Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Modulation of the exfoliated graphene work function through nitrile imines cycloaddition

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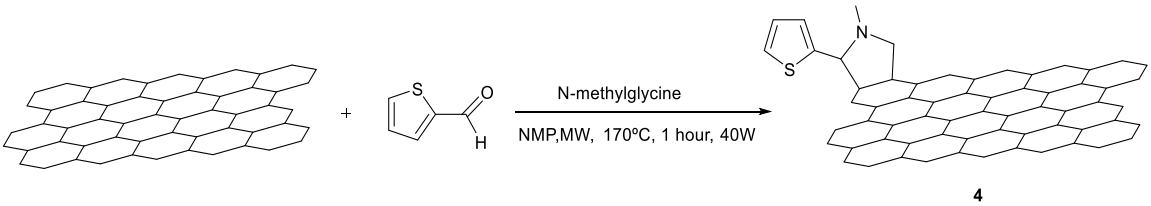
The supporting information contains following items:

Instrumentation. Microwave irradiations were carried out in a CEM Discover reactor with a fiber optic, pressure control system, stirring and air-cooling option FT-IR spectra were measured using a Fourier Transform IR spectrometer (Avatar 370), in KBr pellets. The spectral range was 3500-400 cm^{-1}. Raman spectroscopy were performed on Renishaw inVia Raman microscope at room temperature with exciting 532 nm laser source. Measurements were taken with 10 s of exposure times at varying numbers of accumulations. The laser spot was focused on the sample surface using a long working distance 50× objective. Raman spectra were collected on numerous spots on the sample and recorded with a Peltier cooled CCD camera. The intensity ratio I_D/I_G was obtained by taking the peak intensities following any baseline corrections. The data were collected and analyzed with Renishaw Wire and Origin software.Thermogravimetric analysis was performed using a TGA/DSC Linea Excellent instrument by Mettler-Toledo, collected under inert atmosphere of nitrogen. The sample (~ 0.5 mg) was introduced inside a platinum crucible and equilibrated at 40 ºC followed by a 10 °C min^{-1} ramp between 40 and 1000 °C. The weight changes were recorded as a function of temperature. Transmission electron microscopy (TEM) was performed using a CM300 UltraTWIN (Philips, Netherlands), equipped with a LaB6 filament and a nominal point resolution of 1.7 Å at the Scherzer defocus. The microscope was operated at an acceleration voltage of 300 kV. TEM images were recorded with a charged coupled device camera (TVIPS, Germany), which has an image size of 2048 × 2048 pixels. TEM samples were prepared by drop casting a sonicated suspension of the sample in ethanol/DMF onto Cu grids coated with a holey carbon film layer. The free available software ImageJ (version 1.48r) was used for image analysis. AFM images were acquired in tapping mode using a Multimode V8.10 (Veeco Instruments Inc., Santa Barbara, USA) with a NanoScope V controller (Digital Instruments, Santa Barbara, USA). The cantilevers (RTESP from Bruker Probes) were silicon cantilevers with a resonance frequency of 300 kHz and a nominal force constant of 40 Nm^{-1}. The functionalized samples (1 mg mL^{-1}) were sonicated (frequency: 37 kHz; power 380 W) *N,N*-dimethylformamide (DMF) for 90 min, then samples were prepared by dropcast method on SiO_2 surfaces. The images were processed using WSxM (freely downloadable scanning probe microscopy software from www.nanotec.es) operating at room temperature in ambient air conditions. Photoelectron spectra (XPS) were acquired with a Escalab 200R (Vacuum Generators, Ltd., UK) spectrometer provided with a hemispherical electron analyser and a MgKα1 (hv = 1253.6 eV) X-ray source. The spectra were acquired in the constant analyzer energy mode at 200 eV pass energy for survey spectra and 50 eV pass energy for narrow (10-20 eV) scans. The background pressure in the analysis chamber was maintained below 8.10^{-9} mbar during data acquisition. The XPS data signals were taken in increments of 0.07 eV with dwell times of 40 ms. The binding energy scale of the instrument was calibrated with respect to $Au4f_{7/2}$ (84.0 eV) and $Cu2p_{3/2}$ (932.6 eV) emissions. Charge effects on the samples were corrected by taking the C1s line of adventitious carbon at binding energy (BE) of 284.8 eV which gives an accuracy of ± 0.1 eV. High

resolution spectra envelopes were obtained by curve fitting synthetic peak components using the software "XPS peak". The raw data were used with no preliminary smoothing. Symmetric Gaussian-Lorentzian (90%G-10%L) lines were used to approximate the line shapes of the fitting components. Atomic ratios were computed from experimental intensity ratios and normalized by atomic sensitivity factors. All geometries of intermediates and transition states were full optimize without symmetry constraints using the Gaussian 09 program.[1] DFT computations were carried out using the UM06-2X functional and used the 6-31G(d) basis set. Frequency calculations were perform to confirm the nature of the stationary points and to obtain zero-points energies (ZPEs). All transition structures and minima were full characterize by harmonic analysis. For each located transition structures, only one imaginary frequency was obtain in the diagonalized Hessian matrix, and the corresponding vibration was found to be associated with nuclear motion along the reaction coordinate. HOMO-LUMO topologies were visualize using Gausview program. Ultraviolet photoelectron spectroscopy (UPS) system was a Thermo Scientific Multilab 2000 spectrometer fitted with a He(I) and He(II) UV source with a photon flux >1.5 x 1012 s^{-1} and a 110 mm mean radius hemispherical sector analyzer. Binding energy scale was calibrated using a gold foil in thermal and electrical contact with measured samples. All the measurements were taken in the constant analyzer mode at 20 eV pass energy with increments of 0.01 eV. Work function measurements were performed by evaluating the distance between the secondary electron-cut off in UPS spectra and the incident photon energy (21.21 eV), WF = $h\nu$ - BE_{cutoff}. Valence band edge (VBE) was determined by visual inspection.

