

Supplementary Information

Optimization of Stacked aromatic molecules:

Table1. Difference between geometric parameters obtained from MP2/cc-pVTZ optimization¹ and from the implemented Grimme parameterized dispersion empirical potential². Distance between the centres of the rings, and H-bond contacts between staked molecules are in angstrom. The angles between the planes of the rings are in degree.

		adenine/thymine	uracyl dimer	pyrazine dimer	indole/benzene	benzene dimer
Distance	MP2	3.19	3.37	3.48	3.51	3.77
	PBE+D	3.20	3.37	3.51	3.54	3.78
Angle	MP2	4	16	2	5	0
	PBE+D	5	16	2	6	0
H-bonds contacts	MP2	2.91/3.00	2.71/3.15	-	-	-
	PBE+D	2.87/2.93	2.58/3.08	-	-	-

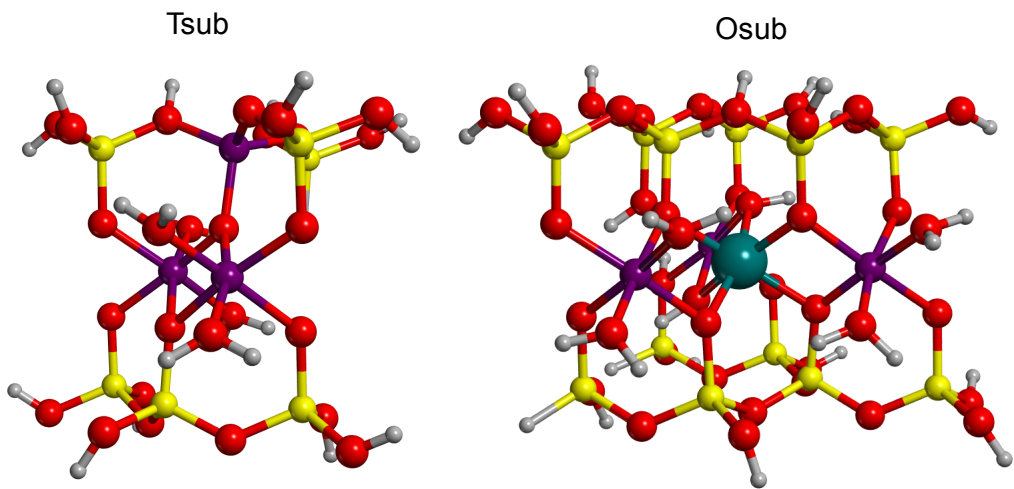
No significant change is observable within the periodic PBE/PAW+DISP_{Grimme} relaxation as compared to the gas phase MP2/cc-pVTZ. Only a strengthened of the H-bond contacts between stacked molecules can be seen which lead only to minor moves. Complexes without H-bond contacts show mainly a small augmentation of the distance between the centres of the aromatic cycles at a maximum of 0.03Å.

Proton affinities:

Table2. Proton Affinities of isolated bases and Osub/Tsub Montmorillonite model surface, computed from a cluster approach with G09³ at the PBE/6-31G* level:

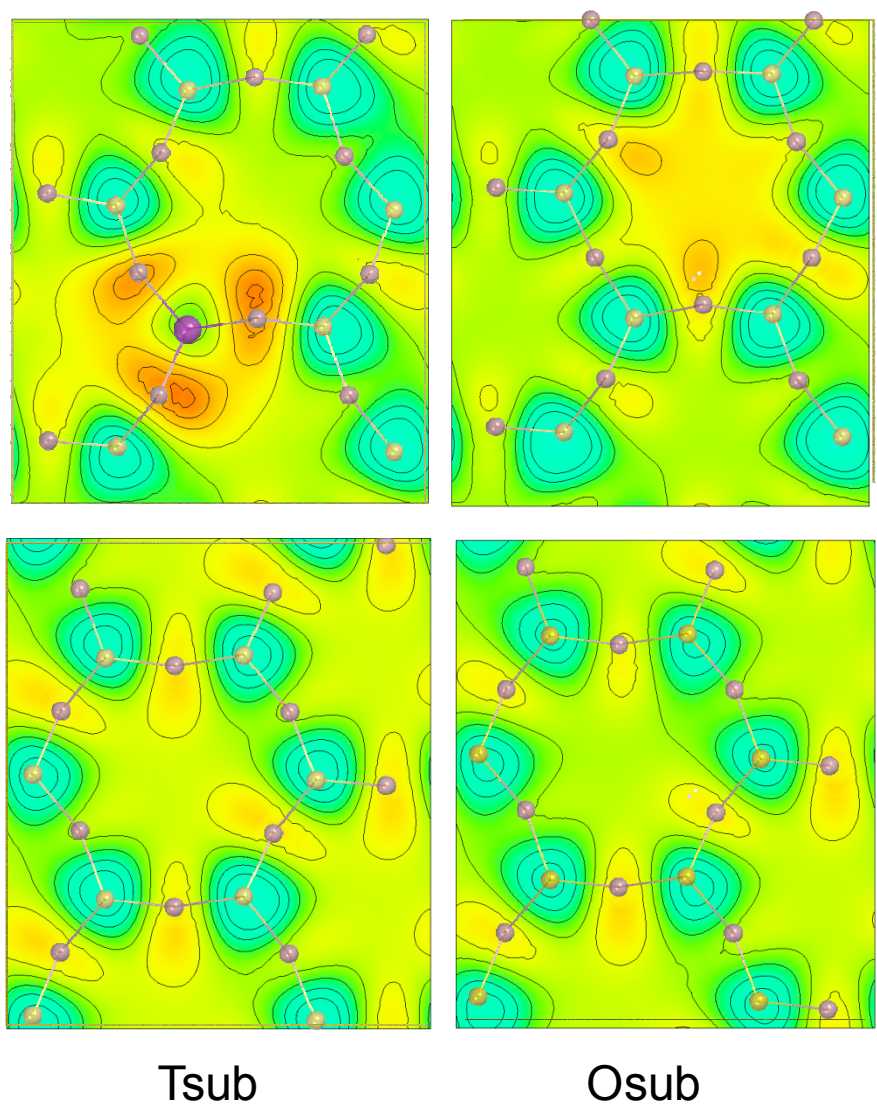
		PBE/6-31G*
MNT	Osub	248.8
	Tsub	279.7

Figure1. Cluster structures used to compute the proton affinities of the Osub and Tsub structures.



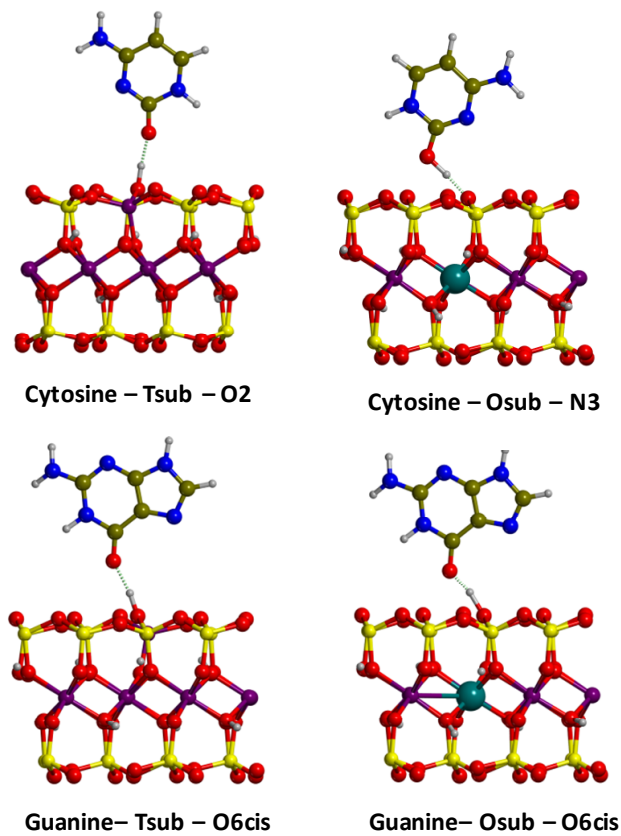
Molecular Electrostatic Potential Maps of Montmorillonite surface.

