1.0	0.47381	0.65421	0.64870	1.0000
O	O100	1.0	0.66844	0.96171	0.68282	1.0000
O	O101	1.0	0.85833	0.02107	0.65004	1.0000
O	O102	1.0	0.33932	0.69895	0.18920	1.0000
O	O103	1.0	0.17017	0.66244	0.24868	1.0000
O	O104	1.0	0.14537	0.76309	0.16165	1.0000
O	O105	1.0	0.19154	0.55535	0.16446	1.0000
O	O106	1.0	0.50074	0.67008	0.25432	1.0000

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O	O107	1.0	0.53634	0.75138	0.16252	1.0000
O	O108	1.0	0.48787	0.54777	0.17323	1.0000
O	O109	1.0	0.33372	0.30248	0.18428	1.0000
O	O110	1.0	0.17152	0.16511	0.18566	1.0000
O	O111	1.0	0.14318	0.35567	0.14755	1.0000
O	O112	1.0	0.49400	0.16139	0.18569	1.0000
O	O113	1.0	0.52253	0.34981	0.14612	1.0000
O	O114	1.0	0.33230	0.02471	0.19425	1.0000
O	O115	1.0	0.15093	0.97375	0.14954	1.0000
O	O116	1.0	0.52063	0.96258	0.16128	1.0000
O	O117	1.0	0.00110	0.84798	0.99699	1.0000
O	O118	1.0	0.99927	0.50864	0.00004	1.0000
O	O119	1.0	0.98891	0.17173	0.49787	1.0000
O	O120	1.0	0.00079	0.51742	0.50186	1.0000
O	O121	1.0	0.15902	0.00275	0.25012	1.0000
O	O122	1.0	0.49702	0.01405	0.25833	1.0000
O	O123	1.0	0.83109	0.99361	0.74887	1.0000
O	O124	1.0	0.49960	0.03057	0.73397	1.0000
O	O125	1.0	0.55513	0.12007	0.55806	1.0000
O	O126	1.0	0.33703	0.15301	0.61590	1.0000
O	O127	1.0	0.52073	0.23766	0.66115	1.0000
O	O128	1.0	0.48303	0.99890	0.63300	1.0000
Si	Si1	1.0	0.33041	0.79191	0.05790	1.0000
Si	Si2	1.0	0.33803	0.53845	0.05364	1.0000
Si	Si3	1.0	0.70661	0.80423	0.05306	1.0000
Si	Si4	1.0	0.71288	0.55064	0.06251	1.0000
Si	Si5	1.0	0.95025	0.80935	0.05055	1.0000
Si	Si6	1.0	0.95689	0.55114	0.05480	1.0000
Si	Si7	1.0	0.52951	0.85738	0.12658	1.0000
Si	Si8	1.0	0.66234	0.44740	0.55968	1.0000
Si	Si9	1.0	0.28044	0.20217	0.56520	1.0000
Si	Si10	1.0	0.29013	0.45763	0.55898	1.0000
Si	Si11	1.0	0.03528	0.21077	0.55295	1.0000
Si	Si12	1.0	0.04636	0.46894	0.55520	1.0000

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Si	Si13	1.0	0.21448	0.33838	0.30669	1.0000
Si	Si14	1.0	0.46548	0.34409	0.30518	1.0000
Si	Si15	1.0	0.20163	0.71299	0.30366	1.0000
Si	Si16	1.0	0.45831	0.71767	0.30813	1.0000
Si	Si17	1.0	0.19613	0.95483	0.30513	1.0000
Si	Si18	1.0	0.45467	0.96017	0.31088	1.0000
Si	Si19	1.0	0.13840	0.52518	0.37559	1.0000
Si	Si20	1.0	0.79257	0.65674	0.80462	1.0000
Si	Si21	1.0	0.53995	0.65360	0.80769	1.0000
Si	Si22	1.0	0.79141	0.27756	0.81475	1.0000
Si	Si23	1.0	0.53467	0.27659	0.81027	1.0000
Si	Si24	1.0	0.78724	0.03342	0.80379	1.0000
Si	Si25	1.0	0.53075	0.03950	0.79405	1.0000
Si	Si26	1.0	0.85143	0.46795	0.87928	1.0000
Si	Si27	1.0	0.66273	0.78642	0.93797	1.0000
Si	Si28	1.0	0.65561	0.53366	0.94754	1.0000
Si	Si29	1.0	0.29315	0.79992	0.94125	1.0000
Si	Si30	1.0	0.28785	0.54841	0.93742	1.0000
Si	Si31	1.0	0.04988	0.80534	0.94374	1.0000
Si	Si32	1.0	0.04370	0.54662	0.94464	1.0000
Si	Si33	1.0	0.47233	0.85275	0.86808	1.0000
Si	Si34	1.0	0.34051	0.19571	0.45201	1.0000
Si	Si35	1.0	0.33193	0.44941	0.44470	1.0000
Si	Si36	1.0	0.72589	0.21636	0.43346	1.0000
Si	Si37	1.0	0.71251	0.46916	0.44421	1.0000
Si	Si38	1.0	0.96459	0.21977	0.44114	1.0000
Si	Si39	1.0	0.95609	0.47699	0.44716	1.0000
Si	Si40	1.0	0.52402	0.14723	0.37891	1.0000
Si	Si41	1.0	0.80026	0.33635	0.70082	1.0000
Si	Si42	1.0	0.54518	0.34118	0.69602	1.0000
Si	Si43	1.0	0.78875	0.70587	0.69069	1.0000
Si	Si44	1.0	0.53329	0.71438	0.69530	1.0000
Si	Si45	1.0	0.79651	0.95059	0.69262	1.0000
Si	Si46	1.0	0.53855	0.95840	0.68608	1.0000

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Si	Si47	1.0	0.86384	0.51463	0.62751	1.0000
Si	Si48	1.0	0.21224	0.66988	0.19043	1.0000
Si	Si49	1.0	0.46546	0.66674	0.19462	1.0000
Si	Si50	1.0	0.20580	0.28879	0.19162	1.0000
Si	Si51	1.0	0.46170	0.28576	0.19097	1.0000
Si	Si52	1.0	0.20393	0.04169	0.19518	1.0000
Si	Si53	1.0	0.46020	0.04066	0.20007	1.0000
Si	Si54	1.0	0.14981	0.47292	0.12117	1.0000
Si	Si55	1.0	0.13341	0.86100	0.12127	1.0000
Si	Si56	1.0	0.52634	0.47244	0.12629	1.0000
Si	Si57	1.0	0.85111	0.14150	0.62729	1.0000
Si	Si58	1.0	0.47400	0.53205	0.62861	1.0000
Si	Si59	1.0	0.16208	0.13834	0.37704	1.0000
Si	Si60	1.0	0.52815	0.52597	0.37547	1.0000
Si	Si61	1.0	0.86395	0.84370	0.87346	1.0000
Si	Si62	1.0	0.47500	0.45942	0.87639	1.0000
Si	Si63	1.0	0.66060	0.19538	0.54966	1.0000