Materials. The graphite from TIMCAL (TIMREX KS15, ρ = 2.255 g/cc, particle size = 8.0 µm, specific surface = 12 m^2/g, ashes ≤ 0.100%, interlamelar distance = 0.3354-0.3359 nm) was used to obtain graphene. Organic solvents and reagents were purchased from commercials suppliers. Hydrazones **1a-d** were synthesized by following the previously reported method.[2]

For the exfoliation of graphene, graphite flakes (100 mg) were dispersed in NMP (100 mL) and sonicated at a low-power sonication bath for 15 hours. The dispersion was centrifuged at 500 rpm for 45 minutes, the supernatant was decanted and stored in solution. Sample sonication was carried out by using an Elmasonic P 300 H sonicator bath (37 kHz). The concentration, after the exfoliation process, was estimated from the absorbance at 660 nm by using the extinction coefficient of graphene (α = 3620 mL mg^{-1} $m^{-}1$) previously determined by Coleman.[3] Graphene concentrations were calculated according to the Lambert-Beer law.



Scheme S1. Synthetic procedure for the preparation of the pyrrolidine graphene derivative **4**.

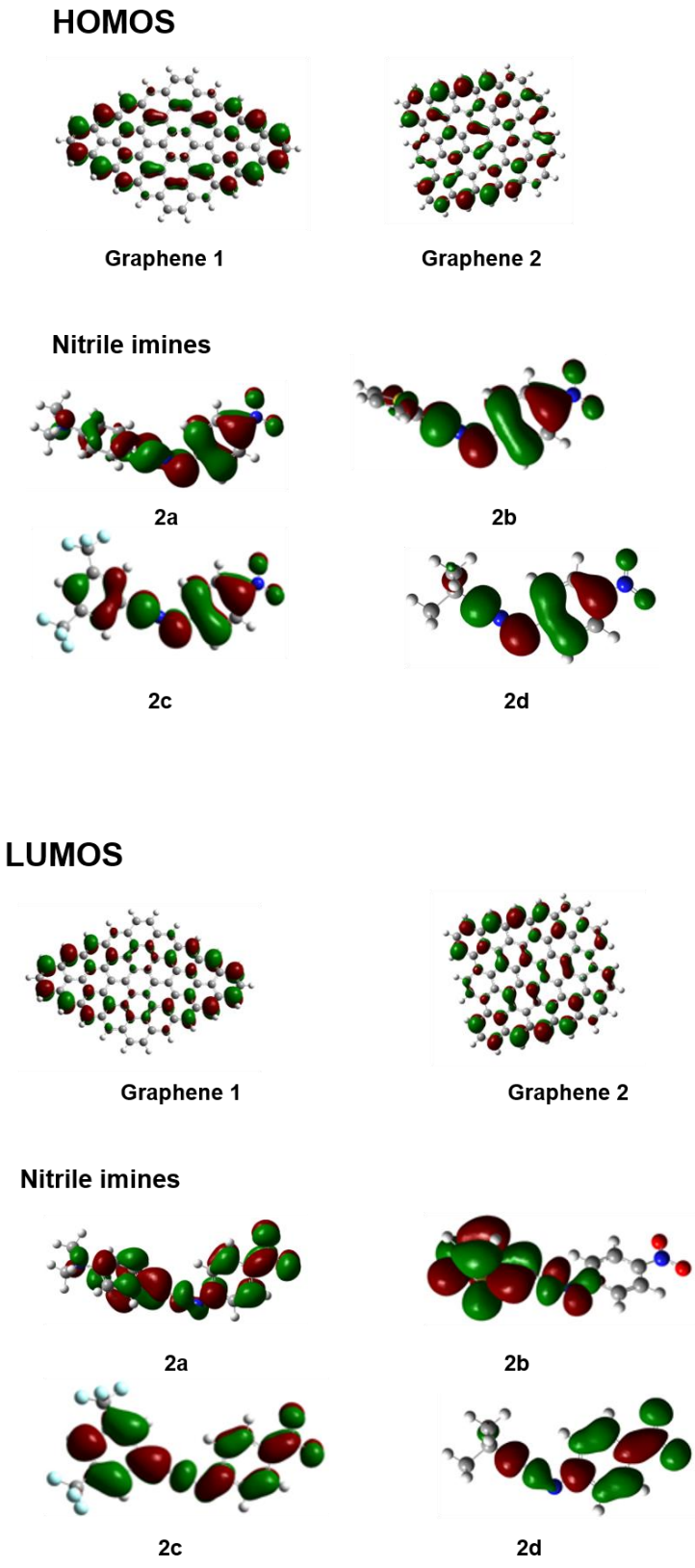


Figure S1. Topology of frontier molecular orbital of graphene model 1 and 2 and nitrile imines **2a-d**.

