

Supplementary Information

A High Energy Density Azobenzene/Graphene Hybrid: A Nano-Templated Platform for Solar Thermal Storage

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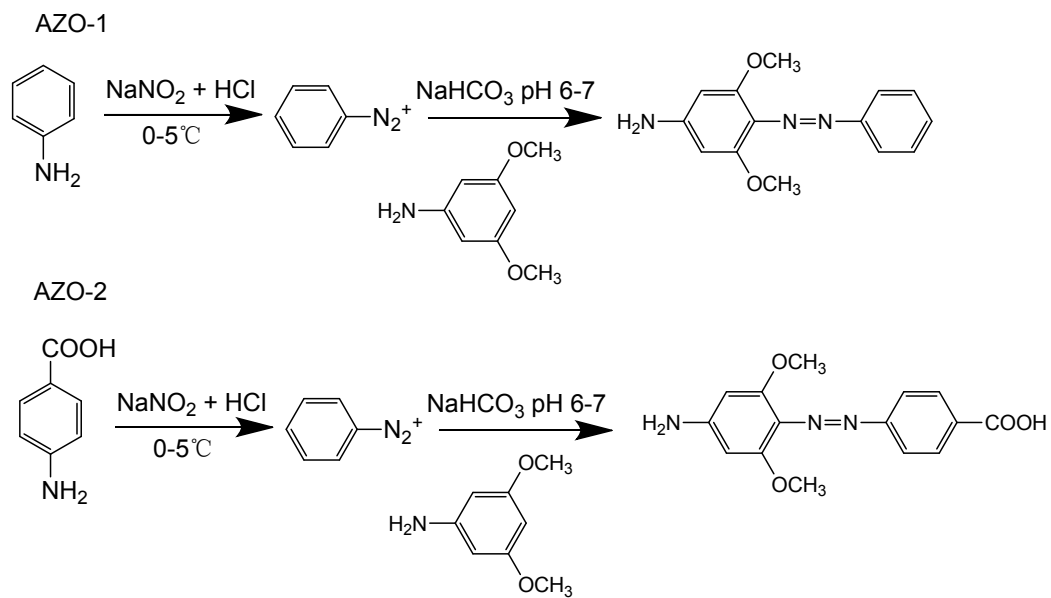


Figure S1. Synthetic route of AZO-1 and AZO-2 by coupling of the diazonium salts.

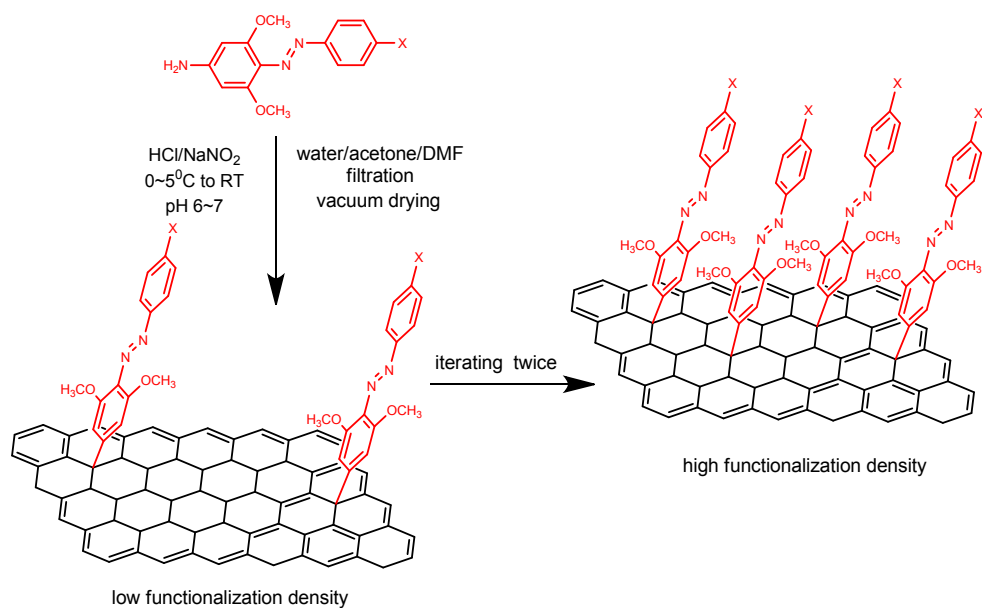


Figure S2. Preparation process of AZO-RGO solar thermal fuels. Azobenzene chromophores are covalently attached on reduced graphene oxide by a triple iterating aryl radical reaction to increase functionalization density.



Figure S3. Dispersion of AZO-RGO in DMF. AZO-RGO hybrid (1 mg mL^{-1}) shows well dispersion after standing undisturbed for three month (left) and dilute dispersion with an initial absorbance 1.5 of AZO-RGO is used for photoisomerization measurements (right) without any precipitate.

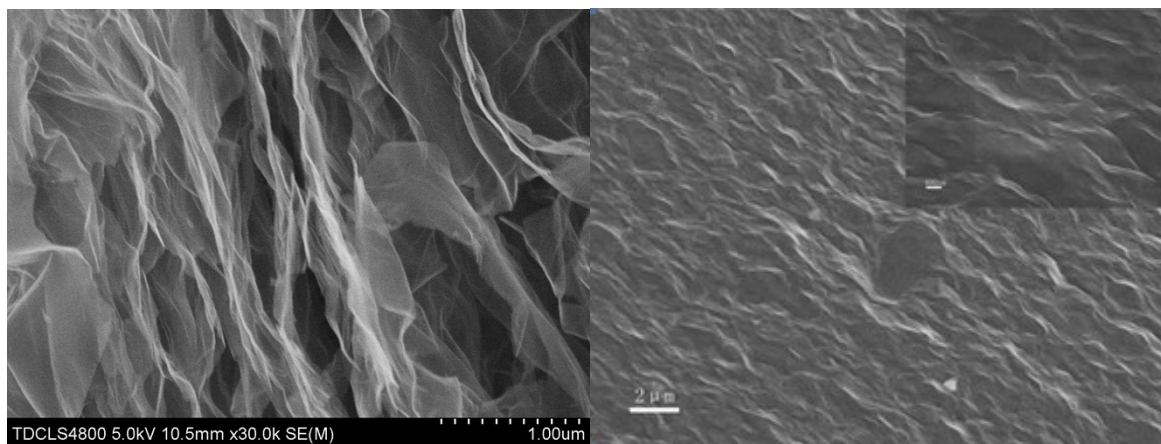


Figure S4. SEM of RGO (left) and AZO-RGO (right).