RAI-T9-T1XT5YT5XT1Y

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H H4 1.0 0.88580 0.11793 0.57650 1.0000
O O1 1.0 0.31563 0.65699 0.06143 1.0000
O O2 1.0 0.35504 0.82355 0.00131 1.0000
O O3 1.0 0.22599 0.84265 0.07912 1.0000
O O4 1.0 0.43693 0.82173 0.09215 1.0000

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O	O5	1.0	0.34817	0.50711	0.99105	1.0000
O	O6	1.0	0.23062	0.46366	0.07147	1.0000
O	O7	1.0	0.44257	0.49133	0.07935	1.0000
O	O8	1.0	0.70762	0.67443	0.06901	1.0000
O	O9	1.0	0.83152	0.84457	0.05564	1.0000
O	O10	1.0	0.64441	0.86532	0.09920	1.0000
O	O11	1.0	0.83256	0.50258	0.05787	1.0000
O	O12	1.0	0.64818	0.48710	0.10424	1.0000
O	O13	1.0	0.95889	0.67292	0.05476	1.0000
O	O14	1.0	0.01833	0.85132	0.10128	1.0000
O	O15	1.0	0.02690	0.49432	0.09709	1.0000
O	O16	1.0	0.67331	0.32898	0.56092	1.0000
O	O17	1.0	0.67364	0.16839	0.49215	1.0000
O	O18	1.0	0.75664	0.14265	0.58334	1.0000
O	O19	1.0	0.54418	0.16081	0.56906	1.0000
O	O20	1.0	0.65921	0.49635	0.50092	1.0000
O	O21	1.0	0.77141	0.51022	0.58593	1.0000
O	O22	1.0	0.55936	0.49752	0.58795	1.0000
O	O23	1.0	0.32447	0.32774	0.56536	1.0000
O	O24	1.0	0.16080	0.18182	0.56575	1.0000
O	O25	1.0	0.34958	0.13676	0.60297	1.0000
O	O26	1.0	0.16550	0.46218	0.56602	1.0000
O	O27	1.0	0.35227	0.52762	0.59935	1.0000
O	O28	1.0	0.00176	0.31945	0.55939	1.0000
O	O29	1.0	0.96454	0.11259	0.58342	1.0000
O	O30	1.0	0.98143	0.50887	0.60316	1.0000
O	O31	1.0	0.33345	0.36636	0.31485	1.0000
O	O32	1.0	0.17698	0.34617	0.24602	1.0000
O	O33	1.0	0.18329	0.21498	0.32387	1.0000
O	O34	1.0	0.13483	0.42018	0.33727	1.0000
O	O35	1.0	0.48618	0.34513	0.24543	1.0000
O	O36	1.0	0.49360	0.23044	0.32878	1.0000
O	O37	1.0	0.52961	0.44145	0.33091	1.0000
O	O38	1.0	0.32706	0.70335	0.31533	1.0000

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O	O39	1.0	0.15511	0.82421	0.30384	1.0000
O	O40	1.0	0.13676	0.63414	0.34304	1.0000
O	O41	1.0	0.49484	0.83512	0.31470	1.0000
O	O42	1.0	0.50719	0.64557	0.35739	1.0000
O	O43	1.0	0.32260	0.95894	0.30716	1.0000
O	O44	1.0	0.13567	0.01392	0.34582	1.0000
O	O45	1.0	0.49934	0.02743	0.35370	1.0000
O	O46	1.0	0.66878	0.69160	0.81276	1.0000
O	O47	1.0	0.83507	0.66346	0.75057	1.0000
O	O48	1.0	0.85967	0.76922	0.83581	1.0000
O	O49	1.0	0.82481	0.55663	0.83420	1.0000
O	O50	1.0	0.50960	0.67058	0.74760	1.0000
O	O51	1.0	0.47165	0.73554	0.84223	1.0000
O	O52	1.0	0.51871	0.53623	0.82432	1.0000
O	O53	1.0	0.65558	0.28493	0.81578	1.0000
O	O54	1.0	0.83065	0.16435	0.81350	1.0000
O	O55	1.0	0.83774	0.35326	0.85850	1.0000
O	O56	1.0	0.48720	0.15107	0.81453	1.0000
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O	O58	1.0	0.66252	0.03475	0.82497	1.0000
O	O59	1.0	0.85028	0.97784	0.85874	1.0000
O	O60	1.0	0.47303	0.94365	0.82913	1.0000
O	O61	1.0	0.64763	0.66599	0.93215	1.0000
O	O62	1.0	0.65140	0.82157	0.00127	1.0000
O	O63	1.0	0.78661	0.82908	0.92539	1.0000
O	O64	1.0	0.57962	0.85940	0.90809	1.0000
O	O65	1.0	0.64976	0.51957	0.00570	1.0000
O	O66	1.0	0.77396	0.49649	0.92700	1.0000
O	O67	1.0	0.56180	0.47338	0.91808	1.0000
O	O68	1.0	0.29976	0.67434	0.93420	1.0000
O	O69	1.0	0.17848	0.84460	0.94498	1.0000
O	O70	1.0	0.36723	0.86490	0.90411	1.0000
O	O71	1.0	0.16967	0.50455	0.93534	1.0000
O	O72	1.0	0.35813	0.49666	0.89073	1.0000