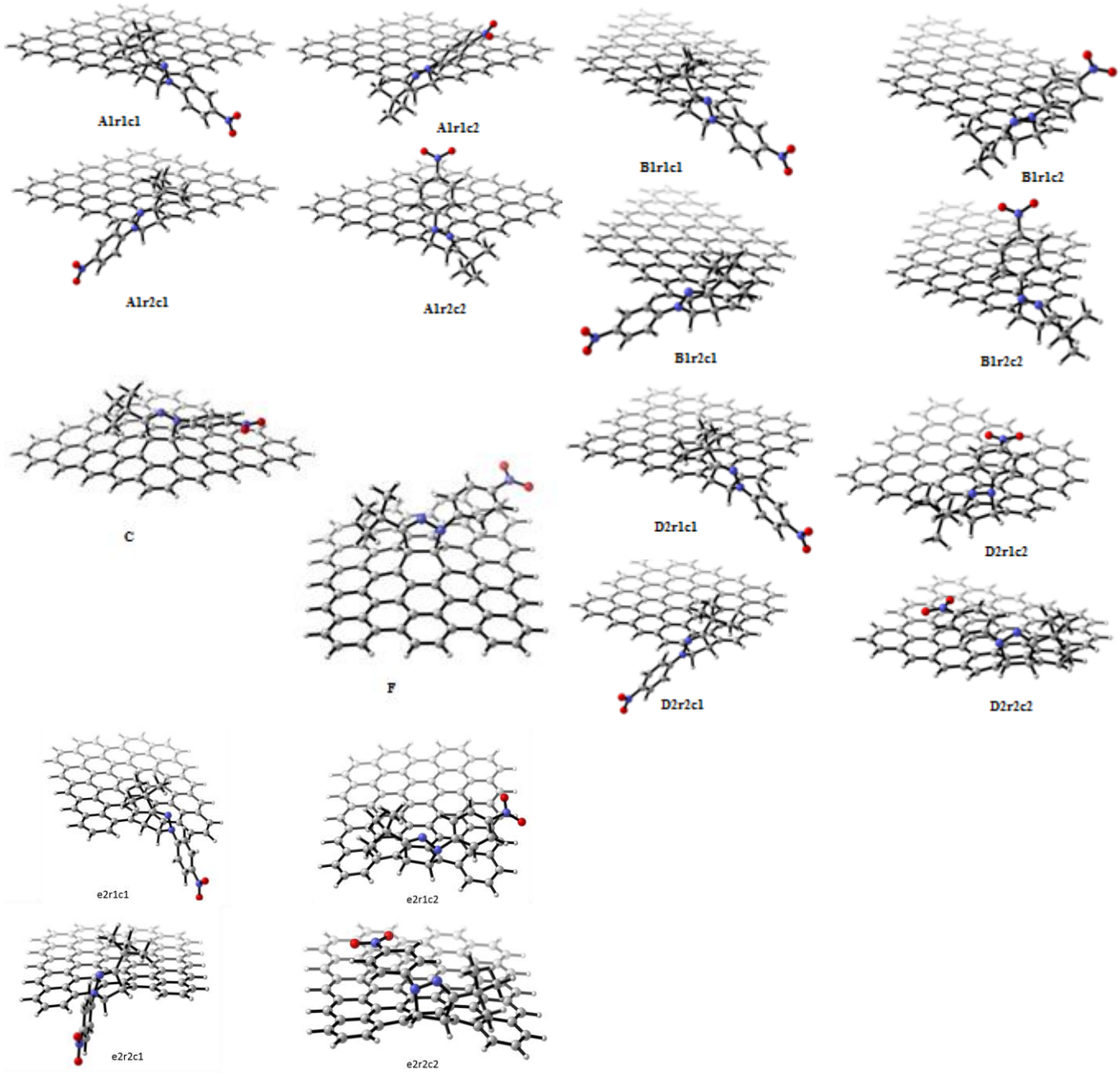


Figure S2. All possible cycloaducts optimized at U)M06-2X/6-31G(d) theory level.

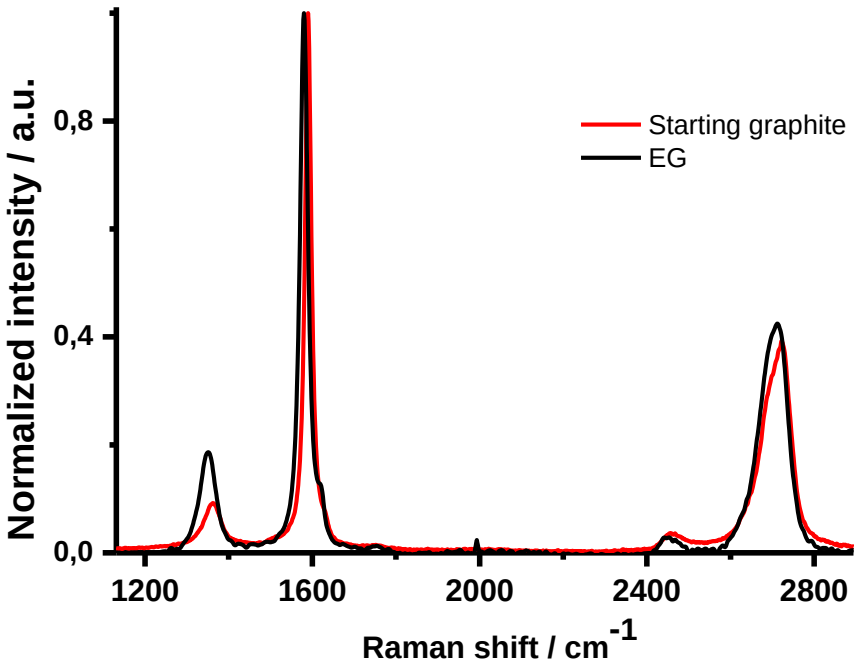


Figure S3. Raman spectrum of starting graphite (red) in comparison with exfoliated graphene (**EG**) (black) upon excitation at 532 nm.

