

Supporting Information

Silicon-Doped Carbon Nanotubes: Promising CO₂/N₂ Selective Agents for Sequestering Carbon Dioxide

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Optimized geometries of the transition states:

TS-T2a-V

\\C,0.8511829463,3.3983494842,-0.6476813
669\C,-5.6927961789,3.067076627,0.0839177777\C,-5.5650765391,0.6121178
107,3.3665377368\C,-5.703459146,2.7655911606,1.4133589983\C,-4.4778872
577,2.4768882761,2.0908398978\C,-5.5372180849,-0.7544846459,3.43488083
37\C,-4.3363318941,-1.4563009207,3.1412321023\C,-4.4016295815,1.345820
0636,3.0031075123\C,-5.5282734127,-3.2410254627,1.8370023349\C,-4.3316
677374,-2.699190164,2.3975639403\C,-5.4782370159,-3.096154626,-2.29090
74837\C,-5.5207375401,-3.7794304191,0.5800147704\C,-4.3139720121,-3.81
84030857,-0.1828341354\C,-5.4553861659,-2.0423043139,-3.1611581268\C,-
4.2482340657,-1.3064180736,-3.3689334946\C,-4.2929547849,-3.4839640065
, -1.5946551263\C,-5.4456009818,0.8964023377,-3.3752647296\C,-4.2418114
,0.138979626,-3.4403778188\C,-5.49018004,2.055444523,-2.6532860292\C,-
4.3376641181,2.517718118,-1.9539015364\C,-4.4542754297,3.0968959935,-0
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0.6997445816,3.1346978595\C,-3.2859200394,2.9664327051,1.5457741086\C,
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,1.4413918494,2.9064660134\C,-3.1181973877,-3.1246325677,1.8392388088\
C,-1.8806642165,-2.6027564207,2.3418338176\C,-3.0702375444,-3.07587347
98,-2.1535341014\C,-3.1094189982,-3.7192124049,0.5342955167\C,-1.86174
41464,-3.7822891501,-0.1633598916\C,-3.0464461417,-1.9505279026,-3.043
4170078\C,-1.7997957299,-1.2632285721,-3.214818033\C,-1.8416576936,-3.
4563458232,-1.5263782137\C,-3.0467234094,0.8140547429,-3.1292412581\C,
-1.7918102404,0.1395902002,-3.2316264895\C,-3.0852588948,2.0263722006,
-2.3777025379\C,-1.8713999522,2.5584231032,-1.7986936146\C,-2.04505835
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\C,-0.6565624059,-0.64519924,3.1846516263\C,0.5497313362,-1.3733975809
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, -0.5973744062,-3.0979313786,-2.1253225967\C,-0.6365763035,-3.74750214
72,0.5666057748\C,0.5848325321,-3.8246177125,-0.1243338925\C,-0.579429

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3443,-1.963215473,-2.9939155134\C,0.6315566442,-1.289079562,-3.2038370
129\C,0.6047558455,-3.4992650244,-1.5174410077\C,-0.5649131964,0.85205
29129,-3.0115878716\C,0.6386937057,0.143409071,-3.2347209205\C,-0.5644
82271,2.1052306762,-2.3044507778\C,0.6996965779,2.5556578189,-1.803832
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,1.5796622719\C,3.2103057954,2.427525324,2.1512761635\C,1.7999123543,-
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96467,5.7937918808,-1.3055729315\\

TS-T2b-II

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-1.4464166515,-3.6294688488\H,-6.4215766635,-1.5574745753,-3.535264907
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59,-3.5581583248\H,-6.5259738362,2.4660990913,-2.2112310112\Si,-0.7671
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TS-T2b-IV

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-3.1299030299,2.3831948705\C,-4.2049530745,-3.5250824105,1.7090993337\
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,-3.200941163\C,0.6339687622,-1.6820330065,-3.0293819294\C,-0.60231259

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,3.6859204365,-0.6878077589\Si,-0.5454374511,4.1052025827,0.9489721935
\O,0.630413231,6.557885805,0.4853814805\O,2.1643543495,5.555145291,-0.
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\C,4.0912838621,-2.847965076,-2.5943177592\C,5.3060298847,-2.344867986
5,-3.1436398889\C,5.2514518044,-4.0595463462,-0.7241923771\C,4.2500375
28,-0.179523825,-3.4478949053\C,5.376879297,-1.0493496623,-3.570970414
5\C,4.3836407065,1.1922347085,-3.0053917378\C,5.6706660056,1.640057217
3,-2.5916108185\C,5.8087128788,2.3788040522,-1.4473647712\H,6.79832390
45,2.5177008007,-1.0317012786\H,6.5579650787,1.2503332584,3.0096587975
\H,6.728459886,2.6792493411,1.0852227732\H,-6.519119215,3.21062631,1.1
909879877\H,6.3801023698,-0.7410581584,3.7815135309\H,-6.4454938202,-0
.1453828724,3.8474858715\H,-6.4072516502,2.1613944632,3.1025530211\H,6
.2348055274,-3.0306210955,3.0229913026\H,-6.5674843398,-2.1766249498,3
.0563567226\H,6.1936366337,-4.1393241278,-1.2499613074\H,6.1980585859,
-4.1967116015,1.1616126288\H,-6.6571057883,-3.5763220829,1.0924449765\
H,6.2070391037,-2.9435721064,-3.1163793116\H,-6.5864431445,-2.16605009
65,-3.0684482582\H,-6.6623689382,-3.5757170546,-1.1109467285\H,6.33410
94198,-0.6549653409,-3.8824689271\H,-6.4837787333,-0.1140810845,-3.806

7230453\H,6.5571036973,1.2270287628,-3.050272313\H,-6.4278707534,2.177
9176124,-3.0470045684\H,-6.4717392244,3.2581787202,-1.2211403246\C,0.9
579471524,3.0732272856,1.604430884\Si,2.1348197166,3.9433492385,-0.850
6723006\Si,-0.4649891148,3.737265954,0.7670946223\O,-0.093483872,5.770
6386319,0.9543611605\O,1.4586109696,7.3161253968,0.1695771059\C,0.7688
757586,6.4507656626,0.486169446\