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O	O73	1.0	0.04417	0.67465	0.94220	1.0000
O	O74	1.0	0.99101	0.85977	0.90222	1.0000
O	O75	1.0	0.97549	0.49322	0.89843	1.0000
O	O76	1.0	0.30501	0.32812	0.43913	1.0000
O	O77	1.0	0.32404	0.16257	0.50296	1.0000
O	O78	1.0	0.23616	0.13490	0.41339	1.0000
O	O79	1.0	0.44606	0.17377	0.42290	1.0000
O	O80	1.0	0.32788	0.49293	0.50193	1.0000
O	O81	1.0	0.23820	0.52024	0.41242	1.0000
O	O82	1.0	0.44604	0.48663	0.42017	1.0000
O	O83	1.0	0.70714	0.33958	0.43594	1.0000
O	O84	1.0	0.83951	0.17171	0.43115	1.0000
O	O85	1.0	0.64504	0.15854	0.39235	1.0000
O	O86	1.0	0.83606	0.50887	0.44566	1.0000
O	O87	1.0	0.64938	0.53050	0.40294	1.0000
O	O88	1.0	0.96686	0.34085	0.43860	1.0000
O	O89	1.0	0.03023	0.16765	0.39025	1.0000
O	O90	1.0	0.02530	0.52975	0.40590	1.0000
O	O91	1.0	0.65560	0.36944	0.69330	1.0000
O	O92	1.0	0.81963	0.34073	0.75876	1.0000
O	O93	1.0	0.79535	0.22254	0.67432	1.0000
O	O94	1.0	0.85144	0.43244	0.67210	1.0000
O	O95	1.0	0.49196	0.31812	0.75275	1.0000
O	O96	1.0	0.50097	0.23513	0.66091	1.0000
O	O97	1.0	0.46450	0.44363	0.67425	1.0000
O	O98	1.0	0.67791	0.70168	0.68682	1.0000
O	O99	1.0	0.85110	0.83346	0.69048	1.0000
O	O100	1.0	0.86512	0.64150	0.65245	1.0000
O	O101	1.0	0.52269	0.84201	0.68864	1.0000
O	O102	1.0	0.48736	0.64979	0.64931	1.0000
O	O103	1.0	0.69582	0.97149	0.67686	1.0000
O	O104	1.0	0.50354	0.02578	0.64389	1.0000
O	O105	1.0	0.34528	0.69309	0.18664	1.0000
O	O106	1.0	0.18029	0.64872	0.24682	1.0000

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O	O107	1.0	0.15517	0.77167	0.16753	1.0000
O	O108	1.0	0.18716	0.56149	0.15719	1.0000
O	O109	1.0	0.49398	0.65863	0.25741	1.0000
O	O110	1.0	0.54242	0.76714	0.17464	1.0000
O	O111	1.0	0.50420	0.55678	0.17076	1.0000
O	O112	1.0	0.32963	0.29508	0.18095	1.0000
O	O113	1.0	0.15942	0.16831	0.19026	1.0000
O	O114	1.0	0.14010	0.35574	0.14723	1.0000
O	O115	1.0	0.49924	0.16719	0.19095	1.0000
O	O116	1.0	0.51819	0.35238	0.14655	1.0000
O	O117	1.0	0.32921	0.03896	0.19378	1.0000
O	O118	1.0	0.15155	0.98012	0.14678	1.0000
O	O119	1.0	0.51171	0.97324	0.15450	1.0000
O	O120	1.0	0.00732	0.84404	0.00140	1.0000
O	O121	1.0	0.00325	0.50363	0.99786	1.0000
O	O122	1.0	0.01716	0.16721	0.48973	1.0000
O	O123	1.0	0.00617	0.49765	0.50414	1.0000
O	O124	1.0	0.15557	0.99539	0.24676	1.0000
O	O125	1.0	0.49609	0.00201	0.25358	1.0000
O	O126	1.0	0.81443	0.98148	0.76059	1.0000
O	O127	1.0	0.54310	0.02107	0.74168	1.0000
O	O128	1.0	0.90270	0.04195	0.67791	1.0000
Si	Si1	1.0	0.33395	0.78617	0.05897	1.0000
Si	Si2	1.0	0.33480	0.52983	0.05114	1.0000
Si	Si3	1.0	0.70868	0.80125	0.05590	1.0000
Si	Si4	1.0	0.71073	0.54626	0.05888	1.0000
Si	Si5	1.0	0.95350	0.80241	0.05322	1.0000
Si	Si6	1.0	0.95569	0.54346	0.05168	1.0000
Si	Si7	1.0	0.53334	0.85661	0.13028	1.0000
Si	Si8	1.0	0.66168	0.20082	0.55098	1.0000
Si	Si9	1.0	0.66546	0.45832	0.55932	1.0000
Si	Si10	1.0	0.28821	0.20242	0.55887	1.0000
Si	Si11	1.0	0.29234	0.45250	0.55763	1.0000
Si	Si12	1.0	0.03630	0.19501	0.54959	1.0000

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Si	Si13	1.0	0.03871	0.44533	0.55786	1.0000
Si	Si14	1.0	0.47515	0.14076	0.61996	1.0000
Si	Si15	1.0	0.20702	0.33696	0.30558	1.0000
Si	Si16	1.0	0.46040	0.34504	0.30515	1.0000
Si	Si17	1.0	0.20051	0.70354	0.30198	1.0000
Si	Si18	1.0	0.45598	0.71093	0.31081	1.0000
Si	Si19	1.0	0.19340	0.94823	0.30083	1.0000
Si	Si20	1.0	0.45245	0.95617	0.30707	1.0000
Si	Si21	1.0	0.13536	0.52441	0.37463	1.0000
Si	Si22	1.0	0.79691	0.67001	0.80873	1.0000
Si	Si23	1.0	0.54260	0.65834	0.80656	1.0000
Si	Si24	1.0	0.78513	0.28568	0.81188	1.0000
Si	Si25	1.0	0.52647	0.27450	0.80811	1.0000
Si	Si26	1.0	0.78987	0.04031	0.81383	1.0000
Si	Si27	1.0	0.54167	0.03701	0.80227	1.0000
Si	Si28	1.0	0.85288	0.47498	0.87955	1.0000
Si	Si29	1.0	0.66591	0.79419	0.94166	1.0000
Si	Si30	1.0	0.65836	0.53930	0.94556	1.0000
Si	Si31	1.0	0.29973	0.80134	0.94637	1.0000
Si	Si32	1.0	0.29358	0.54533	0.93814	1.0000
Si	Si33	1.0	0.05530	0.80402	0.94799	1.0000
Si	Si34	1.0	0.04804	0.54474	0.94371	1.0000
Si	Si35	1.0	0.47456	0.85073	0.87121	1.0000
Si	Si36	1.0	0.32828	0.20034	0.44463	1.0000
Si	Si37	1.0	0.32979	0.45651	0.44307	1.0000
Si	Si38	1.0	0.71673	0.21028	0.43789	1.0000
Si	Si39	1.0	0.71294	0.46768	0.44678	1.0000
Si	Si40	1.0	0.96318	0.21147	0.43791	1.0000
Si	Si41	1.0	0.95810	0.46819	0.44875	1.0000
Si	Si42	1.0	0.52068	0.14816	0.37435	1.0000
Si	Si43	1.0	0.78146	0.34119	0.70004	1.0000
Si	Si44	1.0	0.52806	0.34024	0.69512	1.0000
Si	Si45	1.0	0.80652	0.71109	0.69527	1.0000
Si	Si46	1.0	0.54988	0.71615	0.69340	1.0000