Figure 2. MEP maps projected on the ab plane, around 1.3 Å above the upper and lower surface of montmorillonite slab, for the tetrahedral and octahedral substitutions. MEP scale: from -6.2 to -2.0 eV. Most negative values are shown in red. Substituted sites are indicated with larger atom size.



Adsorption structures

Figure 3. Structures for wich the proton transfer did not occur (completely)



Free Cell parameters optimization:

Calculations with the cell parameters allowed to moved have been performed for the face to face orientation with cytosine interacting via O2 with Octahedral montmorillonite. The results are shown in the Supporting Information. For the cell parameters the changes are: $\Delta a = 8.9 - 9.055 = -0.155$ Å, $\Delta b = 10.28 - 10.438 = -0.158$ Å, $\Delta c = 30.00 - 30.038 = 0.038$ Å; i.e. less than 2%. The structural parameters are as follow:

	d H-Base (Å)	d H-O.MNT (Å)	d Base-MNT (Å)	θ Base-MNT (°)	H-Bond (Å)
a, b, c fixed	0.98	2.61	2.91	16.00	1.92/2.94
a, b, c free	0.98	2.73	2.87	15.00	2.00/2.83

The major difference is the difference in the distance between the proton and the surface oxygen atom ($\Delta d = 0.12$ Å) and a H-bond distance ($\Delta d = 0.08$ Å). However one can see that the proton has been transferred, and that the base is at almost the same distance and orientation (see angle) by letting the cell parameters free. Hence the fixed cell parameters may not include much difference in the obtained structures via the present methodology.

Optimization with a supplementary water molecule:

- (1) Valdes, H.; Pluhackova, K.; Pitonak, M.; Rezac, J.; Hobza, P. *Physical Chemistry Chemical Physics* **2008**, *10*, 2747.
- (2) Grimme, S. *J. Comput. Chem.* **2006**, *27*, 1787.
- (3) Frisch, M. J., et al. Gaussian 09, Revision A.1, Gaussian, Inc. Wallingford CT; Gaussian 09, Revision A.1, Gaussian, Inc. Wallingford CT, 2009.

Structures:

READ-ME:

- Coordinates are given in the moldraw format
- Names are difined as follow: NUCLEOBASE.Substitution-[ll for face-to-face, nothing for orthogonal orientation].Atom accepting the proton[vdw for the inclusion of VanDerWaals forces]
- Copy/paste from TITLE to the end of FRAG in a file: name.mol and open it with moldraw.

ADE.Osub-ll.N1vdw

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TITLE

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47	O	0.138644008018	0.850751349501	0.107488675567
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14	0.13805719058157431	0.87154040650317599	5.34495335467378013E-002
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BONDS

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6	0.68952354074707800	0.21933147264622571	0.38868259037458519
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7	0.56090817696691087	0.40996966741509261	0.33597271578649279
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BONDS

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1	0.73924463723368450	0.33487311598122682	0.10108724895824441
1	0.73615952464272461	0.83221616112693186	0.10285252630931339
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1	0.24345755136293190	8.70293599636100951E-002	9.93494806158777971E-002
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6	0.77103142248004575	0.17146695723369679	0.39477449674858189
6	0.56254853434255048	0.23549667237373209	0.35341829534004421
6	0.62191034256294175	0.36336976345432132	0.35579324668920759
6	0.68728641290802861	0.56962478473196576	0.34912018648490728
7	0.83940765450072818	0.28788734732144838	0.39813681392901412
7	0.64203230964205815	0.14121264726339089	0.37426662752032941
7	0.43396381434829612	0.20379159806093011	0.33270343676760078
7	0.579260338451550232	0.48431172915923559	0.33944294874005970
7	0.79534806607651809	0.51060560917436759	0.37310761104742368
8	0.77709507111650578	0.56623782218434593	0.25974704867115228
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8	0.25963866837751431	0.31976351758140192	0.25765187596977168
8	0.18553176031550470	0.56532337152813184	0.24796784949893391
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8	0.33207596808061057	0.44038626896923683	0.18145073681855059
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8	0.83680969727319365	0.68982656761467198	0.18146916104904151
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BONDS

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6	0.48458085240244608	0.47491806842722328	0.40916942426445152
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7	0.47711943566014309	0.70814524934847412	0.40567082301313162
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2 16 3 20 4 20 5 19 6 52 7 26 8 43 9 37 12 66 13 60 14 22 15 16 15 19
16 17 17 20 17 21 18 19 18 21 18 22 23 79 23 83 24 79 24 91 25 80
25 82 26 72 26 76 27 71 27 73 27 80 28 73 28 82 29 79 29 81 30 81
30 93 31 81 31 88 32 72 32 76 33 71 33 73 33 81 34 71 34 76 34 79
35 83 36 83 36 84 37 71 37 75 38 74 38 76 38 83 39 75 39 88 40 85
40 90 41 80 41 86 42 85 42 86 43 74 44 75 44 85 45 75 45 90 46 84
46 87 47 87 47 88 48 74 49 75 49 87 50 84 51 86 51 89 52 71 52 75
53 74 53 76 53 89 54 71 54 76 54 86 55 82 57 90 58 82 59 91 60 73
60 77 61 72 61 78 61 91 62 73 62 93 63 92 64 80 64 92 65 92 65 94
66 73 66 77 67 72 67 78 67 94 68 77 68 78 68 92 69 91 70 93 71 75 1 1
10 10 11 11 56 56

BONDS

1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 3 3 3 3 3 2 2 2 2 2 3 3 2 2 2 2 2 3 3 1
2 3 3 2 2 2 2 2 2 2 2 1 2 1 2 3 3 3 1 1 1 1 1 3 3 2 1 2 2 3 3 3 1 1
7 4 6 4 7 6 3 3 4 4 4 4 4 3 3 4 3 3 2 3 4 4 3 2

FRAG

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1 1

CYT.Osub-N3O2vdw

TITLE

formed from CONTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

COORD

1	0.49258802907145882	0.60193235480042873	0.46287804296783408
1	0.47620206541823490	0.35816506952979638	0.45731092211840579
1	0.46825400398208522	0.20580614855544310	0.34313833352612078
1	0.46486943076830428	0.17233132041706190	0.40070091348598108
1	0.50089705276327645	0.72506929961108491	0.39541861842820603
1	0.25034699106473263	0.61057825393447884	9.00549143625972021E-002
1	0.75145404683045036	0.34380713473633001	9.58134847526222050E-002
1	0.73995739804821814	0.83532436261145337	0.10290120156327590
1	0.54633996166443022	0.75484196829909678	0.18420564434063269
1	6.33580416072379998E-002	0.49332750701189149	0.17834826740623549
1	5.11343894781425001E-002	0.99550891823112286	0.18501049858877111
1	0.23737603545508110	8.30214230372656042E-002	0.10462838809787900
1	0.55541187472921161	0.24800816169757900	0.18169038767138360
1	0.49038246832076621	0.59427719308077720	0.28869204654866171
6	0.48942957178220081	0.55070389585223278	0.43110183018447801
6	0.48069772100690628	0.41875248185732511	0.42756878433768020
6	0.47833640446499842	0.36548124256700920	0.38323340025633662
6	0.49016396049139649	0.56964045629914983	0.35195424073988762
7	0.49455267384218388	0.62628496007051970	0.39374691715120608
7	0.47103203094016483	0.23735482481328610	0.37543853755206541