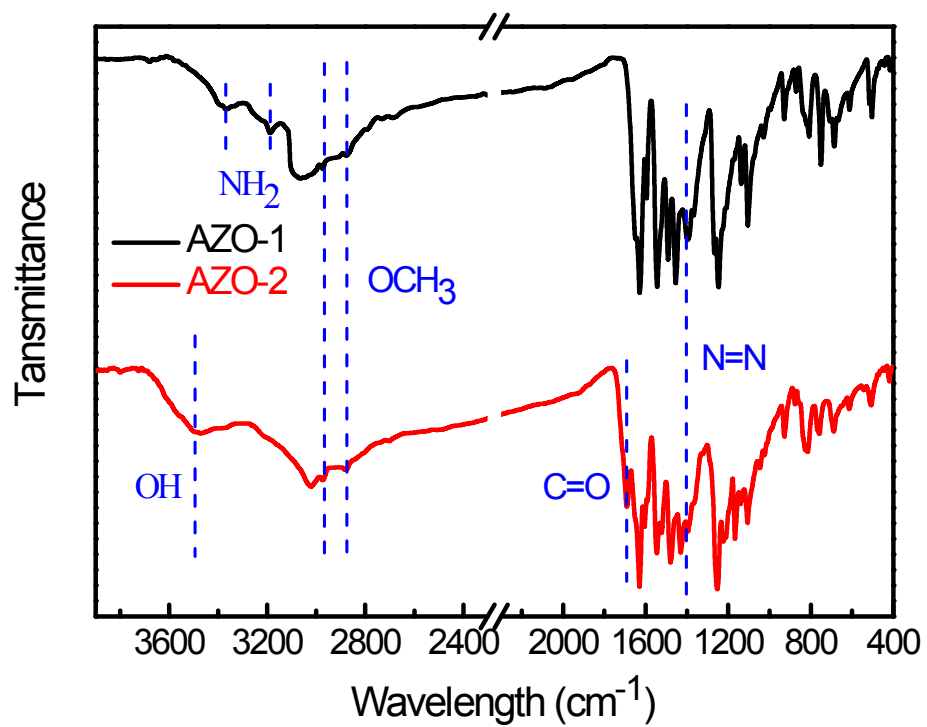


Figure S5. FTIR spectra of AZO molecules.

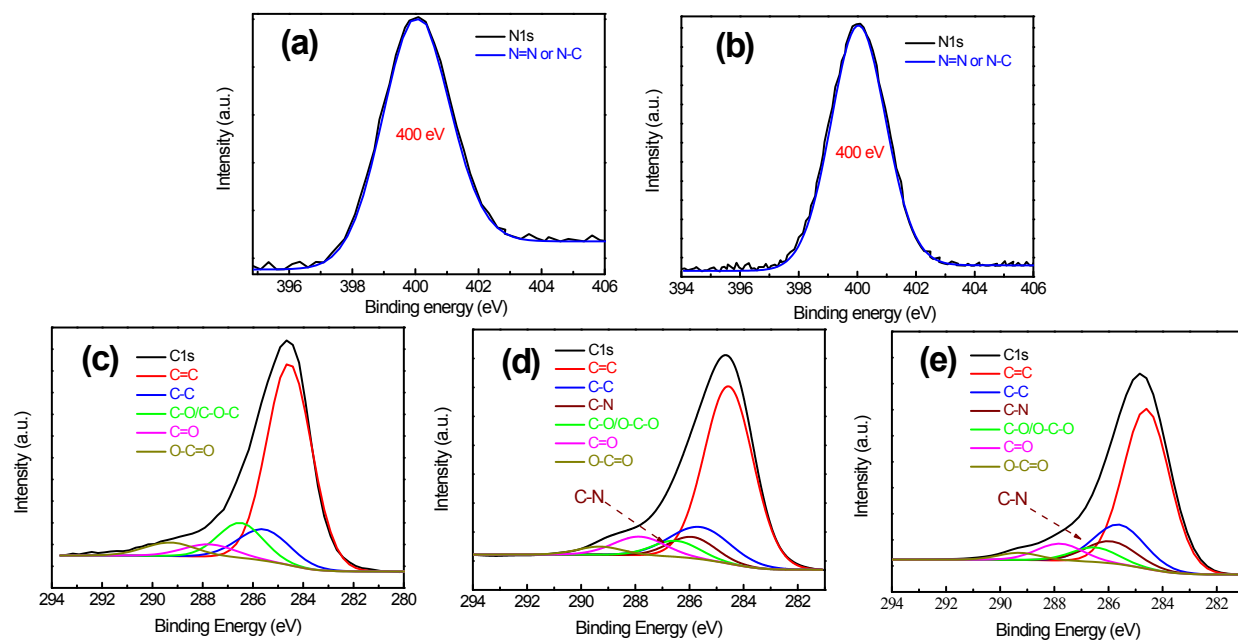


Figure S6. N 1s peak and C 1s peak in XPS spectra. N 1s region of (a) AZO-1-RGO and (b) AZO-2-RGO. C 1s region of (c) RGO, (d) AZO-1-RGO and (e) AZO-2-RGO.

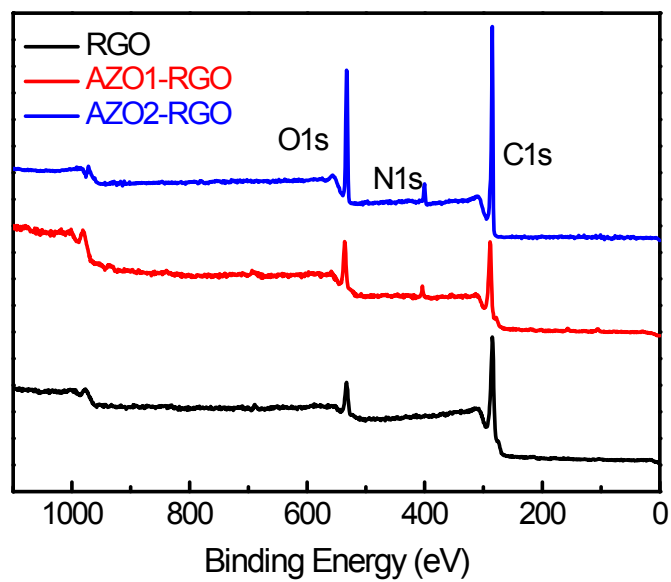


Figure S7. XPS spectra of RGO and AZO-RGO.