TS-T2e-VI

\C,-0.534131,2.755775,2.309377\C,5.606997,2.89339,1.388663\C,5.512613,2.0986
78,-2.696567\C,5.63606,3.151235,0.049561\C,4.420827,3.127773,-0.69919\C,5.4
9984,0.924248,-3.39041\C,4.30913,0.139477,-3.446645\C,4.336485,2.55219
9,-2.025669\C,5.571516,-1.994105,-3.045701\C,4.349124,-1.298145,-3.302
271\C,5.630761,-3.6227,0.764367\C,5.608611,-3.006526,-2.128299\C,4.423
992,-3.396461,-1.431014\C,5.609546,-3.073659,2.016979\C,4.393691,-2.55
8562,2.560877\C,4.43497,-3.698648,-0.01207\C,5.543435,-0.554824,3.5461
92\C,4.361553,-1.304918,3.289197\C,5.535634,0.807891,3.412625\C,4.3480
9,1.490689,3.024532\C,4.375909,2.569829,2.04559\C,3.179643,2.964937,1.
436272\C,3.098346,2.044147,-2.480957\C,3.221908,3.264292,0.010358\C,2.
012299,3.299837,-0.758218\C,3.096087,0.802973,-3.188886\C,1.857511,0.0
96402,-3.261909\C,1.867375,2.557715,-1.933199\C,3.158378,-1.953031,-2.
956892\C,1.8996,-1.302269,-3.171917\C,3.218985,-3.618087,0.689885\C,3.
198919,-3.03795,-2.017971\C,1.973131,-3.42765,-1.39314\C,3.196695,-3.0
19249,1.992856\C,1.94001,-2.527198,2.479727\C,1.982288,-3.720351,-0.02
1684\C,3.141288,-0.606267,3.352975\C,1.906312,-1.294214,3.146981\C,3.1
32447,0.814383,3.218462\C,1.893222,1.478687,2.924267\C,1.926499,2.6262
3,2.112874\C,0.683939,3.239422,1.815941\C,0.567509,2.068702,-2.435619\
C,0.609338,0.787213,-3.079097\C,-0.577676,0.042832,-3.274042\C,-0.7107
85,2.535143,-1.986546\C,0.693053,-2.019548,-2.929317\C,-0.531777,-1.38
8802,-3.184911\C,0.746144,-3.699979,0.690474\C,0.73026,-3.121179,-2.02
1915\C,-0.468602,-3.537504,-1.419189\C,0.72438,-3.056174,1.967961\C,-0
.499062,-2.571765,2.462567\C,-0.458847,-3.827072,-0.018899\C,0.664397,
-0.59978,3.285548\C,-0.538394,-1.302209,3.120517\C,0.637055,0.830463,3
.187416\C,-0.605116,1.501072,2.988535\C,-1.909446,1.91075,-2.460745\C,
-2.091393,3.423697,-0.111298\C,-3.306022,3.006041,-0.716222\C,-1.84123
3,0.672877,-3.127766\C,-3.045367,-0.077908,-3.355334\C,-3.209975,2.336
711,-1.986648\C,-1.738008,-2.099638,-2.916378\C,-2.995979,-1.503234,-3
.229862\C,-1.69419,-3.737855,0.685619\C,-1.70952,-3.177862,-2.01826\C,
-2.942079,-3.597053,-1.419761\C,-1.708779,-3.102544,1.933775\C,-2.9535
78,-2.677733,2.479711\C,-2.932672,-3.885327,-0.014766\C,-1.797714,-0.6
24735,3.249073\C,-2.995301,-1.424013,3.175836\C,-1.865224,0.781243,3.1
80927\C,-3.205138,1.35318,2.993065\C,-3.401297,2.492793,2.147188\C,-4.
601792,2.65697,1.428886\C,-4.373958,1.812112,-2.575595\C,-4.543317,2.9
60599,-0.001938\C,-5.705451,2.807521,-0.807164\C,-4.290246,0.564177,-3
.304862\C,-5.444829,-0.232217,-3.566571\C,-5.621692,2.267093,-2.062596
\C,-4.183853,-2.228569,-3.02599\C,-5.395609,-1.591419,-3.420689\C,-4.1
39319,-3.872641,0.703793\C,-4.1604,-3.305881,-2.054299\C,-5.34998,-3.7
44283,-1.395759\C,-4.143258,-3.270794,2.022818\C,-5.345732,-2.877524,2
.681078\C,-5.34014,-4.018043,-0.055197\C,-4.243217,-0.849155,3.432188\
C,-5.388358,-1.704212,3.377578\C,-4.352128,0.58326,3.290748\C,-5.63622
3,1.140677,2.991816\C,-5.76888,2.101394,2.029994\H,-6.759483,2.358965,
1.677715\H,-6.537441,2.043392,-2.592931\H,-6.684003,2.984027,-0.380421
\H,6.591252,3.236231,-0.450752\H,-6.402202,0.240596,-3.738843\H,6.4292

84,0.52982,-3.779116\H,6.451221,2.613869,-2.541608\H,-6.314728,-2.1596
78,-3.479774\H,6.501701,-1.628957,-3.459897\H,-6.28114,-4.197193,0.447
744\H,-6.298549,-3.714212,-1.915123\H,6.567314,-3.4167,-1.83942\H,-6.2
57841,-3.441299,2.53513\H,6.547828,-2.89933,2.526339\H,6.584439,-3.866
852,0.315429\H,-6.334764,-1.368151,3.777907\H,6.485746,-1.061152,3.706
963\H,-6.527533,0.666974,3.377113\H,6.473329,1.343496,3.476227\H,6.542
473,2.781304,1.918766\C,-0.885485,3.432788,-0.862156\Si,-2.06721,3.627
67,1.735502\Si,0.563836,3.818833,0.111681\O,0.280431,5.758998,-0.03222
6\O,-1.282112,6.380847,-1.652074\C,-0.570665,5.902793,-0.88827\