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Si	Si47	1.0	0.56757	0.96437	0.68792	1.0000
Si	Si48	1.0	0.86521	0.52204	0.62842	1.0000
Si	Si49	1.0	0.21700	0.66813	0.18905	1.0000
Si	Si50	1.0	0.47148	0.66842	0.19720	1.0000
Si	Si51	1.0	0.20175	0.29143	0.19141	1.0000
Si	Si52	1.0	0.45762	0.28937	0.19135	1.0000
Si	Si53	1.0	0.19975	0.04602	0.19465	1.0000
Si	Si54	1.0	0.45851	0.04479	0.19847	1.0000
Si	Si55	1.0	0.14604	0.46930	0.11803	1.0000
Si	Si56	1.0	0.13896	0.86053	0.12368	1.0000
Si	Si57	1.0	0.52727	0.47315	0.12512	1.0000
Si	Si58	1.0	0.46726	0.52915	0.62799	1.0000
Si	Si59	1.0	0.14613	0.13426	0.36881	1.0000
Si	Si60	1.0	0.53106	0.52621	0.37774	1.0000
Si	Si61	1.0	0.86994	0.85875	0.88035	1.0000
Si	Si62	1.0	0.47630	0.46432	0.87166	1.0000
Si	Si63	1.0	0.81574	0.95622	0.70054	1.0000

RAI-T7T7T7T7T9T9

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H H6 1.0 0.42177 0.03283 0.61968 1.0000
H H7 1.0 0.36843 0.18093 0.63667 1.0000
H H8 1.0 0.51667 0.23090 0.62307 1.0000

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H	H9	1.0	0.93062	0.02771	0.62664	1.0000
H	H10	1.0	0.79141	0.08092	0.58976	1.0000
H	H11	1.0	0.81910	0.21041	0.63342	1.0000
H	H12	1.0	0.97017	0.17765	0.64294	1.0000
H	H13	1.0	0.02713	0.93158	0.12007	1.0000
H	H14	1.0	0.17681	0.97213	0.10401	1.0000
H	H15	1.0	0.20996	0.82115	0.11361	1.0000
H	H16	1.0	0.08065	0.79290	0.15691	1.0000
H	H17	1.0	0.57766	0.97058	0.11968	1.0000
H	H18	1.0	0.63300	0.82256	0.13620	1.0000
H	H19	1.0	0.48517	0.77003	0.12238	1.0000
H	H20	1.0	0.45594	0.89923	0.08137	1.0000
H	H21	1.0	0.03103	0.42298	0.12809	1.0000
H	H22	1.0	0.17991	0.37019	0.11137	1.0000
H	H23	1.0	0.22940	0.51799	0.12463	1.0000
H	H24	1.0	0.09786	0.54761	0.16502	1.0000
O	O1	1.0	0.30841	0.67016	0.05428	1.0000
O	O2	1.0	0.31372	0.83249	0.98442	1.0000
O	O3	1.0	0.32128	0.49845	0.99212	1.0000
O	O4	1.0	0.45585	0.52323	0.07220	1.0000
O	O5	1.0	0.70040	0.68062	0.06893	1.0000
O	O6	1.0	0.83659	0.83429	0.04630	1.0000
O	O7	1.0	0.83219	0.51487	0.06311	1.0000
O	O8	1.0	0.64734	0.49777	0.11247	1.0000
O	O9	1.0	0.96374	0.67623	0.07992	1.0000
O	O10	1.0	0.68877	0.33393	0.55418	1.0000
O	O11	1.0	0.68784	0.17057	0.48515	1.0000
O	O12	1.0	0.68182	0.50583	0.49184	1.0000
O	O13	1.0	0.54448	0.48361	0.57089	1.0000
O	O14	1.0	0.29843	0.32158	0.56835	1.0000
O	O15	1.0	0.16476	0.16495	0.54638	1.0000
O	O16	1.0	0.16800	0.48846	0.56338	1.0000
O	O17	1.0	0.35359	0.50341	0.61217	1.0000
O	O18	1.0	0.03828	0.32554	0.57879	1.0000

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O	O19	1.0	0.32618	0.37044	0.30729	1.0000
O	O20	1.0	0.15818	0.35429	0.24304	1.0000
O	O21	1.0	0.15394	0.27220	0.34208	1.0000
O	O22	1.0	0.14474	0.47695	0.32735	1.0000
O	O23	1.0	0.48810	0.34497	0.24018	1.0000
O	O24	1.0	0.50244	0.27032	0.33786	1.0000
O	O25	1.0	0.50587	0.47648	0.32129	1.0000
O	O26	1.0	0.33975	0.72317	0.32015	1.0000
O	O27	1.0	0.17826	0.85990	0.32491	1.0000
O	O28	1.0	0.16074	0.67018	0.36759	1.0000
O	O29	1.0	0.50026	0.85812	0.31583	1.0000
O	O30	1.0	0.52393	0.66921	0.36151	1.0000
O	O31	1.0	0.33683	0.99233	0.30099	1.0000
O	O32	1.0	0.14921	0.06496	0.33079	1.0000
O	O33	1.0	0.52716	0.06315	0.32421	1.0000
O	O34	1.0	0.67369	0.63295	0.80788	1.0000
O	O35	1.0	0.84155	0.64944	0.74365	1.0000
O	O36	1.0	0.84680	0.73017	0.84267	1.0000
O	O37	1.0	0.85482	0.52558	0.82777	1.0000
O	O38	1.0	0.51214	0.65717	0.74012	1.0000
O	O39	1.0	0.49614	0.73165	0.83768	1.0000
O	O40	1.0	0.49425	0.52560	0.82108	1.0000
O	O41	1.0	0.66078	0.27875	0.82092	1.0000
O	O42	1.0	0.82271	0.14248	0.82494	1.0000
O	O43	1.0	0.84017	0.33173	0.86820	1.0000
O	O44	1.0	0.50012	0.14441	0.81513	1.0000
O	O45	1.0	0.47581	0.33268	0.86113	1.0000
O	O46	1.0	0.66415	0.01058	0.80068	1.0000
O	O47	1.0	0.47394	0.93925	0.82365	1.0000
O	O48	1.0	0.63872	0.67568	0.93875	1.0000
O	O49	1.0	0.64814	0.84240	0.00445	1.0000
O	O50	1.0	0.73008	0.85373	0.90597	1.0000
O	O51	1.0	0.52519	0.85435	0.92012	1.0000
O	O52	1.0	0.65462	0.51499	0.00749	1.0000