7	0.48338404041347172	0.44206480166007700	0.34716603173234462
8	0.49273472222740339	0.64965996085010391	0.31888466261735032
8	0.76475777044845228	0.57128574772599305	0.25849672783550443
8	0.70260997708424711	0.31791922806022183	0.25242416816421059
8	0.30337617855570742	0.33690449932906730	3.25691662760980993E-002
8	0.83609914922063600	0.38344200433700232	0.11109334358212480
8	0.45154223270515448	0.37538082748976742	0.10836890987573430
8	0.14427451941687930	0.34378571606510938	0.10938990098029230
8	0.48821002752030690	0.49746989764001032	0.25376308515474838
8	0.26710430239487221	0.32324160263205048	0.25885224622764957
8	0.20953342437290151	0.57341573751890473	0.25195521207853983
8	0.96665717960467812	0.44850436106889580	0.17763373538853869
8	0.32206155861220659	0.44016461864927142	0.18118664750080679
8	0.65883522124360205	0.47246579452930421	0.18108347239692851
8	0.98727045002019698	0.73891476294635217	0.25834954457124648
8	0.70464814827783917	0.81901276369222276	0.25072679605699238
8	0.45226578117725208	0.70762035038326809	0.18142580385282461
8	0.83746695277517980	0.69451188845369449	0.18182261371853520
8	0.14416774477921920	0.73258415015970291	0.18186754256335980
8	0.30326062709147472	0.83920655573941194	3.46058908734781026E-002
8	0.52399002335862666	0.50996097186988365	3.47495472556558979E-002
8	0.58947233818825118	0.76318849416731260	4.16866804069875030E-002
8	0.82827500049337910	0.88249790802818151	0.11310545031825890
8	0.45466025277908018	0.88872707059991540	0.11053585728592190
8	0.14193410546779700	0.85565002636427590	0.11044146641946739
8	0.48768652497817350	0.99049955182827787	0.25859215819217712
8	0.26387786915057199	0.82485803875389596	0.25851036637125929
8	0.95797981589174974	0.94856638987247954	0.17930578666658140
8	0.33220122599461749	0.95135914812634181	0.18208193046230170
8	0.64467733594595134	0.98171291291504337	0.18204357002816049
8	0.80633717627128854	0.58870191292589391	3.26740066575353996E-002
8	0.32887555113151928	0.64617583891316555	0.10867944374464331
8	0.95781190986964004	0.63682931159085132	0.10982182411418710
8	0.65809437810668636	0.60438595557067365	0.10888110481094020
8	1.93016089543222996E-002	0.26058406162704889	3.41287891632384016E-002
8	8.90106031086933952E-002	1.32722395319937996E-002	4.14024064764094979E-002
8	2.39218355337535993E-002	0.76023884816149090	3.43229768265453997E-002
8	9.21753012038250968E-002	0.51215402521328102	4.22562958874320022E-002
8	0.98702191282007024	0.24221393727543061	0.25829427168573299
8	0.46177180276319091	0.19938989982203861	0.17898897880319201
8	0.83478245648758687	0.19641353534651071	0.18211688663535819
8	0.14410435458962681	0.22635271700125181	0.18199172552059831
8	0.52021324470679720	1.05721522896382002E-002	3.44212385393988032E-002
8	0.59216411054911677	0.26192552793363427	4.04109854431429008E-002
8	0.80284677613329958	8.48243932054244948E-002	3.43698616229332968E-002
8	0.32787484116079768	0.13033000592226801	0.11275835216619180
8	0.95188023950171030	0.13415843783598549	0.11003787964305790
8	0.64399121386222558	0.10002170303300220	0.11006648646405290
8	0.76748612310540221	7.03947210955570973E-002	0.25836731511114058
8	0.20637063549003501	7.28169631808845974E-002	0.25259432219686972
12	0.47611586142287737	0.54303423335002954	0.14400126599469160
13	0.97689603121187563	0.29042518323932193	0.14501493222275830
13	0.31244022461041288	0.28841680884775361	0.14443878922964781
13	0.97682866702256499	0.79171863503480977	0.14527816863304710
13	0.31159052421633898	0.78919049623142934	0.14507668264134219
13	0.81332271269092171	0.53840794910374157	0.14442804802218651
13	0.47625575480082200	4.27552023063726000E-002	0.14566381076566870
13	0.81058347424869870	3.88758328231055966E-002	0.14548324211044539
14	0.65928495836724343	0.46231774558689998	0.23433879761545590
14	0.46675036138369841	0.37054280230036851	5.44977792122506022E-002
14	0.31891583214694191	0.45796040844068647	0.23430716259974380
14	0.13931942238147330	0.36364911192483368	5.48413599101970975E-002
14	0.82472715702278043	0.70728498442267174	0.23613410429054510
14	0.65276166500686772	0.96476861110305079	0.23643500019289759
14	0.46650668073826090	0.87235153192770853	5.58084630661892997E-002
14	0.64135907580976548	0.61604329817562431	5.50201156644481992E-002
14	0.32326694612042439	0.96048876212876133	0.23651396864652319
14	0.15307798141459539	0.71704531300567842	0.23626753050250951
14	0.96787047976195784	0.62205079354785264	5.50394506161625968E-002
14	0.13789637958856721	0.8666333906167861	5.54137399234983022E-002
14	0.82434888086014857	0.20759874331928249	0.23673961068561220

14	0.63715897928978227	0.11486236459003581	5.50803859017562972E-002
14	0.15279878811625119	0.21670578041837549	0.23655317693617051
14	0.96553805135170601	0.12208559300888530	5.50705928359519967E-002

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BARICE

4.75869503382583 5.12434548723093 4.8696332177631

CONNB
117

1 15 2 16 3 20 4 20 5 19 6 52 7 26 8 43 9 37 12 66 13 60 14 22 14 29
15 16 15 19 16 17 17 20 17 21 18 19 18 21 18 22 23 79 23 83 24 79
24 91 25 80 25 82 26 72 26 76 27 71 27 73 27 80 28 73 28 82 29 79
29 81 30 81 30 93 31 81 31 88 32 72 32 76 33 71 33 73 33 81 34 71
34 76 34 79 35 83 36 83 36 84 37 71 37 75 38 74 38 76 38 83 39 75
39 88 40 85 40 90 41 80 41 86 42 85 42 86 43 74 44 75 44 85 45 75
45 90 46 84 46 87 47 87 47 88 48 74 49 75 49 87 50 84 51 86 51 89
52 71 52 75 53 74 53 76 53 89 54 71 54 76 54 86 55 82 57 90 58 82
59 91 60 73 60 77 61 72 61 78 61 91 62 73 62 93 63 92 64 80 64 92
65 92 65 94 66 73 66 77 67 72 67 78 67 94 68 77 68 78 68 92 69 91
70 93 71 75 10 10 11 11 56 56

BONDS

1 1 1 1 1 1 1 1 1 1 1 1 1 2 3 3 3 3 3 3 2 2 2 2 2 3 3 2 3 2 2 2 3 3 1
2 3 3 2 2 2 2 2 2 2 2 1 2 1 2 3 3 3 1 1 1 1 1 3 3 2 1 2 2 3 3 1 1
7 4 6 4 7 6 3 3 4 4 4 4 4 3 3 4 3 3 2 3 4 4 3 2