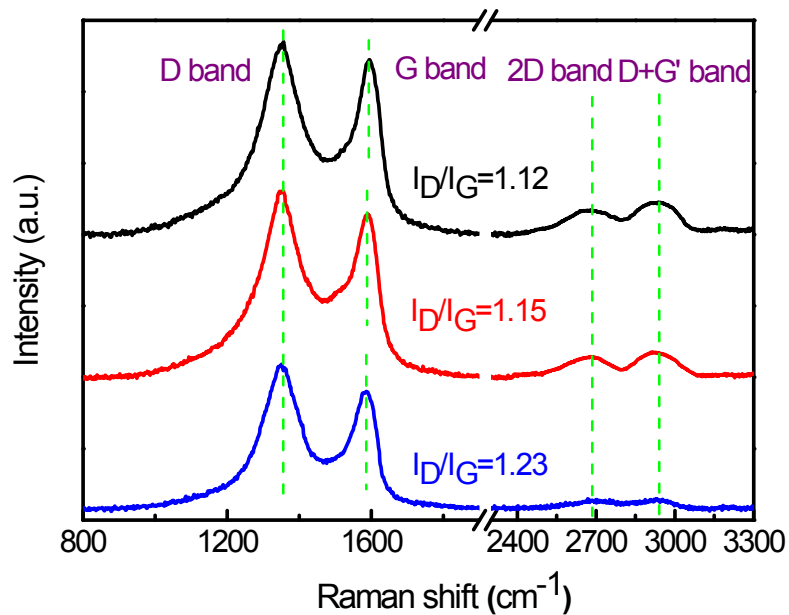


Figure S8. Raman spectrum of RGO and AZO-2-RGO under different functionalization density. It shows black curve for RGO, red curve for low functional density AZO-2-RGO and blue curve for high functional density AZO-2-RGO, respectively.

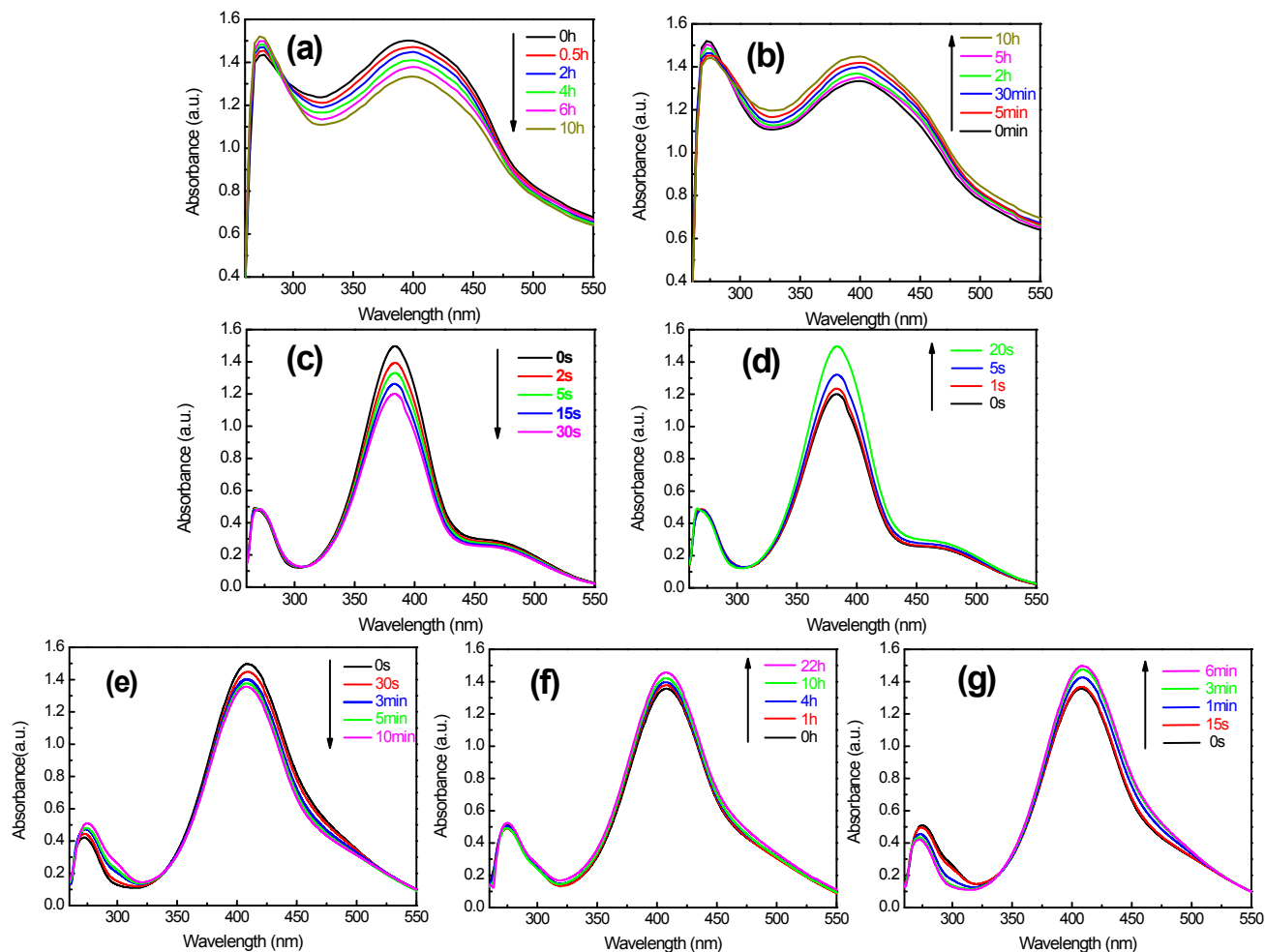


Figure S9. Time-evolved UV-Vis spectra of AZO-1-RGO and AZO. (a) and (b) AZO-1-RGO irradiated by UV light to the PSS and reversion in darkness; (c) and d) AZO-1 irradiated by UV light to the PSS and reversion in darkness; (e) , (f) and (g) AZO-2 irradiated by UV light to the PSS, reversion in darkness or by visible light at 540 nm, respectively.