TS-T33-II

\C,-5.0508404434,-0.5819802961,3.5510392786\
C,-5.2653903964,2.6739974834,2.3989670425\C,-5.1374201
536,3.4737274355,1.285452733\C,-4.9620624039,2.470196218,-2.9047145096
\C,-4.7253937811,3.3459605671,-1.8638554187\C,-4.7985544574,-2.1569802
915,-3.4691866794\C,-4.7620033498,-0.8680151847,-3.942880019\C,-5.2743
732263,-4.0682962103,-0.6820005673\C,-5.2918831923,-4.00576265,0.68982
31619\C,-3.846289447,0.1545247663,3.6899662943\Si,-3.8090908735,1.8565
499201,3.0538919773\Si,-3.5765352028,4.1644165376,0.5823486698\C,-3.46
94438281,3.6320749421,-1.2561144343\Si,-3.5435515868,1.6535485024,-3.6
153623193\C,-3.5357104073,-0.156292604,-3.9585530283\C,-3.6139845011,-
2.8143602056,-3.0426959838\Si,-3.8131357857,-4.0080845963,1.7666729789
\C,-3.8184180114,-2.574191701,2.9611252155\C,-2.2444634461,-3.96912649
27,0.8170852577\C,-2.3551961671,-2.2379422304,-3.3520599904\C,-2.03906
68627,2.3048207208,-2.8719188711\C,-2.1844612638,2.4591354639,2.548410
8331\C,-2.1236649882,3.3198004177,1.4042510047\C,-2.6227842448,-1.9198
970755,3.3579609793\Si,-0.821677133,-3.2096158189,-3.0019358798\C,-0.7
486762856,1.7267094065,-3.2003457166\C,-0.8486183575,3.5789717427,0.84
6825267\Si,-1.0535234997,0.3787864096,4.2220133131\C,-0.9946811641,1.8
683121541,3.080000648\C,4.7803947066,1.6280503461,-3.20909201\C,3.249
2433358,-2.3224287038,-3.198258881\C,2.0029757418,-2.8960958905,-2.828
5378517\C,0.5560511254,2.2090915744,-2.7642666805\C,3.5165811505,2.174
9724145,-2.7654627115\Si,2.0426507253,1.5383584087,-3.5316654649\C,0.5
337578261,-1.9697594555,3.4821369817\C,1.7784631362,0.0642815693,3.959
1635868\C,4.5498975127,1.918659532,3.530353581\C,0.2627691431,2.380283
9838,2.6317975518\C,3.3945244979,2.464265534,2.8482913519\C,0.25133224
97,-3.9655658463,0.8910355919\C,0.2923464651,-4.0201968123,-0.52749989
81\Si,1.9030234305,-3.96750741,-1.3433319369\C,3.4181010241,-4.1634195
527,-0.4027213067\C,3.3648628782,-4.0798189878,1.0188577362\Si,1.77594
73338,-3.9621232619,1.8981262405\C,4.6524539039,-4.100727384,-1.151741
5541\Si,1.9681107691,3.8966385739,0.7692864132\C,3.4593496607,3.230341
1819,1.6622141796\C,4.5516829059,-3.9306525101,1.8197596905\Si,1.81034
45632,1.7566548994,3.2978622453\C,0.3462265382,3.2093716543,1.48243445
26\C,2.9903953482,-0.6754209204,3.9952635045\Si,4.5536374366,0.3194427
086,4.2057897228\Si,4.555847485,-2.9102662685,3.2256118927\C,1.7670004
792,-2.6378028512,3.1894426564\C,2.9877634757,-2.0478776,3.6356514913\
C,0.5094816235,-0.6047208511,3.8655999415\C,0.8025097111,3.1155362783,
-1.7087101288\C,4.7233331301,3.5332043209,1.0453295056\Si,4.838988679,
3.4800495866,-0.6806350885\C,3.3322615292,3.0435468323,-1.6493265161\C
,2.0709836813,3.3615075268,-1.0804473719\Si,4.7812812691,-3.2013773759
,2.6315230235\Si,4.8568501427,-0.0235938098,-3.7493046802\C,2.0690111
718,-0.2777431608,-3.8280280476\C,3.2851800565,-0.9998214499,-3.719664

2266\C,0.8160942987,-0.9482906927,-3.7068019373\C,0.7693439368,-2.2788
093144,-3.2299798792\Si,-1.0406777672,-2.6895004818,2.9489599328\Si,-0
.7217584281,3.8168083572,-0.9552996931\Si,-0.7452348356,0.0219528334,-
3.7283785751\C,-0.918262068,-3.8480866131,-1.2833045874\C,-1.016754312
8,-3.7753720375,1.5355689379\C,-2.6105137134,-0.5420183672,3.737690722
9\C,-2.2300061213,3.2808348591,-1.8405001299\C,-2.3297361528,-0.878306
0827,-3.7974099433\C,-2.1819914964,-4.008411865,-0.614163288\Si,-3.713
6461122,-3.8600491022,-1.5533355289\C,-5.0440311412,-1.9211459387,3.23
67157503\H,-6.2713811041,-4.0092879842,1.1660248102\H,-6.216739844,-4.
1139819365,-1.219983402\H,-5.7594093015,-2.6361838281,-3.3200472873\H,
-5.6892479788,-0.3554731381,-4.1690072797\H,-5.9912286932,2.2985085978
, -3.197191978\H,-5.5985611846,3.7901967294,-1.3946291327\H,-6.07524357
5,3.8249243679,0.8540350133\H,-6.2573233422,2.4398760838,2.7745524653\
H,-6.0012129009,-0.0611817208,3.5935603875\H,-5.9839578416,-2.42720523
6,3.0545855457\H,5.7033884322,2.1865300904,-3.0855222214\H,6.124170319
7,-0.6439148336,-4.1832120344\H,6.0362999023,-3.0833272937,-3.39878602
92\H,5.5566741925,-4.5067958705,-0.7078025633\H,5.4995267649,-4.295841
3826,1.437165473\H,6.1269744856,3.7239817194,-1.365240973\H,5.62585626
91,3.5701216233,1.6469177684\H,5.4790038426,2.4812161863,3.5149553424\
H,5.7266562965,-0.2649510672,4.8841647101\H,5.7827406209,-2.6657430557
,4.0097592408\C,0.3658096981,6.3680225803,-0.6429987828\O,-0.512355710
4,5.7199358411,-1.2002853019\O,1.3033975531,6.4301412086,0.0530706743\