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O	O53	1.0	0.73389	0.49489	0.91107	1.0000
O	O54	1.0	0.52714	0.49829	0.92495	1.0000
O	O55	1.0	0.28070	0.66051	0.92675	1.0000
O	O56	1.0	0.14269	0.82128	0.92221	1.0000
O	O57	1.0	0.33212	0.83967	0.87901	1.0000
O	O58	1.0	0.14549	0.50067	0.93315	1.0000
O	O59	1.0	0.33308	0.47428	0.88722	1.0000
O	O60	1.0	0.00953	0.66354	0.94626	1.0000
O	O61	1.0	0.93784	0.85173	0.91627	1.0000
O	O62	1.0	0.94158	0.47204	0.92338	1.0000
O	O63	1.0	0.36300	0.32631	0.43917	1.0000
O	O64	1.0	0.35371	0.15971	0.50512	1.0000
O	O65	1.0	0.26984	0.14957	0.40670	1.0000
O	O66	1.0	0.47508	0.14708	0.42053	1.0000
O	O67	1.0	0.34448	0.48752	0.50707	1.0000
O	O68	1.0	0.26854	0.50672	0.40976	1.0000
O	O69	1.0	0.47474	0.50319	0.42545	1.0000
O	O70	1.0	0.72103	0.34272	0.42745	1.0000
O	O71	1.0	0.85764	0.18123	0.42233	1.0000
O	O72	1.0	0.66773	0.16428	0.37960	1.0000
O	O73	1.0	0.85642	0.50291	0.43219	1.0000
O	O74	1.0	0.66791	0.52809	0.38681	1.0000
O	O75	1.0	0.99063	0.33908	0.44628	1.0000
O	O76	1.0	0.06214	0.15143	0.41569	1.0000
O	O77	1.0	0.06124	0.52971	0.42372	1.0000
O	O78	1.0	0.66882	0.31105	0.69302	1.0000
O	O79	1.0	0.83152	0.31390	0.76279	1.0000
O	O80	1.0	0.49832	0.32011	0.75601	1.0000
O	O81	1.0	0.51945	0.45666	0.67614	1.0000
O	O82	1.0	0.67930	0.69974	0.67922	1.0000
O	O83	1.0	0.83231	0.83716	0.70090	1.0000
O	O84	1.0	0.51477	0.83350	0.68371	1.0000
O	O85	1.0	0.49673	0.64808	0.63511	1.0000
O	O86	1.0	0.67553	0.96590	0.66716	1.0000

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O	O87	1.0	0.33255	0.68880	0.19320	1.0000
O	O88	1.0	0.16851	0.68981	0.26202	1.0000
O	O89	1.0	0.50326	0.68363	0.25626	1.0000
O	O90	1.0	0.48404	0.54566	0.17743	1.0000
O	O91	1.0	0.32064	0.30034	0.17985	1.0000
O	O92	1.0	0.16450	0.16585	0.20098	1.0000
O	O93	1.0	0.48718	0.16910	0.18340	1.0000
O	O94	1.0	0.50161	0.35533	0.13505	1.0000
O	O95	1.0	0.32461	0.03879	0.16846	1.0000
O	O96	1.0	0.03106	0.82675	0.01213	1.0000
O	O97	1.0	0.02324	0.51106	0.01955	1.0000
O	O98	1.0	0.97085	0.17476	0.51186	1.0000
O	O99	1.0	0.97716	0.49169	0.51933	1.0000
O	O100	1.0	0.17316	0.97173	0.23511	1.0000
O	O101	1.0	0.49033	0.97893	0.22852	1.0000
O	O102	1.0	0.82711	0.03168	0.73473	1.0000
O	O103	1.0	0.51063	0.02396	0.72803	1.0000
O	O104	1.0	0.85201	0.93735	0.83034	1.0000
O	O105	1.0	0.49513	0.00316	0.62065	1.0000
O	O106	1.0	0.86129	0.99065	0.62820	1.0000
O	O107	1.0	0.74940	0.52246	0.59095	1.0000
O	O108	1.0	0.99841	0.50459	0.62668	1.0000
O	O109	1.0	0.82520	0.44424	0.67890	1.0000
O	O110	1.0	0.86872	0.67221	0.63660	1.0000
O	O111	1.0	0.56024	0.17388	0.56993	1.0000
O	O112	1.0	0.32894	0.13326	0.61206	1.0000
O	O113	1.0	0.47947	0.25191	0.65699	1.0000
O	O114	1.0	0.77239	0.15643	0.58302	1.0000
O	O115	1.0	0.01233	0.13366	0.61729	1.0000
O	O116	1.0	0.85851	0.23509	0.66628	1.0000
O	O117	1.0	0.23451	0.86062	0.08073	1.0000
O	O118	1.0	0.99065	0.86191	0.11860	1.0000
O	O119	1.0	0.15604	0.77381	0.16398	1.0000
O	O120	1.0	0.13271	0.01403	0.12972	1.0000