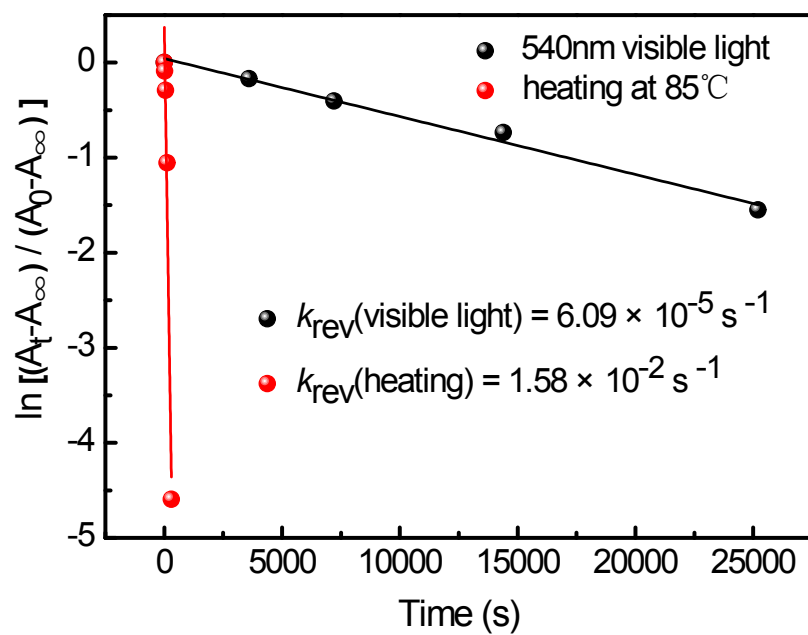


Figure S10. First plots of *cis*-to-*trans* reversion of AZO-2-G after the irradiation in darkness at 85°C or irradiated by visible light at 540 nm with different k_{rev} (the inset).

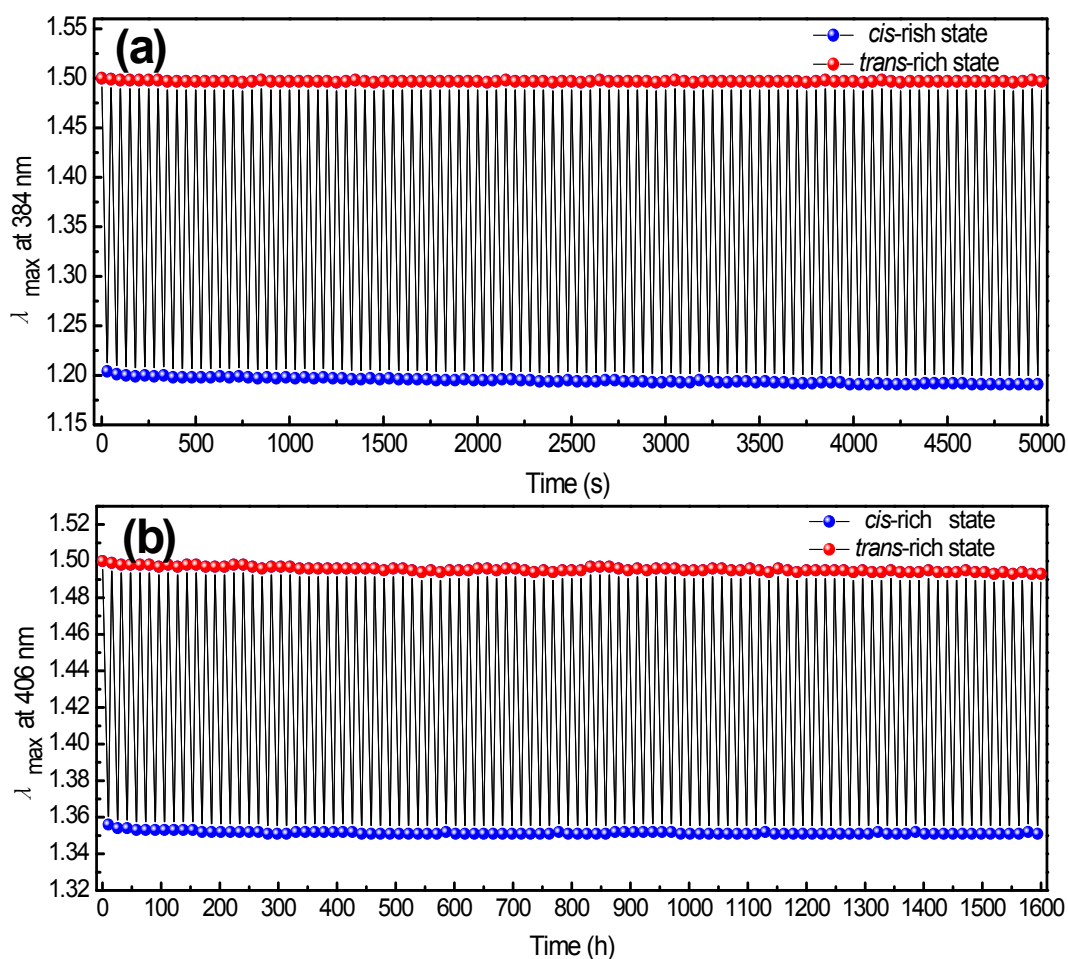


Figure S11. Cycling stabilities of AZO molecules for 100 circles. The absorbance was recorded at the maximum absorption peak with an initial absorbance 1.5 a.u. in DMF of (a) AZO-1 alternatively irradiated at 365 and 540 nm for 30 s and 20 s, respectively and (b) AZO-2 alternatively irradiated at 365 and 540 nm for 10min and 6min, respectively.

Table S1. Functionalization densities of AZO on RGO after one time reaction calculated by TGA and XPS

	TGA			XPS			
	D_g (%)			D_f	Element content (%)		D_f
	600	700	800		C	N	
RGO	80.15	75.81	71.76	/	85.6	/	/
AZO-1-RGO	31.44	31.47	31.45	1:39.4	77.2	2.9	1:39.6
AZO-2-RGO	36.33	36.34	36.35	1:37.8	74.7	2.8	1:38.1

Data S1. The coordinates of optimized Geometries for AZO molecules and AZO-G hybrids by DFT.

cis - AZO-1:

C	13.975118167	11.975460887	15.559656816
C	15.205739910	11.263777639	15.553029619
C	15.236523191	9.865531564	15.584995036
C	14.040999605	9.131390792	15.617456230
C	12.808480086	9.806377590	15.626229847
C	12.782517066	11.200231286	15.614847837
C	10.402153061	11.227107697	15.800886459
C	17.594051776	11.360415168	15.673981532
C	15.691528322	13.553514828	11.854701755
C	16.478665566	14.950925445	14.136882442
C	17.271474749	14.986524956	12.992678055
C	16.882804798	14.286904260	11.844953802
C	14.908868553	13.483239637	13.007293825
C	15.310207029	14.170843273	14.166535841
N	14.491703714	14.294953459	15.322431426
N	13.821788982	13.357004210	15.835058788
N	14.068285790	7.739937125	15.587757677
O	11.628773342	11.928173480	15.616724670
O	16.335581078	12.026140349	15.600305153
H	13.976034884	12.916744422	13.007603376
H	10.194427018	10.551430052	14.954246146
H	9.622402246	11.995978793	15.849773079
H	10.408042308	10.646300822	16.738722403
H	16.186071204	9.331183391	15.598213419