TS-T33-IV

\C,-5.0561497498,-0.5818651018,3.5493259021\C,
-5.2739274118,2.6763421956,2.3990829083\C,-5.1504755979,3.4791993935,1
.2896007086\C,-4.9688008261,2.4618926365,-2.9095786429\C,-4.7341040117
,3.3378953008,-1.8692966654\C,-4.797900911,-2.1666459141,-3.4714149548
\C,-4.7635927833,-0.8788566377,-3.9486281982\C,-5.2736723596,-4.071430
3954,-0.6816993003\C,-5.2928342461,-4.00713283,0.6896242403\C,-3.85210
56837,0.1559038015,3.6913987749\Si,-3.8175184419,1.8597027615,3.064912
9294\Si,-3.5802112878,4.1305074751,0.5751974628\C,-3.4772396098,3.6196
429215,-1.259055175\Si,-3.5523141854,1.6473846452,-3.6327222085\C,-3.5
388551076,-0.16456246,-3.9657896987\C,-3.6126812388,-2.8206757081,-3.0
418208766\Si,-3.813315547,-4.0051828359,1.7656887883\C,-3.8197513289,-
2.5728185621,2.9596639902\C,-2.2436891518,-3.9702423543,0.8187142968\C
, -2.3546041769,-2.2428881592,-3.3525132338\C,-2.0462760251,2.299928037
8,-2.894989143\C,-2.1950577769,2.4647117141,2.5687910636\C,-2.13683378
6,3.3040640322,1.4118488473\C,-2.6248281077,-1.9189663523,3.3583488535
\Si,-0.8192505537,-3.2093432365,-2.9982911223\C,-0.7538204353,1.726719
881,-3.2279849163\C,-0.8581366851,3.5307594703,0.8391559987\Si,-1.0558
503266,0.3758068804,4.2028404561\C,-0.9978510165,1.8801892345,3.100118
0607\C,4.7727434624,1.6382772225,-3.218243797\C,3.2488029761,-2.314428
4743,-3.1910691103\C,2.0030139511,-2.8926248662,-2.8244953271\C,0.5524
733002,2.203831305,-2.7974893559\C,3.5070707336,2.1852190675,-2.774085
0959\Si,2.0413305816,1.5564029175,-3.5824153564\C,0.5328927504,-1.9652
109873,3.4839109509\C,1.7778906161,0.0714095686,3.9634864891\C,4.54810
23921,1.9209429823,3.5130152932\C,0.2614495839,2.396525335,2.659721484
6\C,3.3870429231,2.4729876315,2.8404048556\C,0.2529117409,-3.965486848
8,0.895009054\C,0.2940107144,-4.0201861233,-0.5238919744\Si,1.90458825
64,-3.9629315224,-1.3385778552\C,3.4193596854,-4.1585054555,-0.3975761
354\C,3.3640592459,-4.0767277976,1.0232729145\Si,1.7746023943,-3.96695

51614,1.9045522616\C,4.654774238,-4.0933675894,-1.1455654192\Si,1.9414
224439,3.8909370093,0.7551397872\C,3.4448221654,3.2437294824,1.6545252
362\C,4.5507654628,-3.9291887321,1.8255794724\Si,1.8092023681,1.775225
1626,3.3189837234\C,0.3487841793,3.1945824965,1.4862372441\C,2.9885198
786,-0.6701528403,3.9946830479\Si,4.5559146586,0.322708665,4.189092364
4\Si,4.5538263063,-2.9081113853,3.2303170544\C,1.7648149797,-2.6349637
823,3.1923629349\C,2.9845906358,-2.0428652717,3.6363160773\C,0.5113431
174,-0.6006132799,3.8702321338\C,0.7956732197,3.0910827081,-1.71929891
63\C,4.7078414855,3.5355329334,1.03433944\Si,4.827381022,3.487118568,-
0.692842565\C,3.3264757681,3.0546956648,-1.6631600564\C,2.0566365462,3
.3418819918,-1.0773770853\Si,4.783190485,-3.1906516703,-2.6229417576\Si,
4.8512974874,-0.0147449866,-3.7497352882\C,2.0666311481,-0.272041152
2,-3.828292963\C,3.2820227585,-0.9948885456,-3.7161051426\C,0.81577484
79,-0.947049977,-3.709152401\C,0.7705879936,-2.2774045878,-3.228579857
9\Si,-1.0416952862,-2.6889163979,2.9512098581\Si,-0.7277757311,3.69511
89678,-0.9409145837\Si,-0.7472353996,0.0156118616,-3.7378263877\C,-0.9
160144723,-3.8499929871,-1.280712483\C,-1.0168749739,-3.7738237425,1.5
378527985\C,-2.6155754624,-0.540450032,3.7387152215\C,-2.2394287324,3.
2641362275,-1.8503993662\C,-2.3313374516,-0.8843793489,-3.802293021\C,
-2.1806111035,-4.0115652135,-0.6127301096\Si,-3.7114792334,-3.86649738
34,-1.5527300344\C,-5.0470060233,-1.9195332467,3.2324992442\H,-6.27248
82808,-4.0101942513,1.1654811144\H,-6.215507786,-4.1180035365,-1.22059
67353\H,-5.7580098691,-2.6471962493,-3.3219926061\H,-5.6917809789,-0.3
690291149,-4.1769548874\H,-5.9985848646,2.2854714372,-3.1970644916\H,-
5.607809629,3.7779478031,-1.3971531046\H,-6.0861802673,3.84039178,0.86
2990473\H,-6.2655834158,2.4441657902,2.7765510141\H,-6.0066208733,-0.0
611835642,3.5905407479\H,-5.9860799134,-2.426104466,3.0477099972\H,5.6
957498896,2.1971710457,-3.0969033309\H,6.1201625084,-0.633938277,-4.18
15120234\H,6.0371174026,-3.0732917387,-3.3922023911\H,5.5586011851,-4.
5008792024,-0.7022004621\H,5.4982738061,-4.297251033,1.4448668444\H,6.
1250768963,3.7060765915,-1.3678528023\H,5.6136504927,3.5509149546,1.63
24258129\H,5.4783594825,2.4816730452,3.4973367481\H,5.7280157729,-0.25
95457257,4.8717077898\H,5.7778826289,-2.6703472002,4.0209754305\C,0.52
7164357,6.3774159204,-0.3982574948\O,-0.3136210073,5.7573397023,-0.984
6378773\O,1.1660777794,7.2485589153,0.0109858427\