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O	O121	1.0	0.44344	0.82537	0.06856	1.0000
O	O122	1.0	0.67216	0.86984	0.11131	1.0000
O	O123	1.0	0.52112	0.75088	0.15706	1.0000
O	O124	1.0	0.50376	0.99838	0.12100	1.0000
O	O125	1.0	0.25129	0.48062	0.09088	1.0000
O	O126	1.0	0.00100	0.49621	0.12691	1.0000
O	O127	1.0	0.17183	0.56148	0.17760	1.0000
O	O128	1.0	0.13223	0.33085	0.13603	1.0000
Si	Si1	1.0	0.33431	0.54327	0.05237	1.0000
Si	Si2	1.0	0.71329	0.80663	0.05779	1.0000
Si	Si3	1.0	0.70925	0.55296	0.06290	1.0000
Si	Si4	1.0	0.95629	0.80122	0.06382	1.0000
Si	Si5	1.0	0.95504	0.54884	0.07171	1.0000
Si	Si6	1.0	0.67665	0.20684	0.54700	1.0000
Si	Si7	1.0	0.66614	0.46148	0.55204	1.0000
Si	Si8	1.0	0.28742	0.19517	0.55807	1.0000
Si	Si9	1.0	0.29060	0.44943	0.56264	1.0000
Si	Si10	1.0	0.04569	0.20020	0.56366	1.0000
Si	Si11	1.0	0.04535	0.45323	0.57159	1.0000
Si	Si12	1.0	0.19710	0.36766	0.30462	1.0000
Si	Si13	1.0	0.45457	0.36543	0.30160	1.0000
Si	Si14	1.0	0.21208	0.73624	0.31856	1.0000
Si	Si15	1.0	0.46679	0.73401	0.31319	1.0000
Si	Si16	1.0	0.20951	0.97251	0.29781	1.0000
Si	Si17	1.0	0.46327	0.97274	0.29228	1.0000
Si	Si18	1.0	0.15820	0.54465	0.38249	1.0000
Si	Si19	1.0	0.80282	0.63527	0.80515	1.0000
Si	Si20	1.0	0.54525	0.63707	0.80171	1.0000
Si	Si21	1.0	0.78857	0.26626	0.81905	1.0000
Si	Si22	1.0	0.53388	0.26853	0.81303	1.0000
Si	Si23	1.0	0.53769	0.02998	0.79184	1.0000
Si	Si24	1.0	0.84317	0.45724	0.88290	1.0000
Si	Si25	1.0	0.63608	0.80492	0.94263	1.0000
Si	Si26	1.0	0.63872	0.54717	0.94544	1.0000

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Si	Si27	1.0	0.26669	0.78826	0.92830	1.0000
Si	Si28	1.0	0.26963	0.53369	0.93510	1.0000
Si	Si29	1.0	0.03011	0.79083	0.94934	1.0000
Si	Si30	1.0	0.03035	0.53735	0.95568	1.0000
Si	Si31	1.0	0.45785	0.84193	0.86472	1.0000
Si	Si32	1.0	0.36474	0.19718	0.44318	1.0000
Si	Si33	1.0	0.36253	0.45479	0.44534	1.0000
Si	Si34	1.0	0.73404	0.21493	0.42872	1.0000
Si	Si35	1.0	0.73235	0.46970	0.43485	1.0000
Si	Si36	1.0	0.97057	0.21173	0.44922	1.0000
Si	Si37	1.0	0.97095	0.46540	0.45552	1.0000
Si	Si38	1.0	0.54204	0.16061	0.36517	1.0000
Si	Si39	1.0	0.54166	0.33508	0.69559	1.0000
Si	Si40	1.0	0.80528	0.71350	0.69003	1.0000
Si	Si41	1.0	0.55169	0.71027	0.68463	1.0000
Si	Si42	1.0	0.54833	0.95657	0.67557	1.0000
Si	Si43	1.0	0.46019	0.66732	0.19588	1.0000
Si	Si44	1.0	0.19425	0.28889	0.18989	1.0000
Si	Si45	1.0	0.44852	0.29183	0.18469	1.0000
Si	Si46	1.0	0.45222	0.04615	0.17586	1.0000
Si	Si47	1.0	0.52177	0.48090	0.12426	1.0000
Si	Si48	1.0	0.47900	0.52247	0.62361	1.0000
Si	Si49	1.0	0.15943	0.16019	0.37381	1.0000
Si	Si50	1.0	0.54226	0.54354	0.37381	1.0000
Si	Si51	1.0	0.45838	0.45831	0.87368	1.0000
Si	Si52	1.0	0.79608	0.32528	0.70082	1.0000
Si	Si53	1.0	0.32446	0.79730	0.04646	1.0000
Si	Si54	1.0	0.20538	0.67800	0.20030	1.0000
Si	Si55	1.0	0.79150	0.03034	0.79756	1.0000
Si	Si56	1.0	0.84118	0.84261	0.87384	1.0000
Si	Si57	1.0	0.19925	0.04677	0.18342	1.0000
Si	Si58	1.0	0.80055	0.95706	0.68309	1.0000

RAI-T1T1T7T7T7T7T9T9

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H H4 1.0 0.06944 0.78090 0.15738 1.0000
H H5 1.0 0.58840 0.97459 0.11726 1.0000
H H6 1.0 0.63553 0.82330 0.13706 1.0000
H H7 1.0 0.48608 0.78055 0.12629 1.0000
H H8 1.0 0.45635 0.90753 0.08262 1.0000

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H	H9	1.0	0.03409	0.42381	0.12471	1.0000
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H	H11	1.0	0.23682	0.51130	0.12255	1.0000
H	H12	1.0	0.10584	0.54143	0.16177	1.0000
H	H13	1.0	0.96788	0.58387	0.62530	1.0000
H	H14	1.0	0.82027	0.64628	0.61124	1.0000
H	H15	1.0	0.76351	0.49847	0.62304	1.0000
H	H16	1.0	0.89324	0.46693	0.66203	1.0000
H	H17	1.0	0.54724	0.09788	0.58300	1.0000
H	H18	1.0	0.41347	0.03333	0.61759	1.0000
H	H19	1.0	0.36715	0.18520	0.63704	1.0000
H	H20	1.0	0.51666	0.22566	0.62684	1.0000
H	H21	1.0	0.92870	0.02881	0.62048	1.0000
H	H22	1.0	0.79728	0.09066	0.58774	1.0000
H	H23	1.0	0.82820	0.22158	0.63394	1.0000
H	H24	1.0	0.97775	0.18077	0.64016	1.0000
H	H25	1.0	0.26285	0.02448	0.34249	1.0000
H	H26	1.0	0.15264	0.89931	0.34696	1.0000
H	H27	1.0	0.29164	0.97715	0.26739	1.0000
H	H28	1.0	0.13440	0.93579	0.24265	1.0000
H	H29	1.0	0.86560	0.07949	0.74033	1.0000
H	H30	1.0	0.85057	0.10848	0.84512	1.0000
H	H31	1.0	0.74029	0.98245	0.84206	1.0000
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O	O1	1.0	0.31651	0.66761	0.05521	1.0000
O	O2	1.0	0.32308	0.83510	0.98834	1.0000
O	O3	1.0	0.32897	0.49879	0.99116	1.0000
O	O4	1.0	0.46252	0.51813	0.07168	1.0000
O	O5	1.0	0.70040	0.67952	0.06689	1.0000
O	O6	1.0	0.83299	0.83647	0.04334	1.0000
O	O7	1.0	0.83797	0.51463	0.06245	1.0000
O	O8	1.0	0.65356	0.49765	0.11319	1.0000
O	O9	1.0	0.96495	0.68110	0.07799	1.0000
O	O10	1.0	0.68478	0.34111	0.55537	1.0000