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CYT.Osub-O2-TRANS

TITLE

formed from OUTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

COSYMB

1	H	0.465149210789	0.776748450170	0.344153707738
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3	H	0.482165804886	0.457075714861	0.488382884020
4	H	0.471308436859	0.625930696940	0.495813671372
5	H	0.481367766078	0.572978416548	0.306293555359
6	H	0.246050852662	0.603137491812	0.092839084770
7	H	0.746589815502	0.336755774015	0.099933552541
8	H	0.739464718014	0.829668507673	0.105125978714
9	H	0.546520304624	0.747408369600	0.185776917828
10	H	0.064578794183	0.489051297900	0.179237784262
11	H	0.052374035120	0.991732210192	0.186039175051
12	H	0.235880668115	0.075558068583	0.107295842854
13	H	0.557082980444	0.242664394995	0.181700677864
14	H	0.489463732213	0.364918211270	0.307359673107
15	C	0.470753783213	0.688325823810	0.364227899952
16	C	0.469782385393	0.685896822394	0.409794990025
17	C	0.477433577216	0.561143203495	0.430534335310
18	C	0.485406665856	0.458355826945	0.362974194058
19	N	0.478874221151	0.575033671766	0.341037128853
20	N	0.477341206096	0.548047903719	0.475246082197
21	N	0.484905381354	0.449967154065	0.406966425257
22	O	0.492499534427	0.349422877927	0.340186040882
23	O	0.760652805643	0.567505159721	0.260051273397
24	O	0.705656167284	0.313175358763	0.253730580365
25	O	0.302425327833	0.332474553637	0.033446136489
26	O	0.835008550287	0.378030788516	0.112656731645
27	O	0.452068455533	0.368315927150	0.109429104156
28	O	0.144490766813	0.338634347459	0.110261327279
29	O	0.487501451429	0.476336184886	0.257521692480
30	O	0.264675263777	0.317017485014	0.259563201990
31	O	0.212820487462	0.568327505733	0.252773193973
32	O	0.968001513876	0.444022133890	0.178676979178
33	O	0.322618441298	0.434758161732	0.181944901024
34	O	0.657954820428	0.468653828827	0.182575910664
35	O	0.987515425001	0.731403395309	0.259460103600

36	O	0.705112210209	0.814029454771	0.252259631734
37	O	0.452415715473	0.700258840658	0.182818573597
38	O	0.837405666578	0.690118685721	0.183122609082
39	O	0.144325292331	0.728279045029	0.183084725855
40	O	0.303458598645	0.833706884048	0.035753939613
41	O	0.526075955830	0.502427945431	0.036111393225
42	O	0.589132231063	0.755194864578	0.042479315528
43	O	0.828514352021	0.877890215044	0.114201034537
44	O	0.456282299512	0.881752499121	0.111591215441
45	O	0.142862610040	0.851886004694	0.111653200783
46	O	0.488423041947	0.983711874211	0.259693181530
47	O	0.265077046724	0.818440234945	0.259921015779
48	O	0.959060041191	0.945115259852	0.180265614012
49	O	0.334224411501	0.944482271774	0.183195789333
50	O	0.645856554611	0.976502553480	0.183101733357
51	O	0.807870570526	0.582987449345	0.033887108220
52	O	0.327610853939	0.640118305302	0.109959303489
53	O	0.958319699399	0.633270399934	0.111064978054
54	O	0.658657398124	0.599023553984	0.110168007342
55	O	0.018289262564	0.257053518501	0.034870353336
56	O	0.090537538899	0.009698952211	0.042408382921
57	O	0.023385818034	0.757458264401	0.035504161606
58	O	0.093209738421	0.508998297170	0.043883999111
59	O	0.987449451915	0.235800402470	0.259009536073
60	O	0.463154752311	0.194010846143	0.179916554668
61	O	0.834712387790	0.191969276404	0.182937382374
62	O	0.144621724697	0.220619014369	0.182748130216
63	O	0.522558949071	0.002485388721	0.035294682272
64	O	0.589687605724	0.254263705632	0.040900758875
65	O	0.803866079011	0.079839998186	0.035218848550
66	O	0.327246063552	0.123635841453	0.113978771886
67	O	0.952417011195	0.129624831243	0.110804390920
68	O	0.644238752613	0.094954186299	0.110881105697
69	O	0.768181513045	0.065096543792	0.259150746281
70	O	0.206107463306	0.065709167031	0.252956911684
71	MG	0.476365533377	0.537187120736	0.144842239143
72	AL	0.978301196411	0.285011797992	0.145929099927
73	AL	0.312587146249	0.282505200788	0.145556002667
74	AL	0.977729763979	0.788841142772	0.146598862433
75	AL	0.312642606769	0.783299307337	0.146166442684
76	AL	0.814518098406	0.534491309693	0.145613883926
77	AL	0.477178757255	0.037217486046	0.146625842295
78	AL	0.811135595112	0.035221998545	0.146222864881
79	SI	0.658816146359	0.456797907960	0.235724114964
80	SI	0.466039567932	0.363570208850	0.055478395595
81	SI	0.318654537445	0.450892275241	0.234988928055
82	SI	0.138520109575	0.359538849337	0.055679728589
83	SI	0.824110526232	0.701891182463	0.237418203325
84	SI	0.653510162536	0.959571707806	0.237561183326
85	SI	0.467473810044	0.864898736428	0.056739506582
86	SI	0.642799522360	0.609019697024	0.056242788839
87	SI	0.324598705657	0.954108260257	0.237636790625
88	SI	0.153368757266	0.711475349857	0.237380716330
89	SI	0.968551406898	0.619084090612	0.056189851792
90	SI	0.138584254359	0.863050434940	0.056604713386
91	SI	0.824743076926	0.201933382626	0.237679850861
92	SI	0.637806713196	0.108458689200	0.055747162450
93	SI	0.152292941183	0.209373578351	0.237320639214
94	SI	0.966197773628	0.118029782326	0.055779067134

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CYT.Osub-O2vdw

TITLE

formed from OUTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

COSYMB

1	H	0.467630357229	0.774976538078	0.454121383646
2	H	0.474685571628	0.545008935604	0.483599090214
3	H	0.492899001639	0.269389837183	0.403015218583