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\C,-5.0490577993,-0.5567404844,3.524710257\C,-5.278611686,2.6927095625,2.37
77451864\C,-5.156303109,3.5016979613,1.2805398526\C,-4.9850350384,2.42
64122177,-2.9036299808\C,-4.754894493,3.3031777631,-1.861472714\C,-4.7
956869913,-2.1901488212,-3.4803787367\C,-4.7647690206,-0.9048702946,-3
.9641160954\C,-5.2731314307,-4.0730492009,-0.6797741879\C,-5.293420035
4,-4.0009522823,0.6903874848\C,-3.8408266905,0.1823329303,3.6504965613
\Si,-3.8039783093,1.8803124649,3.0181515222\Si,-3.5927563625,4.2055991
181,0.5651803861\C,-3.5007816932,3.5870985416,-1.2510408608\Si,-3.5664
116109,1.6215738473,-3.6298003053\C,-3.5427047754,-0.1867150203,-3.977
3986373\C,-3.6088548237,-2.837141719,-3.0450584581\Si,-3.8145019313,-3
.9983370839,1.7696573466\C,-3.8174476193,-2.5568976164,2.9493864745\C,
-2.2422882833,-3.9707748961,0.8224698803\C,-2.3509395768,-2.2563231831
,-3.3547264692\C,-2.0641244725,2.2653254465,-2.8800408332\C,-2.1841564
07,2.5054058064,2.5359069428\C,-2.1239106068,3.3777316706,1.4036227947
\C,-2.6206088233,-1.9055798459,3.3454759539\Si,-0.8145531836,-3.221631

0435,-2.9996836238\C,-0.7611190628,1.7147437097,-3.2093336141\C,-0.838
8369262,3.642340495,0.8443897871\Si,-1.0465247915,0.3930184551,4.12817
11367\C,-0.9891193655,1.902317026,3.0617239285\C,4.7622728063,1.657349
4234,-3.2379897213\C,3.2511872222,-2.3118343553,-3.1854040237\C,2.0078
296128,-2.8928717919,-2.8191745246\C,0.5395759914,2.2196527094,-2.7813
374477\C,3.5020727421,2.2111337059,-2.7905486763\Si,2.030783003,1.5570
896495,-3.5559401424\C,0.536210167,-1.9560217471,3.4769012629\C,1.7879
482933,0.0755235705,3.9707743266\C,4.5547774012,1.903241323,3.52570051
15\C,0.2871502521,2.4097198348,2.6357318661\C,3.3986877995,2.448093948
8,2.8552883967\C,0.2550188543,-3.9630640155,0.8964458367\C,0.296286866
5,-4.019882363,-0.5210340283\Si,1.9069425581,-3.9761374138,-1.34047231
87\C,3.4188512989,-4.1621557059,-0.396371958\C,3.3624112347,-4.0820204
563,1.02814157\Si,1.7756386247,-3.9644404946,1.9047774768\C,4.65424902
39,-4.0928424303,-1.1414707382\Si,1.9851333564,3.7465717696,0.74623641
75\C,3.4750829749,3.2088716277,1.6445317766\C,4.5463674916,-3.93177572
54,1.8314687004\Si,1.818068953,1.8044366131,3.375232556\C,0.3741283826
,3.2305840155,1.4868880275\C,2.9916434587,-0.6727752515,4.0245214566\Si,
4.5578002538,0.3047041889,4.2130443568\Si,4.5491992115,-2.9173304848
,3.242484618\C,1.7700626965,-2.6370975236,3.2028458532\C,2.9821285992,
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0148063738\Si,4.8537577391,3.4746488804,-0.7166418127\C,3.3340127832,3
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4.7848758481,-3.1862450472,-2.6176440168\Si,4.8449688518,-0.0022788766
, -3.7504351048\C,2.0638147351,-0.2695457032,-3.8151632278\C,3.28077317
96,-0.9878288897,-3.7062113523\C,0.8152456513,-0.9500886481,-3.6985430
493\C,0.7733244908,-2.2805769503,-3.2225467865\Si,-1.0393963599,-2.683
2187905,2.9478656298\Si,-0.7548574018,3.7282070162,-0.968510606\Si,-0.
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.2779072393\C,-1.0171820043,-3.7728013516,1.5395392014\C,-2.6088243133
, -0.5216403287,3.7076332712\C,-2.2678116276,3.2221262937,-1.8364456934
\C,-2.3321700855,-0.8985612232,-3.8059772241\C,-2.1784941036,-4.015500
7829,-0.6094317394\Si,-3.7086308699,-3.8719323789,-1.5497244797\C,-5.0
433172958,-1.8961901633,3.2217810433\H,-6.2733924204,-3.9997810208,1.1
65620003\H,-6.2142735845,-4.1208610931,-1.2197508852\H,-5.7545717029,-
2.6728496639,-3.3298167449\H,-5.6936319283,-0.3978371617,-4.1960960176
\H,-6.0132099257,2.2524860111,-3.1982490917\H,-5.630003573,3.749226359
4,-1.3979406267\H,-6.0931540552,3.8567043644,0.8503905158\H,-6.2660146
164,2.4443240838,2.7559305714\H,-5.9985765456,-0.0349425228,3.57057464
53\H,-5.9839445028,-2.4041594323,3.0488844205\H,5.6865157308,2.2160445
001,-3.1272018932\H,6.115738105,-0.6222111119,-4.1752091615\H,6.041662
5403,-3.0619433752,-3.3811044855\H,5.5595166508,-4.4948730332,-0.69596
12441\H,5.4962909006,-4.293280032,1.4502467748\H,6.1478303098,3.695755
8359,-1.3946018265\H,5.6409827068,3.4995768318,1.6127811065\H,5.494728
1128,2.4460033121,3.4795359328\H,5.7409400091,-0.2820666127,4.87155697
56\H,5.7775444426,-2.6814758127,4.0265037887\C,-0.724401563,5.95870217
61,0.2290462442\O,-0.7151970451,5.6845135699,-0.9626403725\O,-0.689791
5482,6.5865699831,1.1908060878\