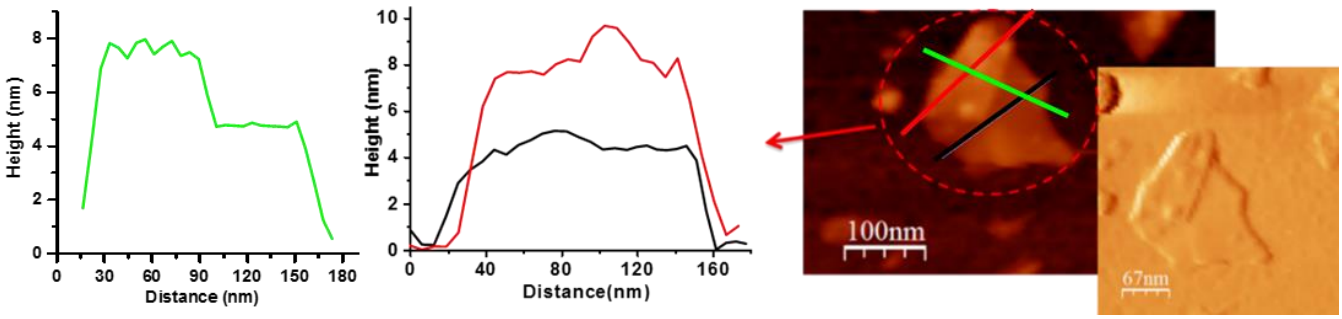


Figure S4. Atomic force microscopy images of exfoliated graphene (EG) deposited onto silicon surface.

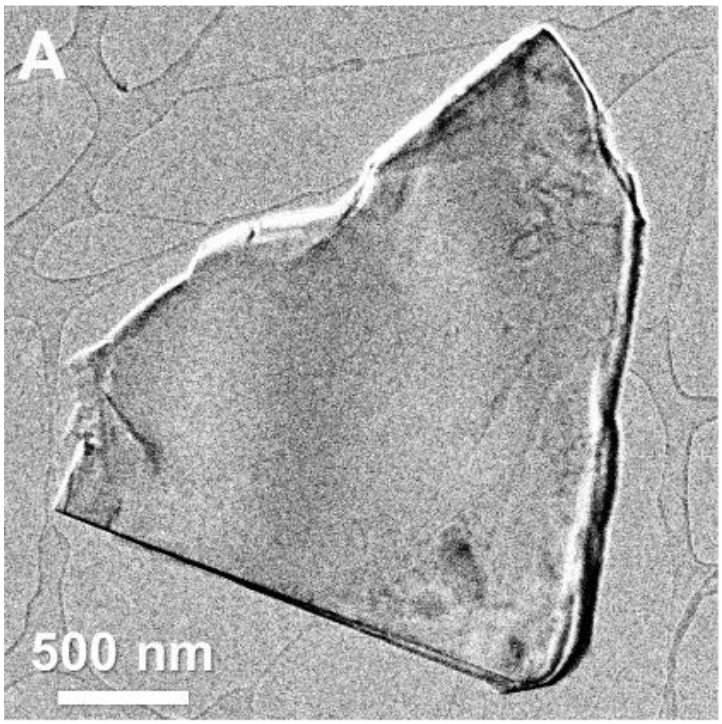


Figure S5. A) TEM image of an exfoliated graphitic flake.

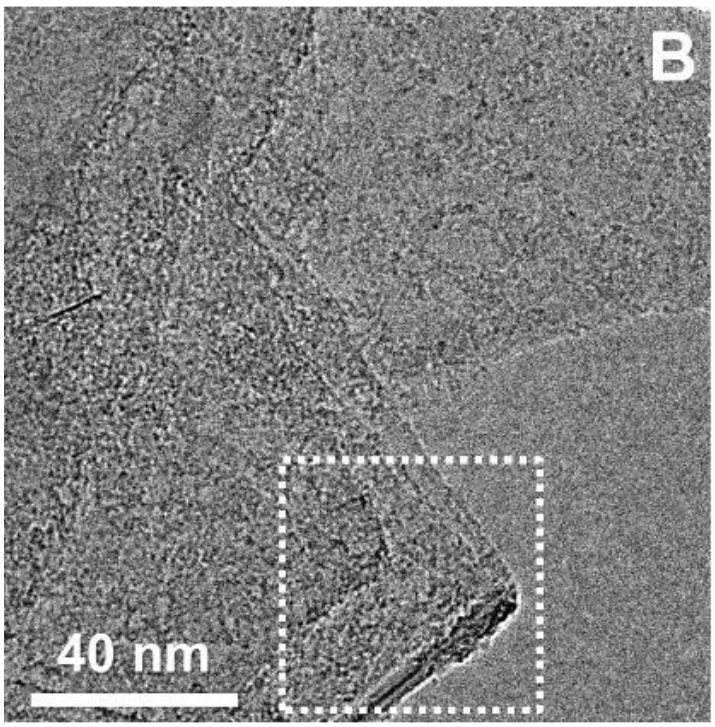


Figure S5. B) Higher TEM image magnification of an exfoliated graphitic flake showing the thin terraces.