4	H	0.486719541577	0.311337453085	0.459836341565
5	H	0.472218836106	0.804763711951	0.374847116142
6	H	0.247978959487	0.601402122647	0.092373815331
7	H	0.744695514785	0.332288022225	0.101254998105
8	H	0.739391317050	0.826539332063	0.104870534081
9	H	0.547502473432	0.745599274833	0.185365706681
10	H	0.063446656037	0.486138197096	0.180075226548
11	H	0.052110360707	0.986820891828	0.186196527615
12	H	0.235235123769	0.074319273703	0.107002115927
13	H	0.556559086311	0.238699066716	0.182370436004
14	H	0.486644518996	0.569953791596	0.291669955168
15	C	0.473150516875	0.690043173260	0.432467786981
16	C	0.476907274334	0.565393647307	0.447990548593
17	C	0.483963203155	0.464155054446	0.415128308886
18	C	0.482859042781	0.611556879599	0.357455090290
19	N	0.476141990121	0.713123767816	0.387880721603
20	N	0.488161887935	0.338144654846	0.427358938392
21	N	0.486722873309	0.488424234521	0.371254491479
22	O	0.484661174795	0.647892921114	0.316825375344
23	O	0.761911202896	0.564506980214	0.260768133397
24	O	0.704184267707	0.309855298340	0.254424540582
25	O	0.302147907180	0.330653476137	0.034113102951
26	O	0.833596929366	0.374244893410	0.113427372218
27	O	0.451831496362	0.366488751247	0.109934160387
28	O	0.144085534701	0.336475550447	0.111123157683
29	O	0.487161567870	0.481443628277	0.258388062639
30	O	0.264971381318	0.312896456454	0.260640844604
31	O	0.210490551725	0.564518661646	0.253478476183
32	O	0.967220775862	0.440584910215	0.179374254519
33	O	0.324803608503	0.430788444285	0.183488189756
34	O	0.656789656389	0.465486848239	0.183742408183
35	O	0.987172637014	0.728677615657	0.259865508515
36	O	0.705786025019	0.812148088099	0.252389970968
37	O	0.452988736816	0.698740303268	0.183074620978
38	O	0.836798323368	0.686161539184	0.183628530708
39	O	0.144181875009	0.723443735136	0.183342042704
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8	0.32932655653683529	0.44689907659713218	0.18091654679346081
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8	0.98133849185938271	0.75804894054595540	0.25656241970022869
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13	0.30792645509739758	0.29289678989542239	0.14497492688757141
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8	0.14647639556049941	0.23307548854306501	0.18126119011545369
8	0.51806715894411703	1.42386397210761007E-002	3.34138500276060027E-002
8	0.59097377967178588	0.26589751016797769	4.19161470918167980E-002
8	0.80225209592110225	8.82353537666866056E-002	3.33165822456846991E-002
8	0.33407578350133732	0.13615959429226579	0.11217550586249510
8	0.95322301066619874	0.13592193403826300	0.10907068842551690
8	0.64543902695209365	9.92949506217631062E-002	0.10907916975400740
8	0.77973442249153002	6.11754486667821021E-002	0.25670338128685238
8	0.20604560145013029	7.06256710181330932E-002	0.24945032088369429
13	0.48170831449653351	0.54370022656210004	0.14547628313976410
13	0.97700165839477482	0.29180899617532191	0.14507078668685491
13	0.31432801231929292	0.29152936735385560	0.14546540705787800
13	0.97867249346969720	0.79130693548165221	0.14489241859172081
13	0.31449444195596482	0.79133518661555502	0.14478493176632801
13	0.80987932938510288	0.54008567607794522	0.14538754006615909
13	0.47938695928221381	4.33523000807789979E-002	0.14491536986940901
13	0.81314575132305544	3.94160792023185019E-002	0.14485357236933191
13	0.65649860671635929	0.46460840029679101	0.23599225168031579
14	0.46577168643914330	0.37510719484091298	5.47105188956122993E-002
14	0.32089324014139597	0.46288406844090851	0.23623198240565571
14	0.13823054214527589	0.36464244910807492	5.48625608509911988E-002
14	0.82999585307261325	0.70936519149773170	0.23654414169462659
14	0.65604894785332624	0.96374261702027486	0.23520950113662900
14	0.46536824464220888	0.87469719609828089	5.38937354852343023E-002
14	0.63665159334490873	0.61843534231685493	5.37207376339133014E-002
14	0.32868472177159269	0.96088354704774404	0.23526329454348871
14	0.15406195593886329	0.72127734414059452	0.23510428714101830
14	0.96510712121656861	0.62128889795085240	5.46938709103318987E-002
14	0.13669211496253661	0.86394256278178538	5.41836986596810968E-002
14	0.82389195317878394	0.20401807204101310	0.23600841269047371
14	0.63688114190849776	0.11727039406926230	5.43408492964230008E-002
14	0.15347709300338550	0.21703441153762620	0.23574826084705661
14	0.96573225470865998	0.12218434717705370	5.43184339380193976E-002

-1 0 0 0

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4.88192262484917 5.02422327105572 4.81228501754542

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116

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29 81 30 81 30 93 31 81 31 88 32 72 32 76 33 71 33 73 33 81 34 71

34 76 34 79 35 83 36 83 36 84 37 71 37 75 38 74 38 76 38 83 39 75

39 88 40 85 40 90 41 80 41 86 42 85 42 86 43 74 44 75 44 85 45 75
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59 91 60 73 60 77 61 72 61 78 61 91 62 73 62 93 63 92 64 80 64 92
65 92 65 94 66 73 66 77 67 72 67 78 67 94 68 77 68 78 68 92 69 91
70 93 10 10 11 11 56 56

BONDS

1 1 1 1 1 1 1 1 1 1 1 1 1 2 3 3 3 3 3 3 2 2 2 2 2 3 3 2 3 2 2 2 3 3 1
2 3 3 2 2 2 2 2 2 2 2 2 1 2 1 2 3 3 3 1 1 1 1 1 3 3 2 1 2 2 3 3 3 1 1
6 4 6 4 6 6 3 3 4 4 4 4 4 3 3 4 3 3 2 3 4 4 3 2

FRAG

1
1
1
1 1

CYT.Tsub-N3O2vdw

TITLE

formed from CONTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

COORD

1	0.48965675891272231	0.59553114509586991	0.46807042407899890
1	0.48176232489687310	0.35141207589999690	0.46146340301555328
1	0.47082165700011680	0.20257507383742651	0.34722081452273518
1	0.47461469038938431	0.16780650769162159	0.40463254269215709
1	0.48775307639397508	0.72101782715104146	0.40115282644261158
1	0.24483318165480669	0.59080899482604843	0.10202603580048300
1	0.74551309409839173	0.34082277170286679	9.98967040241054011E-002
1	0.74210229788484905	0.83792158353293789	0.10115326314141780
1	0.54233878216677545	0.73882628992403943	0.19387566719795810
1	3.55447723886765030E-002	0.48863566749381271	0.19371257016764401
1	5.18353141737702972E-002	0.99335247597196463	0.18603372049436201
1	0.24842628358844190	9.35169363327794934E-002	9.94578051047047967E-002
1	0.54040096785844838	0.23911582217968891	0.19503997413671501
1	0.47776083869908420	0.57784746489754912	0.28696239205215601
6	0.48545410040453107	0.54545878661083680	0.43606349681098810
6	0.48127258394086792	0.41343504409467952	0.43206473039359983
6	0.47638861197101062	0.36225086654205602	0.38744639783131302
6	0.47883179839366707	0.56846382474150636	0.35628992072830262
7	0.48428639502031690	0.62222244162882379	0.39904803475945427
7	0.47214082829566267	0.23347122313706400	0.37953189035223273
7	0.47530715572035431	0.43903951205344488	0.35164125876131580
8	0.47739190126193082	0.64646527015410737	0.32368316046720841
8	0.78525402954581847	0.57215464980169428	0.25937218324511652
8	0.69093021717034320	0.30025868536415901	0.24823655895845040
8	0.30538114893993518	0.33830346270447059	3.29368197708772015E-002
8	0.83501933902947567	0.38529155579676649	0.11051590413625510
8	0.45372112408646648	0.39041179166224388	0.10841835765564679
8	0.14635095504123291	0.34976944769301288	0.10871164512543929
8	0.47971700892396368	0.51119672592970422	0.25679453541602798
8	0.26708189286707479	0.32710943462519421	0.25635890306384829
8	0.19317165176401119	0.57404399442424003	0.24781485217787100
8	0.95436559917272423	0.44508262946408822	0.17815022500458680
8	0.33937421610836560	0.44761686431288622	0.18079649966373240
8	0.64591756600496741	0.48673867611167793	0.17788525804454450
8	0.98854012183615347	0.75915401804947824	0.25552485186976043
8	0.69394010436407216	0.81175023973998772	0.24643153387852559
8	0.45842123559462322	0.70028389970101135	0.17792460431017129
8	0.84388865927578405	0.69468958449757301	0.18074214674705369
8	0.14861055581082430	0.73710548787657160	0.17991994668509209
8	0.30476380939453579	0.83919958252853111	3.24279801807198023E-002
8	0.52096229923709081	0.51455516682657421	3.21743891908300994E-002
8	0.59105938371159661	0.76741241508566549	3.94618299922869994E-002
8	0.83206602661442364	0.88329747491984245	0.11098878506744569
8	0.45475224959660648	0.88934982955550279	0.10815824610665520
8	0.14638948883317729	0.84956465249344792	0.10805501884992960
8	0.49264744785813408	0.99658242473965331	0.25586024470161889
8	0.27383359628627330	0.82438354762370103	0.25588673150161079
8	0.96173916629106326	0.94784876163751663	0.17651745575707720