H	11.885715018	9.227172118	15.631043653
H	17.777160774	10.750135278	14.772912562
H	17.659824189	10.722888259	16.572770232
H	18.345077460	12.157032791	15.731506313
H	13.238442925	7.274143290	15.945334254
H	14.930197192	7.301168358	15.900024335
H	15.366630630	13.031405649	10.951984805
H	17.492413127	14.332468345	10.939902694
H	16.743785319	15.521523417	15.029556044
H	18.187861150	15.579678280	12.986361767

trans - AZO-1:

C	14.458513874	15.591830992	15.691516917
C	13.995338480	9.220757848	15.717441322
C	15.203056799	9.937204410	15.693932397
C	15.199494996	11.333520385	15.671765725
C	17.591105091	11.358870097	15.667181953
C	15.323396387	17.861673365	15.602911543
C	15.533336641	16.484339117	15.541561300
C	12.770901887	9.909484041	15.720912982
C	13.969722202	12.073817669	15.683068947
C	12.759809314	11.302904480	15.705329437
C	13.162855730	16.101639628	15.908304248
C	12.961588949	17.476928271	15.970183694
C	10.368271127	11.316632577	15.727109389
C	14.036984723	18.363679525	15.818897699
N	13.779173581	13.443255847	15.706092024
N	14.795499190	14.215526367	15.620365570

N	14.013330298	7.838460566	15.788934712
O	16.346747090	12.055505413	15.649158754
O	11.605805888	12.022362651	15.701710587
H	16.143078078	9.386556809	15.699517739
H	17.705485006	10.715304452	14.778250907
H	17.699827040	10.749604176	16.580484230
H	14.865889008	7.368811006	15.500457386
H	18.360133759	12.140140078	15.654458310
H	16.165918394	18.546643714	15.484790620
H	16.528448734	16.065448040	15.377221979
H	11.841230358	9.342420728	15.740377317
H	13.163140193	7.347879224	15.530089121
H	12.338581104	15.396807319	16.025546472
H	11.956171939	17.870166829	16.141427929
H	10.269747488	10.702802952	16.638866097
H	10.249558185	10.675217352	14.836802957
H	9.591243191	12.090418700	15.723407992
H	13.869645016	19.441597664	15.872241381

cis - AZO-1-RGO:

C	0.290250000	9.283060000	3.120570000
C	1.660050000	9.282620000	3.123930000
C	2.386210000	10.497420000	3.013440000
C	3.830290000	10.492690000	3.020770000
C	4.551800000	9.283890000	3.120690000
C	5.920700000	9.282740000	3.126780000
C	6.646170000	10.497250000	3.016720000
C	8.090610000	10.493130000	3.020730000

C	0.264020000	11.728100000	2.956220000
C	1.702400000	11.719870000	2.929070000
C	2.406080000	12.970640000	2.941550000
C	3.831400000	12.959950000	2.972430000
C	4.525180000	11.728210000	2.957870000
C	5.963380000	11.719380000	2.932030000
C	6.667140000	12.970200000	2.942250000
C	8.092440000	12.960080000	2.971780000
C	0.291790000	14.209890000	3.086600000
C	1.706000000	14.184110000	3.087670000
C	2.415640000	15.372550000	3.696760000
C	3.872820000	15.410680000	3.332880000
C	4.552900000	14.209960000	3.086840000
C	5.967320000	14.182880000	3.087130000
C	6.676520000	15.371620000	3.695680000
C	8.133690000	15.410220000	3.332690000
C	0.309500000	16.657710000	3.328120000
C	1.707180000	16.673870000	3.384420000
C	2.414100000	17.895420000	3.290360000
C	3.860400000	17.903290000	3.283570000
C	4.570250000	16.657670000	3.327940000
C	5.967970000	16.672830000	3.383990000
C	6.674120000	17.894520000	3.290350000
C	8.121120000	17.903290000	3.285260000
C	0.280770000	19.124560000	3.252650000
C	1.728460000	19.126280000	3.234020000
C	2.450060000	20.342050000	3.206480000

C	3.818160000	20.344460000	3.226640000
C	4.541410000	19.124080000	3.249950000
C	5.989160000	19.125500000	3.233560000
C	6.711360000	20.341650000	3.210280000
C	8.079250000	20.344260000	3.231180000
C	2.195160000	14.808030000	8.104860000
C	1.709260000	13.831110000	7.197220000
C	1.787320000	14.025630000	5.817490000
C	2.371060000	15.167550000	5.268620000
C	2.937980000	16.117680000	6.134970000
C	2.844610000	15.945740000	7.516210000
C	4.062790000	17.958400000	7.944690000
C	0.600540000	11.740470000	6.822620000
C	3.455310000	10.939780000	10.217750000
C	1.773920000	12.402160000	11.884740000
C	2.215150000	11.144490000	12.286490000
C	3.046250000	10.403010000	11.443840000
C	3.019900000	12.198900000	9.811850000
C	2.155630000	12.934670000	10.638700000
C	6.454420000	14.816850000	8.104850000
C	5.964000000	13.839320000	7.200670000
C	6.044020000	14.027990000	5.819110000
C	6.631310000	15.167880000	5.268420000
C	7.199050000	16.118310000	6.132070000
C	7.108090000	15.949300000	7.513530000
C	-0.190780000	17.959440000	7.929150000
C	4.862770000	11.742560000	6.837700000

C	-0.787710000	10.955670000	10.188520000
C	6.028180000	12.386320000	11.858180000
C	6.464930000	11.121020000	12.242640000
C	7.308770000	10.395150000	11.398310000
C	7.298800000	12.219350000	9.796670000
C	6.421360000	12.938740000	10.624570000
N	1.785700000	14.992220000	9.433750000
N	1.644580000	14.245720000	10.430570000
N	6.049710000	15.002070000	9.435930000
N	5.911740000	14.250720000	10.429030000
O	3.348070000	16.820050000	8.424560000
O	1.113810000	12.722580000	7.728430000
O	7.618550000	16.823650000	8.416640000
O	5.365570000	12.734550000	7.739200000
H	1.925820000	21.295320000	3.185340000
H	4.339330000	21.298890000	3.220560000
H	6.186640000	21.294570000	3.189110000
H	0.077900000	21.299990000	3.230830000
H	2.181680000	8.332040000	3.208120000
H	4.031530000	8.331620000	3.191200000
H	6.441910000	8.332660000	3.212100000
H	8.291890000	8.330470000	3.194190000
H	3.389600000	12.633540000	8.887650000
H	4.886370000	17.659380000	7.274980000
H	4.477890000	18.441520000	8.837220000
H	3.394290000	18.659410000	7.412900000
H	1.349520000	13.275810000	5.171150000