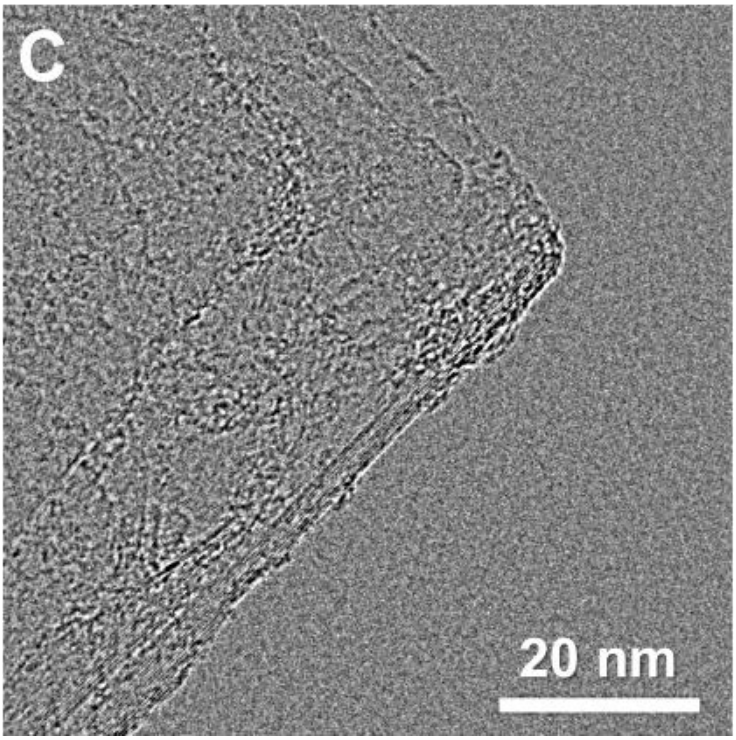


Figure S5. C) Zoom in showing the area marked in (B).

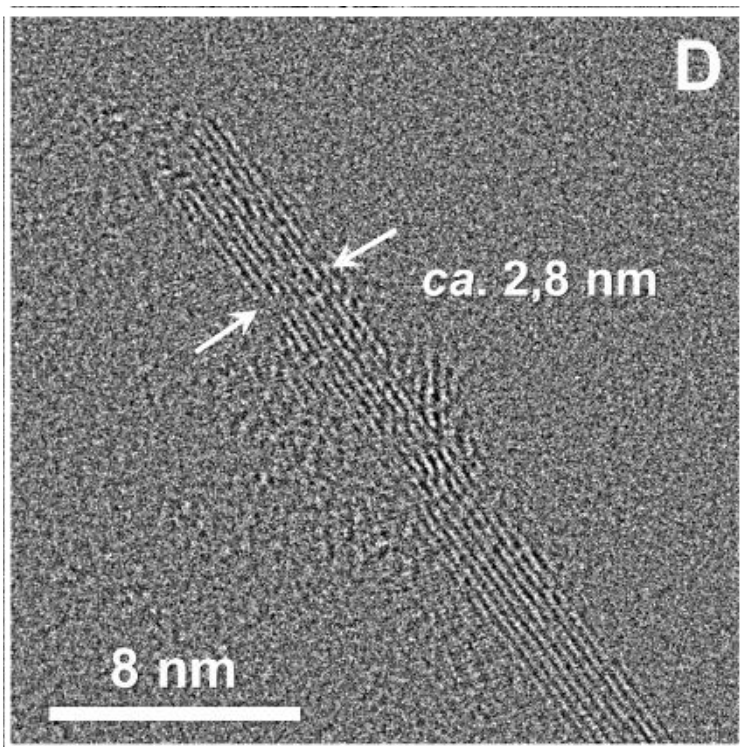


Figure S5. D) HRTEM highlighting the few-layers structure of the exfoliated graphene, with a thickness of ca. 2,8 nm, in excellent accordance with AFM analysis.