CYT.Tsub-O2-TRANS

TITLE

formed from OUTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

COSYMB

1		0.465492835792	0.782175557142	0.352167695837
2	H	0.455250987433	0.766496512858	0.436710408633
3	H	0.465069011547	0.438861763282	0.489881919124
4	H	0.454189701967	0.606267123709	0.500459778067
5	H	0.481337150759	0.582518196463	0.309917860912
6	H	0.245239197845	0.584819123385	0.103318202447
7	H	0.742980598454	0.334429131124	0.104015626577
8	H	0.742442151665	0.832849824065	0.103264336962
9	H	0.546938614231	0.735864710527	0.192726770335
10	H	0.038028641312	0.484223366756	0.195209599365
11	H	0.049669509824	0.987163851624	0.189464897993
12	H	0.246751101008	0.088099001205	0.101766673542
13	H	0.541205662806	0.233999605336	0.196200036271
14	H	0.488435424202	0.381424541153	0.306913055745
15	C	0.468416818823	0.690241021934	0.370290492696
16	C	0.462813700502	0.680295117987	0.415754637177
17	C	0.467276321267	0.552243907666	0.434088125508
18	C	0.481431658576	0.460890957041	0.364673720281
19	N	0.477787024594	0.581217968447	0.344934357399
20	N	0.462075572232	0.531863976800	0.478491654069
21	N	0.476724665594	0.445183047028	0.408507825439
22	O	0.489933660621	0.356949950871	0.339593273922
23	O	0.781895241069	0.568748611776	0.261096326571
24	O	0.692217176792	0.296813929262	0.250227771740
25	O	0.305207081491	0.334394875181	0.034013541509
26	O	0.834483957863	0.379923545489	0.112457989519
27	O	0.454491999914	0.384727619508	0.109634212000
28	O	0.146972835318	0.345634007996	0.110101158721
29	O	0.480235377665	0.488413158356	0.261787279608
30	O	0.264873338120	0.319783078973	0.257997512524
31	O	0.197409783370	0.567825374405	0.249505346435
32	O	0.956154356917	0.441525470570	0.179667525580
33	O	0.339922107582	0.442658906890	0.182337491791
34	O	0.646031535112	0.482114031417	0.179362028353
35	O	0.990207362534	0.751774634229	0.257126102790
36	O	0.695709714781	0.808498382793	0.248578367402
37	O	0.459342690978	0.694829069308	0.179463908918
38	O	0.843325879041	0.690143630281	0.182349714435
39	O	0.149538309154	0.731273009450	0.181468278568
40	O	0.305230000328	0.834757974494	0.033800391906
41	O	0.523134124805	0.508183898153	0.033385938925
42	O	0.591282876181	0.760732495842	0.040496586035
43	O	0.832800568585	0.878560699498	0.112612642783
44	O	0.455920173542	0.883399568020	0.109451203005
45	O	0.147440957863	0.844885243137	0.109640311052
46	O	0.492094314418	0.990381070817	0.257469519525
47	O	0.275818896145	0.817157483129	0.257739979421
48	O	0.961390349204	0.942631268942	0.178137204963
49	O	0.340072793680	0.942053076861	0.181477450823
50	O	0.647430751376	0.977876960295	0.181229408177
51	O	0.806066590715	0.584773998054	0.033172237710
52	O	0.335183102739	0.630544203784	0.112966376163
53	O	0.955235011297	0.631776464077	0.109752988666
54	O	0.647520497106	0.600052400977	0.108556900122
55	O	0.024005666190	0.257459315524	0.033896974766
56	O	0.091562416004	0.009430956380	0.041835662500
57	O	0.023477446461	0.757345110778	0.033915788416
58	O	0.091917216817	0.509484417394	0.042026778705
59	O	0.986797262108	0.236439509460	0.257704829109
60	O	0.459490626085	0.193755960874	0.179507471296
61	O	0.841330341793	0.187417057364	0.181702432551
62	O	0.147766698797	0.229696300448	0.181779293609
63	O	0.522535615226	0.008985330470	0.033983415598

64	O	0.591560140621	0.260510636431	0.042080346128
65	O	0.805079560382	0.084772757540	0.033836742368
66	O	0.335713886616	0.132099133305	0.112982963976
67	O	0.955861869002	0.132452388121	0.109547876134
68	O	0.647541742262	0.095808196269	0.109794724195
69	O	0.781363964261	0.054099107244	0.256951386923
70	O	0.205934427178	0.065738025557	0.249702332730
71	AL	0.484326736417	0.539669418265	0.146134691457
72	AL	0.979143401384	0.287880798212	0.146250574901
73	AL	0.316321257166	0.288387024736	0.145978250592
74	AL	0.980179198499	0.785846892468	0.145570265914
75	AL	0.316325935986	0.786732388677	0.145161969440
76	AL	0.811096623213	0.535940736839	0.145970339611
77	AL	0.481065556425	0.039414195101	0.145939526870
78	AL	0.815431956871	0.035536965347	0.145246240541
79	AL	0.660666103329	0.458287091982	0.236769080619
80	SI	0.468015683494	0.370856531121	0.054903485531
81	SI	0.321757231559	0.457435488304	0.236420989104
82	SI	0.139977275770	0.362113535145	0.055319873887
83	SI	0.828183243339	0.702545835705	0.237279974959
84	SI	0.656578854174	0.958108534847	0.235625969212
85	SI	0.468459499379	0.870125209524	0.054599776989
86	SI	0.640333235134	0.613348220009	0.053998885583
87	SI	0.328958599028	0.955930573092	0.235962702930
88	SI	0.153636950919	0.716983720052	0.235944744441
89	SI	0.968222008328	0.619497572470	0.054948229207
90	SI	0.139845551916	0.861936351289	0.055020239156
91	SI	0.823491197452	0.197626967110	0.236640739733
92	SI	0.639803397911	0.113010097339	0.055081319662
93	SI	0.152152531489	0.212117406714	0.236281925242
94	SI	0.968303662479	0.119761016305	0.054816500374

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CYT.Tsub-O2vdw

TITLE

formed from OUTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

COSYMB

1	H	0.476627979165	0.778239089454	0.459903545367
2	H	0.472276374730	0.580804903004	0.510188525232
3	H	0.464803282324	0.250750940751	0.460346441118
4	H	0.467235930720	0.339855357373	0.510255059825
5	H	0.474349552191	0.742524327408	0.381313512606
6	H	0.246744626023	0.587990219412	0.099565164429
7	H	0.746398377528	0.336961031997	0.098236923102
8	H	0.743475917944	0.834470440298	0.099502146662
9	H	0.543890301907	0.736070169030	0.191800420242
10	H	0.035431236017	0.486078139324	0.192047681353
11	H	0.051028144295	0.989512286959	0.185549075071
12	H	0.248962082441	0.090306570444	0.097780526517
13	H	0.538736532760	0.234195577790	0.194501446289
14	H	0.476152400516	0.509690256216	0.291808873130
15	C	0.474255364370	0.678910254349	0.447201421558
16	C	0.472059697875	0.571813751075	0.474038613461
17	C	0.469159270734	0.448018801988	0.451911276228
18	C	0.468823318255	0.541446507486	0.381374101643
19	N	0.473291647163	0.664557943167	0.402311663542
20	N	0.467627322569	0.337420636850	0.476520401207
21	N	0.467835795132	0.434256613661	0.407699763382
22	O	0.465261759048	0.541645573787	0.339991451542
23	O	0.784890631528	0.569030632079	0.257590448368
24	O	0.689813937381	0.296125495253	0.246189081665
25	O	0.305755768793	0.334905208264	0.031473031292
26	O	0.835557073987	0.381679741963	0.108966563036
27	O	0.453825091663	0.386601562254	0.107131907252
28	O	0.147121190164	0.346100572224	0.107341519601
29	O	0.479957856810	0.495475148018	0.257802841383
30	O	0.264126671880	0.321419100228	0.255397574936
31	O	0.195338939734	0.570051583724	0.246805201516