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\C,-4.6653215992,1.7141169468,3.9802813904\C,-5.0050585265,
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0.0788696469\C,-5.2237193938,1.2391815178,-3.4714004079\
C,-4.9324297249,2.4397213712,-2.8567103537\C,-5.0276938595,-2.97
21511095,-1.8169062902\C,-5.0478444131,-2.1134426022,-2.8924617406\C,-
5.2619352609,-3.2513061976,1.579633691\C,-5.1741575283,-2.5914046434,2
.7837102052\C,-3.4533320083,2.3780639811,3.6620515642\Si,-3.4737299526
,3.6470706614,2.3413413483\Si,-3.5665014629,3.9298939224,-0.9567883419
\C,-3.6357800207,2.8915788183,-2.4820919146\Si,-3.8571140648,0.1976945
308,-3.9875546606\C,-3.8398465858,-1.5658918938,-3.3829413832\C,-3.806
1370351,-3.3445866189,-1.2071417099\Si,-3.6114036673,-2.1687159196,3.6
15630226\C,-3.5036147485,-0.398618487,4.1747586568\C,-2.1231297172,-2.
6341252768,2.6697316677\C,-2.5891948043,-3.0411794391,-1.8755967328\C,
-2.2932403582,1.0237676339,-3.5967480206\C,-1.9444485483,3.7241085638,
1.3845037326\C,-1.9983709728,3.8494939672,-0.0420659286\C,-2.273317092
6,0.304636405,4.1517509053\Si,-1.0192649514,-3.7098081755,-1.168218240
4\C,-1.0211766611,0.3757936892,-3.8258181561\C,-0.7792885247,3.7196390
428,-0.787114987\Si,-0.6342397455,2.6435606497,3.6929379122\C,-0.68426
39529,3.441891681,2.0257047485\C,4.5026454053,0.1403208063,-4.11814383
32\C,2.9981290579,-3.222027464,-2.0827265271\C,1.7886056913,-3.4888717
263,-1.3730965923\C,0.292086425,0.9306546823,-3.6965849804\C,3.2675831
75,0.8599271529,-3.8631192669\Si,1.7414620027,-0.0100653841,-4.3324097
681\C,0.8809834627,0.1893769881,4.0280546643\C,2.1605417678,2.17648004
5,3.4314792921\C,4.8742004158,3.4386248337,1.909157176\C,0.5281280332,
3.612832614,1.2822641476\C,3.6500281196,3.6133911093,1.1544659158\C,0.
3735609357,-2.7081946097,2.5700806356\C,0.2949129237,-3.372691319,1.31
20926678\Si,1.8279251193,-3.7311713732,0.4358046282\C,3.4211250814,-3.
559239127,1.2455873968\C,3.4876645269,-2.8745472602,2.4909668776\Si,1.
9757876252,-2.3442129319,3.3630459669\C,4.5822233469,-3.8803172005,0.4
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6806599131,-0.2653397097\C,4.7395990876,-2.4453241659,3.0626601288\Si,
2.1262153302,3.4151322177,2.084531159\C,0.4871324486,3.7235465368,-0.1
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623220225,3.2694108093\Si,4.8619198272,-0.9216646541,3.8854856444\C,2.
0788228183,-0.5895766303,3.9604612471\C,3.329423096,0.0915144508,3.993
7097867\C,0.8994570908,1.5838665445,3.768992384\C,0.6210061257,2.17139
51502,-3.0642439026\C,4.793185855,3.6173972868,-1.0756236869\Si,4.7622
985718,2.8518020014,-2.6369944639\C,3.1863905293,2.1108923296,-3.21831
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71234,-1.2856667687\Si,4.5410796346,-1.5676330712,-3.8280832562\C,1.76
51808093,-1.7156676573,-3.5646960777\C,2.9821972808,-2.3390165815,-3.1
925055087\C,0.5208923218,-2.2723777554,-3.1004224333\C,0.531820676,-3.
1335080054,-1.9555470883\Si,-0.7364622003,-0.6323833115,3.9862890882\Si,
-0.8472819819,2.9828149009,-2.415533084\Si,-1.049054362,-1.427054328
, -3.640383924\C,-0.9701685507,-3.5115918255,0.6503788043\C,-0.83772735
96,-2.2029606492,3.1500489855\C,-2.2278355987,1.7113108819,3.901305515
3\C,-2.4246023416,2.2860914666,-2.9378083362\C,-2.6193272329,-2.144732
0053,-2.9803931371\C,-2.1816853912,-3.2975028249,1.3996254721\Si,-3.77
90193471,-3.5597479942,0.608387754\C,-4.6926849213,0.3666672689,4.2589
135743\H,-6.1112208912,-2.3371648332,3.2757686128\H,-6.2464540868,-3.4
831202496,1.183157845\H,-5.9670251829,-3.269876497,-1.3648126958\H,-5.
997808409,-1.749776529,-3.2654609174\H,-6.2689125148,0.9870257761,-3.6
082902393\H,-5.7728418107,3.0433495064,-2.5232339429\H,-6.0171344367,4
.1994425618,-0.3847049078\H,-5.945378999,4.0576142027,1.9963139146\H,-
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.3940598851\H,5.4231329958,0.6680225001,-4.348386959\H,5.7569085245,-2
.3819833617,-4.0305352914\H,5.7688269972,-4.0710673576,-2.1075865468\H
,5.5275706825,-4.0588569915,0.9555262426\H,5.6495016459,-2.982489388,2
.8128225894\H,6.0090486243,2.7013137604,-3.4160723717\H,5.7470463157,3
.8861778856,-0.632945298\H,5.7941779024,3.8781431402,1.5345392964\H,6.
1688866328,2.1577091267,4.0778441856\H,6.1434914424,-0.414743897,4.416
2792317\O,-0.8252870585,-2.3747474276,-5.3384358758\O,0.6733515036,-4.
1554400515,-5.2942355294\C,0.0383649864,-3.2126815773,-5.0832221047\