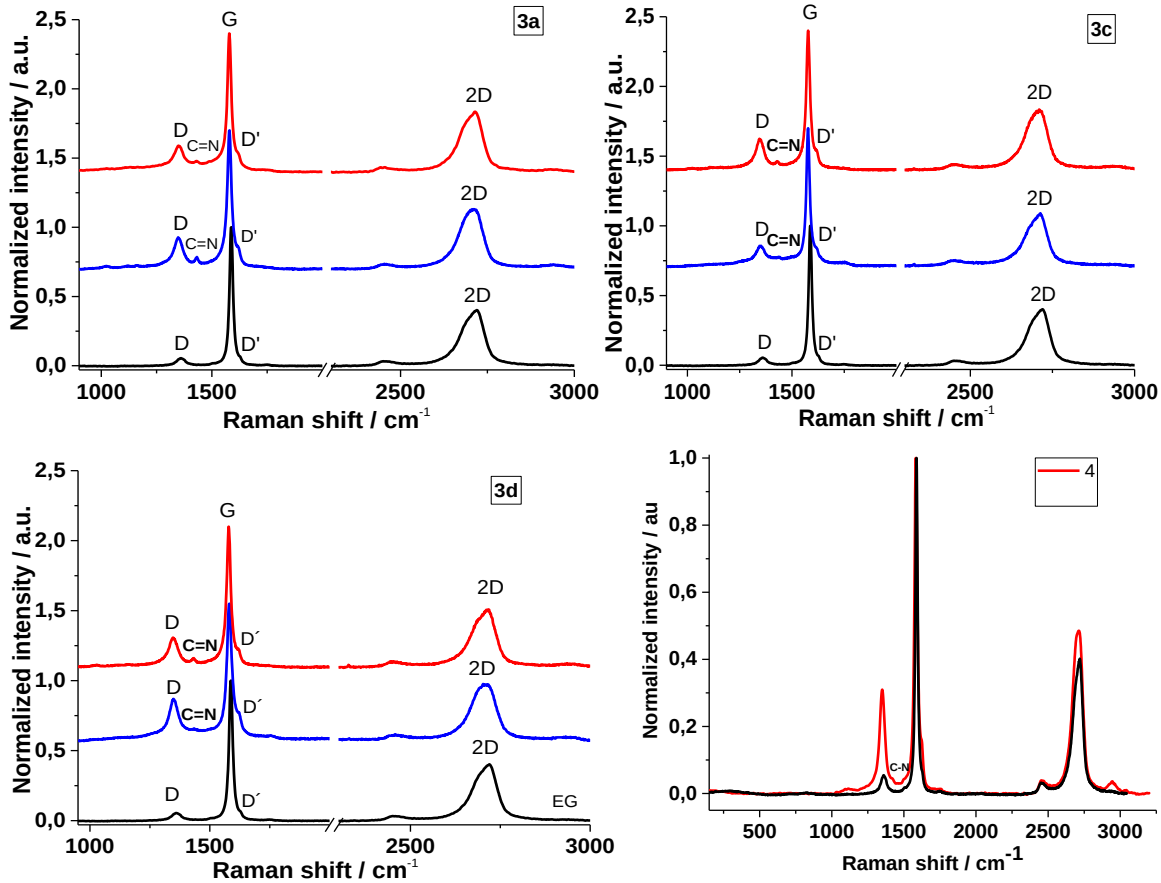


Figure S6. Raman spectra of functionalized materials **3a**, **3c**, **3d** and **4** compared with **EG** (in black). The spectra *in blue* represent the hybrid prepared under classical heating and *in red* under microwave irradiation. λ_{exc}= 532 nm.

XPS. For each sample, high-resolution C1s, O1s, and N1s for **3a**, S2p for **3b** or F1s for **3c**, respectively, core-level spectra were recorded and the corresponding binding energy of peak components are summarized in Table S4. Survey spectrum, C1s and O1s spectra of the raw graphite and exfoliated graphite (**EG**) samples are shown in Figures S7 and S8, respectively. Following the assignment by Boehm[4] and Stankovich,[5] the C1s emission was satisfactorily curve-resolved with six components: thee most intense peak, at 284.8 eV, and the weak π–π* component at about 291.3 eV, come from the sp^2C-atoms of the graphene structure. The components at 286.2, 287.7 and 289.3 eV are due to C–O, C=O and –COOH species, respectively.[6] Similarly, the O1s emission was curve-resolved with two components: a minor one at 532.1 eV and a mayor one at 533.8 eV associated to O=C and O–C groups, respectively[4] (Figures S8b and S9b).

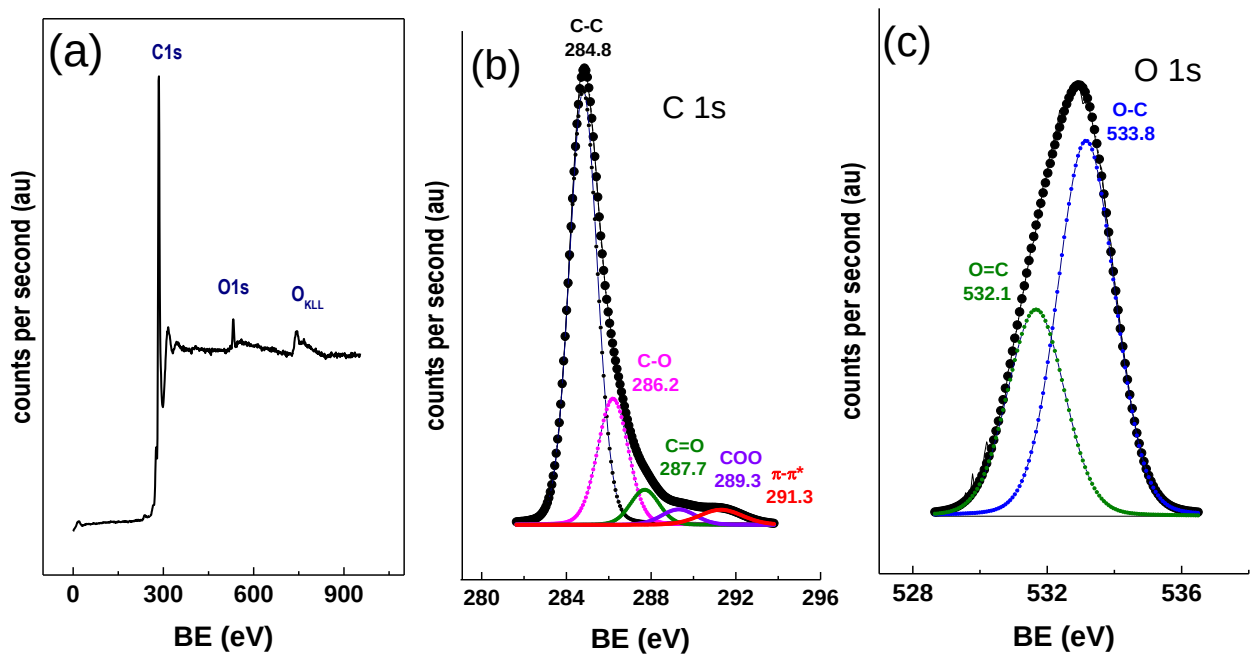


Fig S7. (a) Survey, (b) C1s and (c) O1s core-level spectra of graphite.