32	O	0.954480371955	0.441850595614	0.176601792741
33	O	0.341529979321	0.443865851907	0.180104938449
34	O	0.645275599243	0.483568691412	0.176479745846
35	O	0.990383200493	0.755089482776	0.253800776466
36	O	0.695398060776	0.809386564321	0.245293611748
37	O	0.458881185008	0.696348229049	0.176690662163
38	O	0.843580979258	0.691446342364	0.179274104491
39	O	0.149862815905	0.732747216721	0.178598983417
40	O	0.305400548897	0.835392296188	0.031094807992
41	O	0.522577909758	0.509763900848	0.031153558288
42	O	0.591659296782	0.762644450539	0.038142933615
43	O	0.833501100979	0.879794686462	0.109302517874
44	O	0.455701120408	0.885383912206	0.106775468899
45	O	0.147513266518	0.846112034470	0.106886807284
46	O	0.492682329878	0.994068063086	0.254067652786
47	O	0.276672837330	0.820071051477	0.254419286508
48	O	0.962135848353	0.944394184980	0.174921215567
49	O	0.339684886322	0.944986070949	0.178474834867
50	O	0.647960536809	0.979260227571	0.178214586391
51	O	0.805457891236	0.585798895162	0.030917274397
52	O	0.335969127156	0.632848510664	0.110186699863
53	O	0.955572529705	0.632691948789	0.107216130347
54	O	0.647568500350	0.601668846169	0.106120592362
55	O	0.024540378061	0.257656743445	0.031038487995
56	O	0.091419279369	0.009545042494	0.038920897188
57	O	0.023800401914	0.757151085989	0.031315940090
58	O	0.091706171045	0.509707435051	0.039505151004
59	O	0.985606806265	0.239446334562	0.254385288442
60	O	0.459502447916	0.195196451376	0.176427030518
61	O	0.841890808325	0.188205125425	0.178327334020
62	O	0.148035949259	0.231340328758	0.178981093320
63	O	0.521679349423	0.010399060935	0.031165119568
64	O	0.592757716660	0.262364739284	0.039743029512
65	O	0.805041088649	0.085859740792	0.030852684424
66	O	0.337047528063	0.134162254828	0.109626475567
67	O	0.956182541879	0.133164308970	0.106553517962
68	O	0.648210061653	0.096610428915	0.106758849072
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CONNB

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26 82 26 86 27 82 27 94 28 83 28 85 29 75 29 79 30 74 30 76 30 83
31 76 31 85 32 82 32 84 33 84 33 96 34 84 34 91 35 75 35 79 36 74
36 76 36 84 37 74 37 79 37 82 38 86 39 86 39 87 40 74 40 78 41 77
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47 78 47 88 48 78 48 93 49 87 49 90 50 90 50 91 51 77 52 78 52 90
53 87 54 89 54 92 55 74 55 78 56 77 56 79 56 92 57 74 57 79 57 89
58 85 60 93 61 85 62 94 63 76 63 80 64 75 64 81 64 94 65 76 65 96
66 95 67 83 67 95 68 95 68 97 69 76 69 80 70 75 70 81 70 97 71 80
71 81 71 95 72 94 73 96 74 78 10 10 11 11 59 59

BONDS

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GUA.Osub-O6-CIS

TITLE

formed from OUTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

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4	H	0.432840102707	0.217885791733	0.433230372086
5	H	0.498856785361	0.811408851595	0.368353191500
6	H	0.247156395896	0.604097897943	0.093165289626
7	H	0.744576258128	0.336818488150	0.102390266089
8	H	0.739708468662	0.831193258610	0.106005464918
9	H	0.545260161273	0.746988231418	0.187747137820
10	H	0.062513987524	0.492483203298	0.180815289665
11	H	0.052665627611	0.991313455983	0.187394098729
12	H	0.235514718279	0.075918355627	0.108367852622
13	H	0.555919545277	0.240848328185	0.184120301633
14	H	0.484663783290	0.540554251628	0.292632281365
15	C	0.447637601510	0.321003055245	0.426322650836
16	C	0.497413535236	0.745366436467	0.434302717548
17	C	0.471993790094	0.531083681833	0.440859101117
18	C	0.471268708835	0.505122501833	0.394724659047
19	C	0.483266814137	0.613525954016	0.365564548503
20	N	0.507330059737	0.869235774581	0.450734560457
21	N	0.486007035077	0.646160479506	0.462098218406
22	N	0.456817561881	0.411627685079	0.460543299116
23	N	0.456055279612	0.373579195363	0.386516258736
24	N	0.494915125182	0.731657792023	0.388753039401
25	O	0.484335666335	0.623275950192	0.323837589593
26	O	0.763544902529	0.566866780797	0.261975821872
27	O	0.703948706367	0.312052347060	0.255075559185
28	O	0.302514988881	0.333816229067	0.034916197886
29	O	0.833567983055	0.379013692941	0.114395056047
30	O	0.453146050148	0.368352112970	0.110763010165
31	O	0.144961892983	0.340987565731	0.112046236412
32	O	0.487167246655	0.482397707813	0.259886870613
33	O	0.264091622259	0.316006447658	0.261152968031
34	O	0.210129516597	0.567661154307	0.253986552799
35	O	0.967015869529	0.445808654946	0.180182617363

36	O	0.327026454023	0.433261583356	0.184236444879
37	O	0.656373268475	0.469967152694	0.184852263794
38	O	0.987852831620	0.732789648120	0.260908740655
39	O	0.704656783442	0.814156569766	0.253561827667
40	O	0.451274512543	0.700168360357	0.184082853265
41	O	0.836643244034	0.690272836320	0.184839255972
42	O	0.143631792902	0.727432122945	0.184371365394
43	O	0.303425738710	0.834056070083	0.037096108205
44	O	0.526490312650	0.502567664677	0.037200636585
45	O	0.589387497298	0.755261569152	0.043600780242
46	O	0.828986021311	0.878386668148	0.115501538232
47	O	0.456646578391	0.881400592015	0.112620801381
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50	O	0.265225424161	0.818990664267	0.260714260580
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75	AL	0.977743342585	0.287341431869	0.147646745880
76	AL	0.313517031085	0.281967505339	0.146699446162
77	AL	0.977066121090	0.788019329479	0.148227367510
78	AL	0.312490705465	0.783045360107	0.147259839635
79	AL	0.812605339413	0.535913680995	0.147179782381
80	AL	0.477167219497	0.036144625409	0.147563185086
81	AL	0.811746032373	0.035513239788	0.147610330031
82	SI	0.661835072190	0.456596902470	0.237880844040
83	SI	0.466763969486	0.363890143646	0.056731229548
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86	SI	0.824222236528	0.702266538678	0.239255359426
87	SI	0.653307909637	0.959516769725	0.238611035033
88	SI	0.467974881178	0.865205856751	0.057819323163
89	SI	0.643181594103	0.609063707506	0.057304530349
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91	SI	0.153754020704	0.711890333046	0.238717488980
92	SI	0.968509514274	0.620052144023	0.057656841240
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94	SI	0.823966445817	0.201287115362	0.239156627033
95	SI	0.638552413623	0.109011765429	0.056902533388
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36 74 36 76 36 84 37 74 37 79 37 82 38 86 39 86 39 87 40 74 40 78
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52 90 53 87 54 89 54 92 55 74 55 78 56 77 56 79 56 92 57 74 57 79
57 89 58 85 60 93 61 85 62 94 63 76 63 80 64 75 64 81 64 94 65 76
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BONDS