H	3.450420000	16.993720000	5.739160000
H	1.396760000	11.319980000	6.187070000
H	8.329850000	12.158460000	6.180730000
H	0.183030000	10.949570000	7.453810000
H	4.153680000	10.376890000	9.595660000
H	3.413950000	9.420430000	11.751090000
H	1.118530000	13.006050000	12.512960000
H	1.910480000	10.740590000	13.254750000
H	-0.846100000	12.667820000	8.881160000
H	0.624860000	17.657150000	7.251480000
H	0.235110000	18.443810000	8.816330000
H	7.658220000	18.660160000	7.402890000
H	5.606580000	13.274470000	5.175100000
H	7.711180000	16.991830000	5.732990000
H	5.662930000	11.325390000	6.204830000
H	4.066510000	12.149460000	6.193410000
H	4.452200000	10.951110000	7.473360000
H	-0.076220000	10.407590000	9.568640000
H	7.672220000	9.406840000	11.693610000
H	5.367110000	12.982140000	12.489500000
H	6.144840000	10.698920000	13.197370000

trans - AZO-1-RGO:

C	0.064650000	9.096260000	3.100090000
C	1.433040000	9.098390000	3.104800000
C	2.158730000	10.318570000	3.107750000
C	3.603550000	10.311240000	3.115730000
C	4.324690000	9.096560000	3.103800000

C	5.694810000	9.098480000	3.108790000
C	6.420360000	10.318900000	3.108000000
C	7.865160000	10.311050000	3.115790000
C	0.038710000	11.549000000	3.148350000
C	1.475830000	11.543350000	3.125310000
C	2.180070000	12.789680000	3.198670000
C	3.608290000	12.776370000	3.226850000
C	4.298840000	11.549290000	3.150480000
C	5.737010000	11.542950000	3.127580000
C	6.440650000	12.790560000	3.200020000
C	7.869430000	12.776660000	3.226660000
C	0.065760000	14.026800000	3.313210000
C	1.482540000	14.000370000	3.335050000
C	2.189310000	15.235170000	3.836630000
C	3.647660000	15.239920000	3.474360000
C	4.326380000	14.026380000	3.314790000
C	5.743910000	14.001310000	3.333980000
C	6.449770000	15.236320000	3.838340000
C	7.907910000	15.239950000	3.474110000
C	0.083610000	16.483140000	3.355600000
C	1.481140000	16.504310000	3.404440000
C	2.187150000	17.716880000	3.222150000
C	3.635430000	17.723960000	3.217500000
C	4.344710000	16.483440000	3.355340000
C	5.743140000	16.504170000	3.404740000
C	6.448090000	17.716680000	3.221510000
C	7.896270000	17.722950000	3.217200000

C	0.055200000	18.939750000	3.104100000
C	1.503890000	18.943140000	3.089320000
C	2.227220000	20.155670000	2.994910000
C	3.595290000	20.158010000	3.011190000
C	4.317220000	18.941150000	3.102620000
C	5.764670000	18.942630000	3.092460000
C	6.489260000	20.156230000	2.997620000
C	7.856310000	20.158600000	3.014590000
C	1.692390000	14.825090000	11.780970000
C	2.141740000	15.208450000	5.424640000
C	1.571210000	14.144560000	6.125360000
C	1.546290000	14.130020000	7.527640000
C	0.309090000	12.077500000	7.510560000
C	1.028170000	14.163920000	14.015170000
C	1.134530000	13.879360000	12.653800000
C	2.711940000	16.271900000	6.133810000
C	2.112150000	15.204500000	8.275590000
C	2.705790000	16.270680000	7.528740000
C	2.170770000	16.049450000	12.284180000
C	2.073690000	16.318560000	13.644000000
C	3.899040000	18.336710000	7.563980000
C	1.496000000	15.382620000	14.512610000
C	5.955820000	14.828710000	11.781230000
C	6.403610000	15.209570000	5.425240000
C	5.833380000	14.145220000	6.126160000
C	5.809550000	14.132730000	7.528670000
C	4.570350000	12.078890000	7.512250000

C	5.290690000	14.168910000	14.014900000
C	5.398050000	13.883710000	12.653780000
C	6.974650000	16.272960000	6.133150000
C	6.376900000	15.206780000	8.276090000
C	6.968860000	16.272340000	7.527220000
C	6.435690000	16.052860000	12.283620000
C	6.337280000	16.323260000	13.643320000
C	-0.360730000	18.337850000	7.562190000
C	5.759280000	15.387210000	14.512420000
N	1.749960000	14.450180000	10.414810000
N	2.079470000	15.410590000	9.648000000
N	6.013230000	14.452580000	10.415330000
N	6.343080000	15.412760000	9.648480000
O	0.980160000	13.116720000	8.227530000
O	3.253830000	17.273450000	8.266080000
O	5.242940000	13.118390000	8.227740000
O	7.517580000	17.274420000	8.264170000
H	1.704660000	21.106020000	2.919870000
H	4.120050000	21.108380000	2.951970000
H	5.966880000	21.107490000	2.927640000
H	8.381740000	21.109300000	2.959940000
H	1.956640000	8.144400000	3.101920000
H	3.804470000	8.141610000	3.086670000
H	6.218790000	8.144670000	3.107400000
H	8.065800000	8.141190000	3.082320000
H	1.137210000	13.305690000	5.590220000
H	1.013940000	11.487620000	6.899840000

H	8.028870000	12.479550000	6.870740000
H	8.391490000	11.433770000	8.279680000
H	0.575690000	13.437980000	14.693400000
H	0.773080000	12.937700000	12.235380000
H	3.165360000	17.099610000	5.596660000
H	2.625180000	16.752700000	11.585130000
H	2.464670000	17.258950000	14.041040000
H	3.192510000	18.880410000	6.912270000
H	4.740640000	17.958140000	6.961410000
H	4.279320000	19.013370000	8.337690000
H	1.412480000	15.607710000	15.578810000
H	5.397800000	13.306650000	5.590950000
H	5.274800000	11.489870000	6.901660000
H	3.769040000	12.482240000	6.873330000
H	4.131310000	11.436210000	8.282390000
H	4.837070000	13.444220000	14.693820000
H	5.035170000	12.942830000	12.236270000
H	7.427020000	17.099960000	5.596400000
H	6.889860000	16.755710000	11.584000000
H	6.728780000	17.264050000	14.040520000
H	-1.068120000	18.881760000	6.910680000
H	0.481300000	17.960560000	6.958660000
H	0.020050000	19.015870000	8.335580000
H	5.675000000	15.613370000	15.578690000

cis - AZO-2:

C	13.975943903	11.595815769	14.430258989
C	15.206515223	10.877264774	14.447023072

C	15.244959739	9.485119014	14.424572683
C	14.042133289	8.755297463	14.428576418
C	12.811879147	9.433654303	14.449148498
C	12.776101843	10.829353954	14.443845135
C	10.388368409	10.825622061	14.674408680
C	17.592186092	11.026134998	14.540853596
C	10.116638186	13.823435152	9.470026150
C	13.000253067	13.101817737	11.874922934
C	12.249021643	13.151588147	10.705714702
C	10.980893849	13.760113950	10.682514899
C	10.490902412	14.340127929	11.867189172
C	11.252051526	14.334491422	13.025893306
C	12.503575661	13.689797535	13.053843169
N	13.308768343	13.859275879	14.200898112
N	14.064642590	12.977457411	14.695046680
N	14.070699615	7.371166396	14.473851859
O	11.617463737	11.538560112	14.532488081
O	16.319551038	11.660900548	14.428018052
O	10.729036018	13.622128308	8.256828117
O	8.918113945	14.042792739	9.499797274
H	10.385231215	10.212134780	15.590690883
H	10.193302710	10.186471965	13.797444824
H	9.610708141	11.594864015	14.741913770
H	13.230312375	6.879960500	14.184947828
H	14.932174300	6.914643065	14.191085818
H	17.799611941	10.384056265	13.667818009
H	17.662199018	10.427300217	15.464112492

H	18.325265066	11.840527580	14.575082385
H	16.194725878	8.951809483	14.401643830
H	11.887992643	8.858133823	14.494247164
H	11.696259478	13.567162618	8.383769931
H	12.657734669	12.668024263	9.812241004
H	10.896370924	14.823404371	13.934876297
H	9.506976333	14.811621644	11.840890587
H	13.980996895	12.624761771	11.880141494

trans - AZO-2:

C	12.810428914	39.422249017	14.479829100
C	14.052713564	38.763746641	44.457638350
C	15.244555253	39.509088106	44.422441188
C	15.191159999	40.899625857	44.402320760
C	13.942389561	11.613317251	44.405337432
C	12.746308120	10.815129758	14.453093788
C	13.308961124	15.096028245	14.311971221
C	12.194662261	15.949375408	14.229623562
C	12.360437819	17.330179455	14.226913215
C	13.644676372	17.896743794	44.301821360
C	14.759581727	17.037248090	44.361694302
C	14.601087568	15.660618579	44.374076121
C	17.578471576	41.026605842	44.399813563
C	10.357914242	10.732134546	14.566448040
C	-16.100805164	19.366197902	44.308517967
N	14.069261862	12.982713073	44.376062111
N	13.015323134	13.712703661	14.324329792
N	14.104007070	37.387338905	14.519665408

O	16.306449715	11.672202454	44.371419685
O	11.569173863	11.483267400	14.478701995
O	12.829647641	20.181520610	14.591811197
O	-15.014442492	19.871869700	44.086571676
H	11.898449547	38.828104545	14.522454672
H	16.199333208	38.985498572	44.414734501
H	11.203588766	15.496942750	14.163073807
H	11.469107047	17.957963920	14.127039303
H	-14.247815739	17.490327564	44.402109133
H	15.459723773	14.991326268	44.431966590
H	17.725511268	40.384279370	43.514949455
H	17.705564078	40.426705348	45.316925233
H	-11.683236877	41.836980371	44.388389964
H	10.325115758	10.127980319	15.488675652
H	10.225538751	10.076535364	13.689276989
H	9.556031418	11.479396401	14.588660783
H	14.969478991	36.928381497	44.255805485
H	13.260761456	36.866484330	14.302850468
H	12.058618339	19.633469221	14.836903410

cis -AZO-2-RGO:

C	-0.30432	11.25305	1.96533
C	1.07771	11.29076	1.91964
C	1.77819	12.35010	2.51974
C	3.24749	12.29560	2.57663
C	3.95196	11.17117	2.14841
C	5.33330	11.20917	2.08175
C	6.03737	12.33453	2.54442

C	7.51051	12.31537	2.52714
C	-0.32579	13.45227	3.01697
C	1.09782	13.42985	3.06814
C	1.78488	14.58536	3.77739
C	3.23518	14.63393	3.37041
C	3.93396	13.44823	3.02641
C	5.35838	13.42765	3.06560
C	6.04380	14.59000	3.76234
C	7.49558	14.63524	3.37127
C	-0.32172	15.85961	3.32133
C	1.08735	15.87464	3.36784
C	1.79139	17.08073	3.15145
C	3.23508	17.10054	3.16634
C	3.93829	15.85953	3.31452
C	5.34741	15.87668	3.35283
C	6.05257	17.08166	3.14151
C	7.49616	17.10042	3.16437
C	-0.34550	18.30078	2.95813
C	1.10518	18.29835	2.93038
C	1.82464	19.49308	2.70665
C	3.19489	19.49889	2.72442
C	3.91543	18.30087	2.95597
C	5.36637	18.29945	2.92316
C	6.08673	19.49454	2.70216
C	7.45669	19.49962	2.72383
C	2.13180	14.11962	8.15282
C	1.54627	15.29027	7.57530

C	1.36963	15.42705	6.19726
C	1.76268	14.40135	5.33083
C	2.28273	13.22013	5.87247
C	2.47316	13.07609	7.25077
C	3.50490	10.94244	6.91011
C	0.59853	17.44223	8.01748
C	0.32488	8.76937	12.26305
C	1.16916	11.69702	9.97234
C	0.63654	10.50013	10.44033
C	0.94050	10.02083	11.72718
C	1.76635	10.78439	12.56459
C	2.32436	11.96371	12.08826
C	2.05533	12.42353	10.78306
C	6.39780	14.14394	8.13598
C	5.80240	15.30855	7.55635
C	5.62236	15.44063	6.17914
C	6.01316	14.41035	5.31675
C	6.53079	13.23035	5.86153
C	6.72907	13.09261	7.23898
C	7.74710	10.95263	6.89828
C	4.85486	17.46121	7.99817
C	4.64231	8.85793	12.34221
C	5.45733	11.75347	10.00228
C	4.93051	10.56320	10.49313
C	5.25296	10.10147	11.78230
C	6.09059	10.87466	12.59876
C	6.64247	12.04712	12.09939