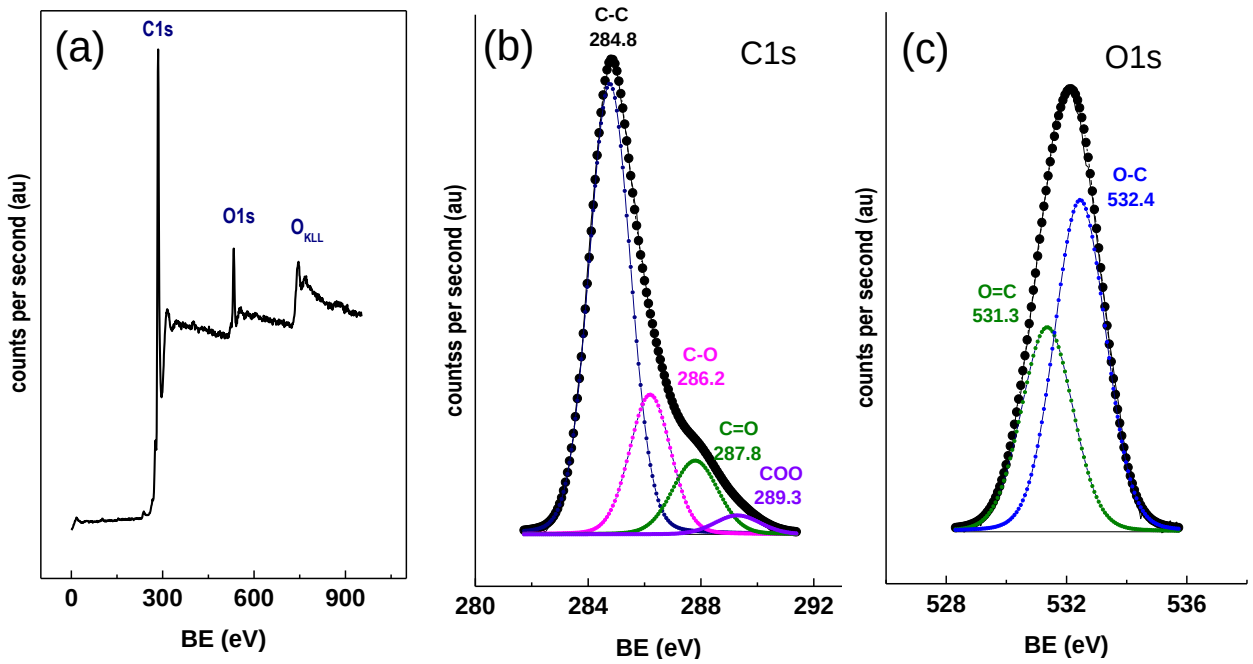


Fig S8. (a) Survey, (b) C1s and (c) O1s core-level spectra of **EG.**

C and O surface composition of the exfoliated graphite and raw substrates and the values are reported in Table S5. The O-content of the raw graphite was 2.4 % O atom and increased slightly to 2.8 % O atom for EG, consistently with the large area increase and subsequent exposure of C-atom at the edges upon liquid exfoliation.[7] In most exfoliation methods, oxygenation of the graphene sheets tends to occur concomitantly.[8]

Photoelectron spectra of *functionalized* graphene surfaces **3a-d** in which the substituent R is a, b, c and d were then recorded. For **3a**, in addition to C1s and O1s spectra, a minor N1s emission was observed (see Figure S9a). The peak was satisfactorily fitted into three components: two peaks at 399.4 and 400.4 eV (for the pyrazoline ring and that for the *N,N*-dimethyl- anilinyl group, respectively) and a third component at ~ 406 eV[9] (that can be assigned to the NO_2 group). These findings unambiguously confirm the molecular anchorage of pyrazoline moiety on graphene sheets (see also Table S4 and Figure S9a).

Functionalization is also effective for R = b. This material (**3b**) shows, in addition to C1s and O1s peaks of graphene substrate, the S2p one at a binding energy of about 164.0 eV which is characteristic of C-S bonds in thiophenic structures[10] (shown in Figure S9b) together with the N1s line whose two components show binding energies and intensities similar to that found in sample **3a**.