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GUA.Osub-O6vdw

TITLE

formed from CONTCAR

CELL

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1	0.54606570720320813	0.74932813794695885	0.19068622759733289
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6	0.49302802396119488	0.48974007498297489	0.41750777282475132
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7	0.49743435773409977	0.73017864101286101	0.42219768671038999
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CONNB

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BONDS

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14	0.63796552845258203	0.11986553475876810	5.48174166209441024E-002
14	0.15460547141883180	0.21881388345712119	0.23688197367549621
14	0.96677221738018448	0.12568879251499940	5.52898089932545994E-002

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BARICE

4.75294069648419 5.25363986255133 5.13503060092554

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30 83 31 76 31 85 32 82 32 84 33 84 33 96 34 84 34 91 35 75 35 79

36 74 36 76 36 84 37 74 37 79 37 82 38 86 39 86 39 87 40 74 40 78

41 77 41 79 41 86 42 78 42 91 43 88 43 93 44 83 44 89 45 88 45 89
46 77 47 78 47 88 48 78 48 93 49 87 49 90 50 90 50 91 51 77 52 78
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65 96 66 95 67 83 67 95 68 95 68 97 69 76 69 80 70 75 70 81 70 97
71 80 71 81 71 95 72 94 73 96 10 10 11 11 59 59

BONDS

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3 3 1 2 3 3 2 2 2 2 2 2 2 2 1 2 1 2 3 3 3 1 1 1 1 1 3 3 2 1 2 2 3 3
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GUA.Tsub-O6-CIS

TITLE

formed from OUTCAR

CELL

8.900 10.280 30.000 90.000 90.000 90.000

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3	H	0.540817162654	0.916287938964	0.447062198880
4	H	0.449297496927	0.192762827499	0.447423182245
5	H	0.480094242138	0.789780946875	0.383298397527
6	H	0.244648345952	0.588909268219	0.102977195007
7	H	0.745396902863	0.340547727781	0.101039620851
8	H	0.743222537689	0.836913711404	0.101829690263
9	H	0.542993972088	0.738161271168	0.194134852862
10	H	0.032833322462	0.486481807910	0.195843367035
11	H	0.050923162947	0.991179965633	0.187883137176
12	H	0.246753163234	0.092310186829	0.101017598475
13	H	0.537855086365	0.235355643028	0.197019940499
14	H	0.476359962530	0.530194953650	0.292264808710
15	C	0.457600892797	0.296383278374	0.440504472909
16	C	0.486011557809	0.722110313497	0.448782112544
17	C	0.471972901943	0.507101819474	0.454936717862
18	C	0.469250192623	0.481662896853	0.408868135745
19	C	0.473666737280	0.590419309537	0.379139115984
20	N	0.489999189921	0.846255516597	0.465632300628
21	N	0.481565308359	0.622366022447	0.476440275747
22	N	0.464520475095	0.387074488209	0.474670345649
23	N	0.460241839660	0.349584032567	0.400704549418
24	N	0.481498831462	0.709158809722	0.403228699708
25	O	0.470410193567	0.597866375891	0.337819814097
26	O	0.785019345525	0.570133943881	0.259385839496
27	O	0.689451105856	0.296974583821	0.247761063772
28	O	0.305994009023	0.338231321489	0.033343797538
29	O	0.835602359539	0.384997629489	0.111130710690
30	O	0.454361234859	0.389832179163	0.108885875791
31	O	0.147097932292	0.349807098453	0.109153677242
32	O	0.480004088177	0.498463979730	0.259743091901
33	O	0.264425897095	0.323514426195	0.257055619501
34	O	0.194881320783	0.571873344594	0.248271544029
35	O	0.954294645507	0.444275508450	0.178743094449
36	O	0.342556637653	0.446021488651	0.181852414045
37	O	0.645915882551	0.486880146888	0.178289218968
38	O	0.989256769291	0.756422355888	0.255685109648
39	O	0.694144218361	0.810155788955	0.246741754516
40	O	0.458907532622	0.699001119719	0.178429926980
41	O	0.844263081007	0.693695248070	0.180994514252
42	O	0.149544671591	0.734916339322	0.180272944646
43	O	0.306060773405	0.839577976032	0.032586706477
44	O	0.521726314254	0.514564008881	0.032716479647
45	O	0.592009530835	0.767429818053	0.039693816576
46	O	0.833631860339	0.882223967254	0.111346529414
47	O	0.455827661815	0.888443685488	0.108332240545
48	O	0.147906233375	0.848895536144	0.108462091325

49	O	0.492851970399	0.994806903878	0.255718453737
50	O	0.275232053698	0.821987957408	0.256115445173
51	O	0.962265498388	0.946280410747	0.176986979981
52	O	0.339803162572	0.946648535311	0.180109891068
53	O	0.647896240486	0.981090537078	0.179762575778
54	O	0.805055757663	0.589575857838	0.032295233410
55	O	0.335112280180	0.634767124334	0.112116122968
56	O	0.956281301848	0.635219242603	0.108651192563
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58	O	0.024856959570	0.259808761515	0.032997741546
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61	O	0.090728407890	0.511619194592	0.040673210167
62	O	0.985802232841	0.240860394618	0.256035497268
63	O	0.459301313482	0.197476020826	0.178408278784
64	O	0.842217226464	0.190153564626	0.180025598931
65	O	0.148011435502	0.234104052279	0.180582798632
66	O	0.521185200915	0.016054390653	0.032931472140
67	O	0.593512560955	0.267377819378	0.041646614118
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69	O	0.336210737173	0.136730037656	0.111705185807
70	O	0.956735457615	0.135436413286	0.108390117575
71	O	0.648054279405	0.100105889873	0.108718572569
72	O	0.783154467732	0.055735554257	0.255130988879
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74	AL	0.485317507498	0.544919893579	0.144869224869
75	AL	0.978995176577	0.291353316995	0.144755650122
76	AL	0.316780723500	0.292162628674	0.144842451565
77	AL	0.981313044312	0.790278374817	0.144508174369
78	AL	0.316507984615	0.791270869482	0.144336473902
79	AL	0.811921198765	0.540669242033	0.144852211944
80	AL	0.481716534330	0.043811356419	0.144664946737
81	AL	0.816037904204	0.038256308682	0.144043794832
82	AL	0.666218589825	0.458793810122	0.235091770264
83	SI	0.468252723884	0.376784187356	0.054184892898
84	SI	0.316324601952	0.460669325811	0.235202081858
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86	SI	0.828119394602	0.705301582453	0.235914737940
87	SI	0.656927658456	0.960282456771	0.234087084720
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41 79 41 86 42 78 42 91 43 88 43 93 44 83 44 89 45 88 45 89 46 77

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53 87 54 89 54 92 55 74 55 78 56 77 56 79 56 92 57 74 57 79 57 89

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