C	6.35597	12.48807	10.79180
N	7.02212	13.70435	10.47493
N	6.94352	14.37342	9.41644
N	2.72511	13.64511	10.49225
N	2.66096	14.33143	9.44303
O	3.05301	11.96071	7.80262
O	1.20763	16.24018	8.48375
O	0.08411	7.77238	11.34437
O	0.00848	8.60798	13.42469
O	7.30766	11.97655	7.79106
O	5.46402	16.25935	8.46470
O	4.41497	7.83930	11.44552
O	4.31844	8.72339	13.50530
H	1.30161	20.42781	2.51648
H	3.71677	20.43491	2.53907
H	5.56476	20.42974	2.51308
H	7.97945	20.43551	2.54062
H	1.61040	10.48823	1.41434
H	3.43169	10.27072	1.82822
H	5.86203	10.34840	1.67857
H	7.70044	10.40367	1.52345
H	4.26577	11.33090	6.21399
H	2.67085	10.50896	6.33313
H	3.94614	10.16498	7.54545
H	8.16945	17.22966	7.50182
H	1.26827	18.00234	7.34105
H	0.40136	18.03632	8.91717

H	0.93474	16.34070	5.79554
H	2.58867	12.41935	5.20253
H	0.54074	7.99561	10.50941
H	8.43393	9.96343	9.82120
H	2.99183	12.56508	12.70754
H	1.98141	10.42312	13.57111
H	0.86947	12.07967	9.00201
H	-0.01719	11.33409	6.19449
H	6.90591	10.51978	6.33105
H	-0.33119	10.17590	7.53283
H	3.90087	17.24916	7.48804
H	5.52196	18.01753	7.31608
H	4.66391	18.05854	8.89727
H	5.18709	16.35330	5.77592
H	6.82708	12.42489	5.19291
H	4.87751	8.04680	10.60957
H	4.19817	10.01850	9.89109
H	7.31747	12.65837	12.70055
H	6.31970	10.52446	13.60634
H	5.14651	12.12218	9.02991

trans- AZO-2-RGO:

C	8.41027	11.45528	2.69085
C	1.26711	11.49312	2.60219
C	1.97159	12.64159	3.00606
C	3.44398	12.60851	3.03286
C	4.15139	11.48142	2.61728
C	5.53258	11.51052	2.58059

C	6.23424	12.63284	3.05226
C	7.70378	12.59356	3.08135
C	8.38805	13.77833	3.44134
C	1.29216	13.76446	3.45365
C	1.97798	14.95822	4.08929
C	3.43075	14.98326	3.70182
C	4.13140	13.77840	3.43685
C	5.55458	13.75749	3.50299
C	6.23883	14.96087	4.13486
C	7.69084	14.98087	3.72702
C	8.39299	16.20390	3.59778
C	1.28037	16.22442	3.62613
C	1.98548	17.42293	3.38467
C	3.42978	17.43958	3.40059
C	4.13405	16.20269	3.58787
C	5.54394	16.22128	3.63814
C	6.24673	17.42050	3.38965
C	7.69024	17.44024	3.41039
C	8.37017	18.63778	3.18224
C	1.29916	18.63897	3.15617
C	2.01964	19.83475	2.93906
C	3.38974	19.83779	2.95517
C	4.10933	18.63765	3.18083
C	5.56014	18.63386	3.14586
C	6.28003	19.82472	2.90306
C	7.65013	19.83065	2.92604
C	2.53264	13.76977	11.87753

C	1.91149	14.83346	5.64566
C	2.37220	13.64964	6.22877
C	2.41636	13.49649	7.61681
C	3.50380	11.37723	7.38658
C	3.04999	14.02133	14.61335
C	3.46744	12.87261	13.92029
C	3.17723	12.73168	12.57081
C	3.48955	14.19839	16.01865
C	1.47976	15.88468	6.45695
C	1.99847	14.56215	8.47413
C	1.51273	15.75177	7.84862
C	2.10776	14.91911	12.56785
C	2.34674	15.03069	13.93013
C	0.52425	17.91052	8.13660
C	6.74530	14.21675	12.03398
C	6.16519	14.88921	5.70106
C	6.63109	13.74231	6.35329
C	6.65859	13.66349	7.75327
C	7.70457	11.51124	7.65330
C	7.20890	14.66878	14.76891
C	7.75599	13.54359	14.13689
C	7.49218	13.30068	12.79172
C	7.58033	14.99587	16.18554
C	5.71261	15.97026	6.46224
C	6.22457	14.76534	8.55844
C	5.73278	15.91168	7.86076
C	6.18264	15.33985	12.66960

C	6.39385	15.54531	14.02953
C	4.73281	18.08056	8.01202
N	2.34003	13.55631	10.49416
N	2.12759	14.63747	9.85265
N	6.61127	13.90941	10.65503
N	6.31734	14.92372	9.94041
O	2.87604	12.36380	8.20698
O	4.55655	13.69305	16.40807
O	1.08391	16.72380	8.69589
O	2.77645	14.94972	16.84923
O	7.10997	12.56601	8.41019
O	0.22197	15.28558	16.48935
O	5.29187	16.93247	8.64487
O	6.63890	15.02727	17.11601
H	1.49728	20.77180	2.76102
H	3.91303	20.77490	2.78044
H	5.75724	20.75537	2.69519
H	8.17275	20.76291	2.72557
H	2.70571	12.83466	5.59080
H	4.33495	11.80992	6.80606
H	2.78192	10.90317	6.69936
H	3.88938	10.62601	8.08619
H	4.02933	12.10772	14.45792
H	3.48335	11.84633	12.01089
H	1.10170	16.79956	6.00572
H	1.59098	15.70337	12.01425
H	2.01214	15.91979	14.46735

H	8.17404	17.67935	7.50291
H	1.26884	18.47350	7.54700
H	0.20384	18.51296	8.99458
H	1.82851	15.10943	16.54768
H	6.98529	12.89910	5.76298
H	0.02389	11.88031	7.04448
H	6.96445	11.01682	7.00041
H	8.07359	10.79663	8.39835
H	8.38929	12.85762	14.70236
H	7.90423	12.42488	12.28701
H	5.33113	16.85979	5.96604
H	5.58149	16.03280	12.07965
H	5.94613	16.41122	14.52348
H	3.86571	17.81074	7.38639
H	5.47815	18.61144	7.39418
H	4.40609	18.73279	8.83064
H	5.77819	14.55648	16.83427
H	1.79179	10.61271	2.23818
H	3.63586	10.58338	2.28508
H	6.06357	10.64537	2.19032
H	7.89237	10.53839	2.41872