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O	O11	1.0	0.67918	0.17374	0.48863	1.0000
O	O12	1.0	0.67125	0.51030	0.49166	1.0000
O	O13	1.0	0.53845	0.48901	0.57270	1.0000
O	O14	1.0	0.29839	0.32796	0.56674	1.0000
O	O15	1.0	0.16857	0.16791	0.54402	1.0000
O	O16	1.0	0.16315	0.49434	0.56262	1.0000
O	O17	1.0	0.34706	0.50942	0.61358	1.0000
O	O18	1.0	0.03644	0.32727	0.57623	1.0000
O	O19	1.0	0.32106	0.35722	0.30920	1.0000
O	O20	1.0	0.15525	0.34693	0.24274	1.0000
O	O21	1.0	0.15654	0.23091	0.32989	1.0000
O	O22	1.0	0.13228	0.44460	0.33383	1.0000
O	O23	1.0	0.48457	0.35299	0.24257	1.0000
O	O24	1.0	0.50959	0.27793	0.33912	1.0000
O	O25	1.0	0.48824	0.48358	0.32498	1.0000
O	O26	1.0	0.33499	0.75260	0.31914	1.0000
O	O27	1.0	0.18124	0.64421	0.36353	1.0000
O	O28	1.0	0.51008	0.86531	0.31060	1.0000
O	O29	1.0	0.52094	0.68024	0.35862	1.0000
O	O30	1.0	0.53303	0.07157	0.31848	1.0000
O	O31	1.0	0.68139	0.65355	0.80958	1.0000
O	O32	1.0	0.84725	0.66178	0.74285	1.0000
O	O33	1.0	0.84912	0.77579	0.83065	1.0000
O	O34	1.0	0.86884	0.56168	0.83321	1.0000
O	O35	1.0	0.51778	0.65590	0.74332	1.0000
O	O36	1.0	0.49105	0.72805	0.84023	1.0000
O	O37	1.0	0.51582	0.52338	0.82506	1.0000
O	O38	1.0	0.66701	0.25487	0.81998	1.0000
O	O39	1.0	0.82264	0.36183	0.86383	1.0000
O	O40	1.0	0.49301	0.14074	0.81107	1.0000
O	O41	1.0	0.48022	0.32703	0.85873	1.0000
O	O42	1.0	0.47065	0.93386	0.81760	1.0000
O	O43	1.0	0.59517	0.67172	0.94912	1.0000
O	O44	1.0	0.63744	0.84447	0.00703	1.0000

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O	O45	1.0	0.74981	0.79905	0.92095	1.0000
O	O46	1.0	0.54753	0.86766	0.91241	1.0000
O	O47	1.0	0.66046	0.50712	0.00877	1.0000
O	O48	1.0	0.74247	0.53322	0.91396	1.0000
O	O49	1.0	0.54029	0.47406	0.92669	1.0000
O	O50	1.0	0.29068	0.66546	0.92850	1.0000
O	O51	1.0	0.15213	0.82875	0.92595	1.0000
O	O52	1.0	0.34229	0.85020	0.88507	1.0000
O	O53	1.0	0.15346	0.50588	0.93203	1.0000
O	O54	1.0	0.34459	0.47921	0.88714	1.0000
O	O55	1.0	0.01504	0.67025	0.94411	1.0000
O	O56	1.0	0.94932	0.86281	0.91358	1.0000
O	O57	1.0	0.94710	0.47656	0.92217	1.0000
O	O58	1.0	0.40693	0.33583	0.44910	1.0000
O	O59	1.0	0.36442	0.16355	0.50731	1.0000
O	O60	1.0	0.25159	0.20879	0.42156	1.0000
O	O61	1.0	0.45380	0.14004	0.41241	1.0000
O	O62	1.0	0.34152	0.50009	0.50910	1.0000
O	O63	1.0	0.25810	0.47319	0.41474	1.0000
O	O64	1.0	0.46031	0.53358	0.42645	1.0000
O	O65	1.0	0.71087	0.34374	0.42902	1.0000
O	O66	1.0	0.84959	0.18066	0.42573	1.0000
O	O67	1.0	0.65916	0.15925	0.38542	1.0000
O	O68	1.0	0.84765	0.50346	0.43267	1.0000
O	O69	1.0	0.65716	0.52960	0.38763	1.0000
O	O70	1.0	0.98600	0.33910	0.44475	1.0000
O	O71	1.0	0.05204	0.14731	0.41219	1.0000
O	O72	1.0	0.05402	0.53247	0.42218	1.0000
O	O73	1.0	0.66965	0.31312	0.68782	1.0000
O	O74	1.0	0.82465	0.33151	0.76084	1.0000
O	O75	1.0	0.50885	0.32215	0.75655	1.0000
O	O76	1.0	0.51271	0.45635	0.67669	1.0000
O	O77	1.0	0.68043	0.70560	0.68052	1.0000
O	O78	1.0	0.83196	0.84971	0.69920	1.0000

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O	O79	1.0	0.51061	0.83403	0.68680	1.0000
O	O80	1.0	0.49444	0.64998	0.63936	1.0000
O	O81	1.0	0.66854	0.96488	0.65986	1.0000
O	O82	1.0	0.33121	0.69504	0.18852	1.0000
O	O83	1.0	0.17467	0.67894	0.26083	1.0000
O	O84	1.0	0.49314	0.68348	0.25625	1.0000
O	O85	1.0	0.48621	0.55105	0.17553	1.0000
O	O86	1.0	0.32177	0.30027	0.18071	1.0000
O	O87	1.0	0.16740	0.15895	0.19879	1.0000
O	O88	1.0	0.49314	0.17380	0.18681	1.0000
O	O89	1.0	0.50610	0.35722	0.13839	1.0000
O	O90	1.0	0.33440	0.04271	0.16204	1.0000
O	O91	1.0	0.02979	0.83342	0.01096	1.0000
O	O92	1.0	0.02889	0.51758	0.01693	1.0000
O	O93	1.0	0.97333	0.17329	0.51007	1.0000
O	O94	1.0	0.97233	0.49285	0.51725	1.0000
O	O95	1.0	0.49953	0.97927	0.22327	1.0000
O	O96	1.0	0.50509	0.02865	0.72293	1.0000
O	O97	1.0	0.22649	0.85151	0.08051	1.0000
O	O98	1.0	0.98541	0.86960	0.11552	1.0000
O	O99	1.0	0.14540	0.76457	0.16366	1.0000
O	O100	1.0	0.13898	0.01730	0.12330	1.0000
O	O101	1.0	0.44080	0.83119	0.07475	1.0000
O	O102	1.0	0.67531	0.86935	0.11187	1.0000
O	O103	1.0	0.52411	0.75820	0.15969	1.0000
O	O104	1.0	0.51696	0.01052	0.11780	1.0000
O	O105	1.0	0.25623	0.47533	0.08839	1.0000
O	O106	1.0	0.00968	0.49957	0.12293	1.0000
O	O107	1.0	0.17910	0.55362	0.17630	1.0000
O	O108	1.0	0.13353	0.32729	0.13623	1.0000
O	O109	1.0	0.48456	0.99660	0.61769	1.0000
O	O110	1.0	0.85874	0.99147	0.62134	1.0000
O	O111	1.0	0.74465	0.53384	0.58856	1.0000
O	O112	1.0	0.99139	0.50791	0.62324	1.0000