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\\Si,5.6329542111,-2.9559742691,-2.3363875209\C
,5.6439864779,-4.1168657072,1.052293622\Si,5.5995042565,-3.4929783995,
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3742420469\Si,5.6909592439,2.0245041195,-3.3243981172\C,4.1255097861,-
3.5797238311,-1.6233592958\Si,4.134449725,-4.0086319503,0.1109334902\C
,4.1052597677,-2.9566125854,3.4806130767\Si,4.1428106128,-1.4257672143
,4.4002063388\C,4.1624022416,2.1170145899,4.5027682923\Si,4.2138302104
,3.5159977861,3.3906899869\C,4.2263346498,4.6846456712,0.0718503347\C,
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.5768098074\Si,2.6534707368,1.9753480256,-3.2756233527\Si,2.6765340957
,4.5895238621,0.9598421513\Si,2.6130826104,1.2314413341,4.6176405948\C
,2.5815017693,-4.0008665706,1.0048735793\Si,2.563726717,-3.3683257865,
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,4.6929653096,0.0730215969\C,1.0753711018,2.1187445628,4.4044034868\C,
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C,-1.9702639368,4.6975291923,0.0726598449\Si,-0.482138269,1.2634449872
,4.569221534\Si,-3.5864528738,1.3128696178,4.6063486322\C,-2.021037649
8,2.1493319722,4.3571903041\C,-0.4661371631,-1.4676338718,-3.381159868
1\C,-2.0640817963,-3.4220108024,-1.6132886842\Si,-5.1008244814,-3.9461
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4.0158061331,-1.5684653195\C,-3.5005841184,3.5896967716,-2.3696714899\
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61,-3.5996308315\Si,-4.995527655,4.1269518632,-1.5714689658\C,-2.08616
471,-2.807368435,3.3648591369\Si,-3.6368216059,-3.3236633558,2.6289426
852\C,-5.0630127629,1.236314437,-3.7026164455\Si,-2.0629262051,-3.9155
468647,0.098742251\Si,-0.5317982196,-3.31586855,2.6364510838\Si,-3.602
2270388,-2.849680699,-2.3325562362\C,-5.1292338425,-3.469241225,-1.653
3971396\Si,-5.0405431305,-0.5023388948,-3.6671826398\Si,-2.0047230353,
-0.5779741732,-3.5734950025\C,-3.5564053222,-1.4618999211,-3.455743163
2\Si,-0.4993023648,-2.8598253661,-2.2748421151\C,-0.4968592805,-0.5106
149416,4.6761553946\C,-5.1514259671,-2.8123299964,3.416991532\Si,-5.09
51269009,-1.3463533388,4.3516110063\C,-3.5896897803,-0.4701488765,4.71
62706331\Si,-2.0575753092,-1.3122454647,4.332312099\C,-5.0396431872,4.
7732470064,0.0435762242\Si,-5.0051293269,3.6804588834,3.4202272584\Si,
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.7147963983\C,-0.4135908026,4.2273540142,2.7072323302\Si,-0.4170276483

,4.7797845773,0.9693369356\Si,1.0882384651,-0.604658969,-3.5402761804\
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3,3.3256204942\Si,1.1320749582,3.9674705742,-1.5472421662\C,1.09610604
6,1.1716859516,-3.6240605062\Si,2.5951232522,-2.9119069014,-2.26723247
52\C,2.6032169061,-0.5490143107,4.6687531286\C,2.678885769,4.111613486
,2.6817829371\C,2.6833664182,3.4550901513,-2.2844902087\Si,4.239696392
7,3.9785055573,-1.5701994353\C,5.6959151854,-1.5715823527,-3.387493722
2\H,6.9689776783,1.4378371503,-3.8005910973\H,6.70782596,3.9202199209,
-2.1212162352\H,7.0085041129,4.8496185333,0.3526987773\H,6.6939708086,
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6126893443,-1.105195455,4.832545528\H,6.8813804392,-3.3235385751,3.405
3592091\H,6.5973211798,-4.3397015796,0.5874557397\H,6.9087110109,-3.61
1164036,-1.9510254404\H,6.6557698364,-1.1903753162,-3.716154321\H,-6.0
430361605,1.8927987772,4.7590092814\H,-6.2778082473,4.3562941275,3.062
3103225\H,-5.9918178835,4.9911534213,0.5128823975\H,-6.279468252,3.936
2043062,-2.292738844\H,-6.0107063054,1.7600325745,-3.7488464408\H,-6.3
741146856,-0.7462312701,4.8080730037\H,-6.1097442081,-3.2470097103,3.1
573632872\H,-6.3909485696,-4.2214693651,0.7002705953\H,-6.0780622182,-
3.3460699346,-2.1624359012\H,-6.3331825495,-1.2290847841,-3.7431674357
\C,-0.407407098,6.5714586793,2.9362879112\O,-0.4238035324,6.7432083839
,1.7405577944\O,-0.3915968229,6.8356427893,4.0639437226\