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O	O114	1.0	0.86918	0.68215	0.63629	1.0000
O	O115	1.0	0.56421	0.17421	0.57583	1.0000
O	O116	1.0	0.32682	0.13881	0.61216	1.0000
O	O117	1.0	0.47703	0.24935	0.65961	1.0000
O	O118	1.0	0.77986	0.16770	0.58212	1.0000
O	O119	1.0	0.01409	0.13368	0.61386	1.0000
O	O120	1.0	0.86693	0.24738	0.66630	1.0000
O	O121	1.0	0.13676	0.84003	0.32264	1.0000
O	O122	1.0	0.34396	0.00346	0.29424	1.0000
O	O123	1.0	0.19910	0.03191	0.36627	1.0000
O	O124	1.0	0.19954	0.95567	0.22432	1.0000
O	O125	1.0	0.86508	0.16753	0.82047	1.0000
O	O126	1.0	0.65945	0.00252	0.79378	1.0000
O	O127	1.0	0.80389	0.97571	0.86584	1.0000
O	O128	1.0	0.80143	0.05467	0.72271	1.0000
Si	Si1	1.0	0.34092	0.53950	0.05148	1.0000
Si	Si2	1.0	0.71034	0.80728	0.05739	1.0000
Si	Si3	1.0	0.71352	0.55066	0.06281	1.0000
Si	Si4	1.0	0.95400	0.80677	0.06149	1.0000
Si	Si5	1.0	0.96051	0.55271	0.06911	1.0000
Si	Si6	1.0	0.67654	0.21281	0.54959	1.0000
Si	Si7	1.0	0.66005	0.46921	0.55202	1.0000
Si	Si8	1.0	0.29081	0.19985	0.55770	1.0000
Si	Si9	1.0	0.28726	0.45706	0.56303	1.0000
Si	Si10	1.0	0.04768	0.20133	0.56082	1.0000
Si	Si11	1.0	0.04054	0.45611	0.56912	1.0000
Si	Si12	1.0	0.19191	0.34472	0.30440	1.0000
Si	Si13	1.0	0.44978	0.36776	0.30375	1.0000
Si	Si14	1.0	0.46331	0.74490	0.31098	1.0000
Si	Si15	1.0	0.47202	0.97944	0.28627	1.0000
Si	Si16	1.0	0.15683	0.52408	0.38337	1.0000
Si	Si17	1.0	0.81093	0.66338	0.80464	1.0000
Si	Si18	1.0	0.55291	0.64018	0.80432	1.0000

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Si	Si19	1.0	0.53882	0.26168	0.81141	1.0000
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Si	Si21	1.0	0.84485	0.48290	0.88309	1.0000
Si	Si22	1.0	0.63194	0.79662	0.94715	1.0000
Si	Si23	1.0	0.63549	0.54705	0.94938	1.0000
Si	Si24	1.0	0.27624	0.79410	0.93211	1.0000
Si	Si25	1.0	0.27907	0.53721	0.93483	1.0000
Si	Si26	1.0	0.03566	0.79836	0.94894	1.0000
Si	Si27	1.0	0.03657	0.54301	0.95379	1.0000
Si	Si28	1.0	0.46439	0.84551	0.86385	1.0000
Si	Si29	1.0	0.36970	0.21109	0.44739	1.0000
Si	Si30	1.0	0.36571	0.46022	0.44958	1.0000
Si	Si31	1.0	0.72546	0.21524	0.43228	1.0000
Si	Si32	1.0	0.72213	0.47197	0.43545	1.0000
Si	Si33	1.0	0.96622	0.21070	0.44843	1.0000
Si	Si34	1.0	0.96457	0.46654	0.45424	1.0000
Si	Si35	1.0	0.53740	0.16181	0.36388	1.0000
Si	Si36	1.0	0.54198	0.33512	0.69537	1.0000
Si	Si37	1.0	0.80708	0.72336	0.68986	1.0000
Si	Si38	1.0	0.55190	0.71099	0.68790	1.0000
Si	Si39	1.0	0.54111	0.95605	0.67215	1.0000
Si	Si40	1.0	0.45905	0.67211	0.19515	1.0000
Si	Si41	1.0	0.19467	0.28470	0.18968	1.0000
Si	Si42	1.0	0.45041	0.29639	0.18752	1.0000
Si	Si43	1.0	0.46210	0.05150	0.17268	1.0000
Si	Si44	1.0	0.52681	0.48197	0.12472	1.0000
Si	Si45	1.0	0.47352	0.52525	0.62564	1.0000
Si	Si46	1.0	0.16566	0.15426	0.38193	1.0000
Si	Si47	1.0	0.53216	0.55481	0.37421	1.0000
Si	Si48	1.0	0.46966	0.45276	0.87411	1.0000
Si	Si49	1.0	0.79539	0.33587	0.69879	1.0000
Si	Si50	1.0	0.32650	0.79608	0.04918	1.0000
Si	Si51	1.0	0.20572	0.67270	0.19900	1.0000
Si	Si52	1.0	0.83728	0.85383	0.88219	1.0000

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Si	Si53	1.0	0.20806	0.04439	0.17616	1.0000
Si	Si54	1.0	0.79400	0.96431	0.67555	1.0000
Si	Si55	1.0	0.79463	0.27735	0.81729	1.0000
Si	Si56	1.0	0.20730	0.73068	0.31765	1.0000