TS-T50-VI

\Si,5.2869219834,-3.4458234587,-2.9134834
204\C,5.2487730106,-4.731020335,0.4328855345\Si,5.1998940425,-4.173473
7465,2.0800754407\Si,5.3103755893,0.4017225449,4.2497953357\C,5.299522
8583,-1.3375374291,4.2727467173\Si,5.4756660939,3.9752029784,0.6553365
269\C,5.4755305713,3.4236399749,2.3043165184\C,5.5128618087,2.99932751
84,-2.801705666\Si,5.4364250338,1.5636966955,-3.7829464692\C,3.7636175
143,-4.0643207536,-2.2326528042\Si,3.7497645342,-4.5587942318,-0.51501
6957\C,3.7081808237,-3.6429222091,2.8931741296\Si,3.7638671688,-2.1407
557045,3.8590595687\C,3.8480638716,1.3913118853,4.0286449319\Si,3.9304
351777,2.8078896234,2.9452594306\C,3.9958773395,4.1405878656,-0.321431
3365\C,3.9212188346,0.716631629,-4.1680529394\Si,3.8957523064,-1.07005
59723,-4.1040551681\Si,2.3989533616,1.5583598,-3.7497847959\Si,2.44304
69222,4.0094122725,0.5513288543\Si,2.2769295546,0.5377438825,4.1187648
499\C,2.1892808581,-4.5574331246,0.3641403979\Si,2.1667793115,-3.99361
55901,2.0547636608\C,2.3212037552,-1.8968668927,-3.8946093632\C,0.9021
734921,4.2726161437,-0.3468865024\C,0.7594087593,1.4564555854,3.915246
2695\C,0.6199323232,-3.5010919889,2.8037825124\C,0.6749692134,-3.92140
96406,-2.2442020902\Si,0.6490799518,-4.4245160036,-0.5370067315\C,-5.3
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1411465\C,-2.209839677,4.2683142265,-0.3559095793\Si,-0.8145689963,0.6
274391736,4.0600282358\Si,-3.9127151296,0.7291078435,4.0783413822\C,-2
.3343712562,1.5448164894,3.8547190235\C,-0.7764191743,-1.8256197361,-3
.9667701735\C,-2.422190385,-3.8015085772,-2.2683046684\Si,-5.481436482
3,-4.3310372993,-0.6797755054\C,-0.9094414895,-4.5046099418,0.32936370
42\C,-4.0015511107,-4.479288791,0.2984829094\Si,-0.6900173649,1.642435
9826,-3.7488976379\C,-0.6441153915,3.1220039034,-2.7597218741\Si,-2.19
14055847,3.6307664024,-2.0098041513\C,-3.7281478562,3.2636234992,-2.85
0592264\Si,-3.7870209322,1.7695100273,-3.8256761233\C,-2.2620270102,0.
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,-2.4768326244,-3.3754614417,2.7318603101\Si,-4.0300623364,-3.83354448
79,1.9645961017\C,-5.3207667312,0.9697347026,-4.2514121438\Si,-2.44486
4475,-4.3563366077,-0.5748518688\Si,-0.9263084879,-3.8838403309,1.9974
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\Si,-2.2980972666,-0.9043543659,-4.1449519504\C,-3.8655879507,-1.76243
23983,-4.0631932778\Si,-0.8428252571,-3.2483272464,-2.8997000247\C,-0.
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\C,-5.276521992,4.3912474295,-0.4184997933\Si,-5.2940064491,3.12807794
54,2.9210870876\Si,-2.2559733106,3.0143640663,2.8449758002\C,-3.773060
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08\Si,-0.6722172267,4.2792815364,0.5786773634\Si,0.7933786762,-0.98746
82466,-4.0922097018\Si,0.6632641323,-2.0111373963,3.7762821996\Si,0.81
93727724,2.8848517503,2.8560893837\Si,0.9026891015,3.5364368911,-1.985
0752214\C,0.8321483128,0.7915609312,-4.1274758516\Si,2.2501328731,-3.3
53092686,-2.8684833138\C,2.2391215605,-1.2431843278,4.1368285743\C,2.4
098641165,3.4322415857,2.2301259217\C,2.4462418578,3.0120607374,-2.716
7789307\Si,4.0105241381,3.493594242,-1.9852189837\C,5.3835090099,-2.03
28296499,-3.9243054077\H,6.7081985553,0.9678476747,-4.2641801507\H,6.4
765933395,3.4162779762,-2.5330315114\H,6.7764332286,4.251532902,-0.004
908818\H,6.4160024293,3.2595664238,2.8174418316\H,6.6159266399,1.10297
33034,4.3439003251\H,6.2364591891,-1.8798882915,4.3245006881\H,6.47817
81092,-4.0584765267,2.8272593583\H,6.2021136051,-4.9533976065,-0.03201
95464\H,6.5487639753,-4.1314228786,-2.5356301457\H,6.3529361696,-1.659
4939134,-4.2333750918\H,-6.3650778989,1.3318897457,4.2241834053\H,-6.5
548396435,3.8261231205,2.5617224926\H,-6.2290971232,4.6127237714,0.048
4445025\H,-6.4990117352,3.6793035402,-2.8077798383\H,-6.2592309574,1.5
104086095,-4.2907222069\H,-6.7386400011,-1.2881916876,4.21161006\H,-6.
5061827265,-3.7302898775,2.4756889293\H,-6.782296692,-4.607504338,-0.0
193078997\H,-6.4297072847,-3.6369720722,-2.8459643897\H,-6.6350386921,
-1.469977732,-4.3616231892\C,0.5547094716,6.5567657583,-0.0006459686\O
,1.3040723641,7.1764792302,-0.6318675445\O,-0.3427522259,6.3385985769,
0.7790930231\