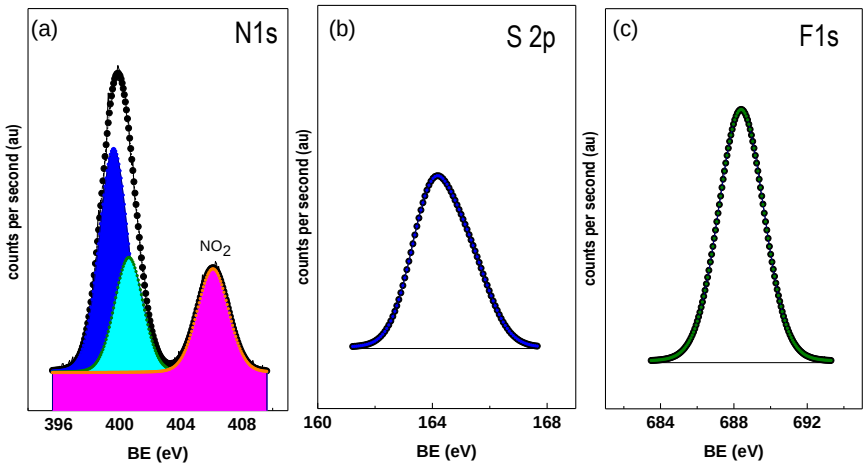
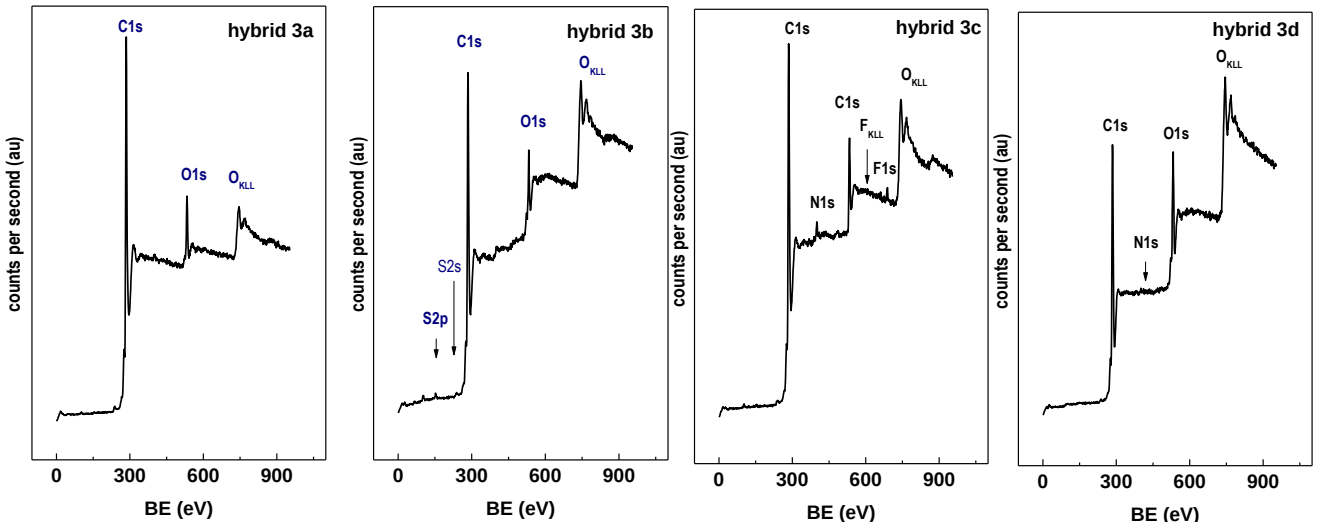


Figure S9. Photoemission spectra and fit of the (a) N1s region of **3a** (b) S2p region of **3b** and the (c) F1s region of **3c**.

Similarly, photoelectron spectra of sample **3c** were recorded. In addition to the C1s and O1s peaks coming from the graphene substrate, the N1s and F1s emissions of the anchored pyrazoline moiety are observed. Figure S9c shows the F1s peak at a binding energy of 688.4 eV in conjunction with the observation of an additional C1s component at 292.7 eV are conclusive of the strong C-F covalent bonding.[11] Surprisingly, in all samples **3a-d** a higher binding energy of N1s peak corresponding to the $–NO_2$ group have been observed (407 eV), when compared with its tabulate value (ca. 405.8 eV[9]). Such binding energy differences have been attributed to the orientation of $–NO_2$ group with respect to the graphene surface.[12]

A



B

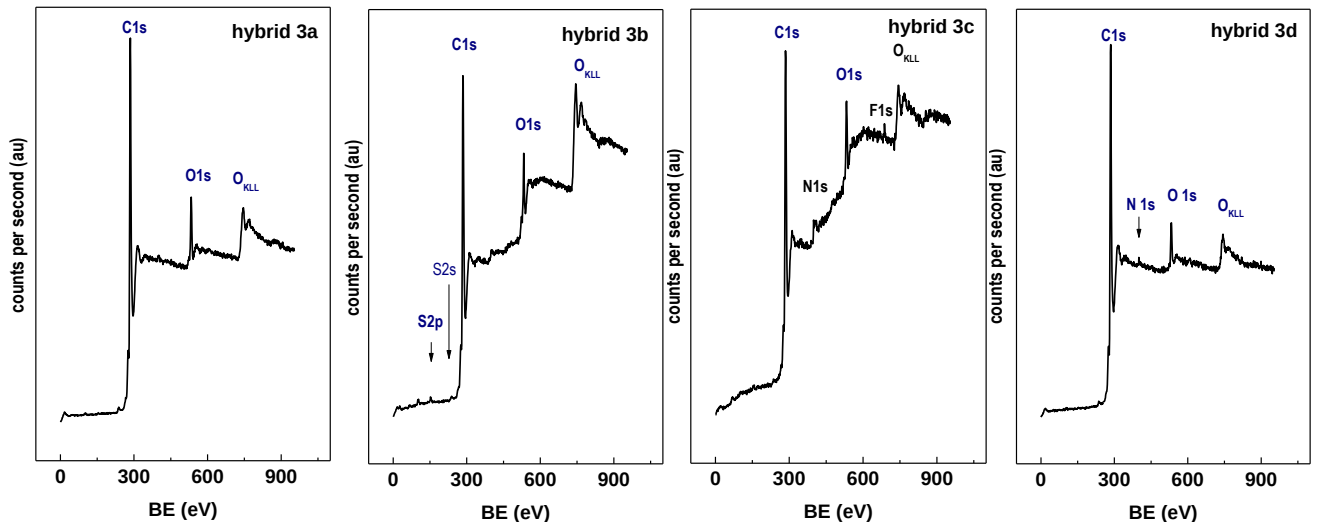


Figure S10. XPS survey spectra of *functionalized* graphene surfaces **3a-d** (A) prepared under classical heating and (B) under microwave irradiation.

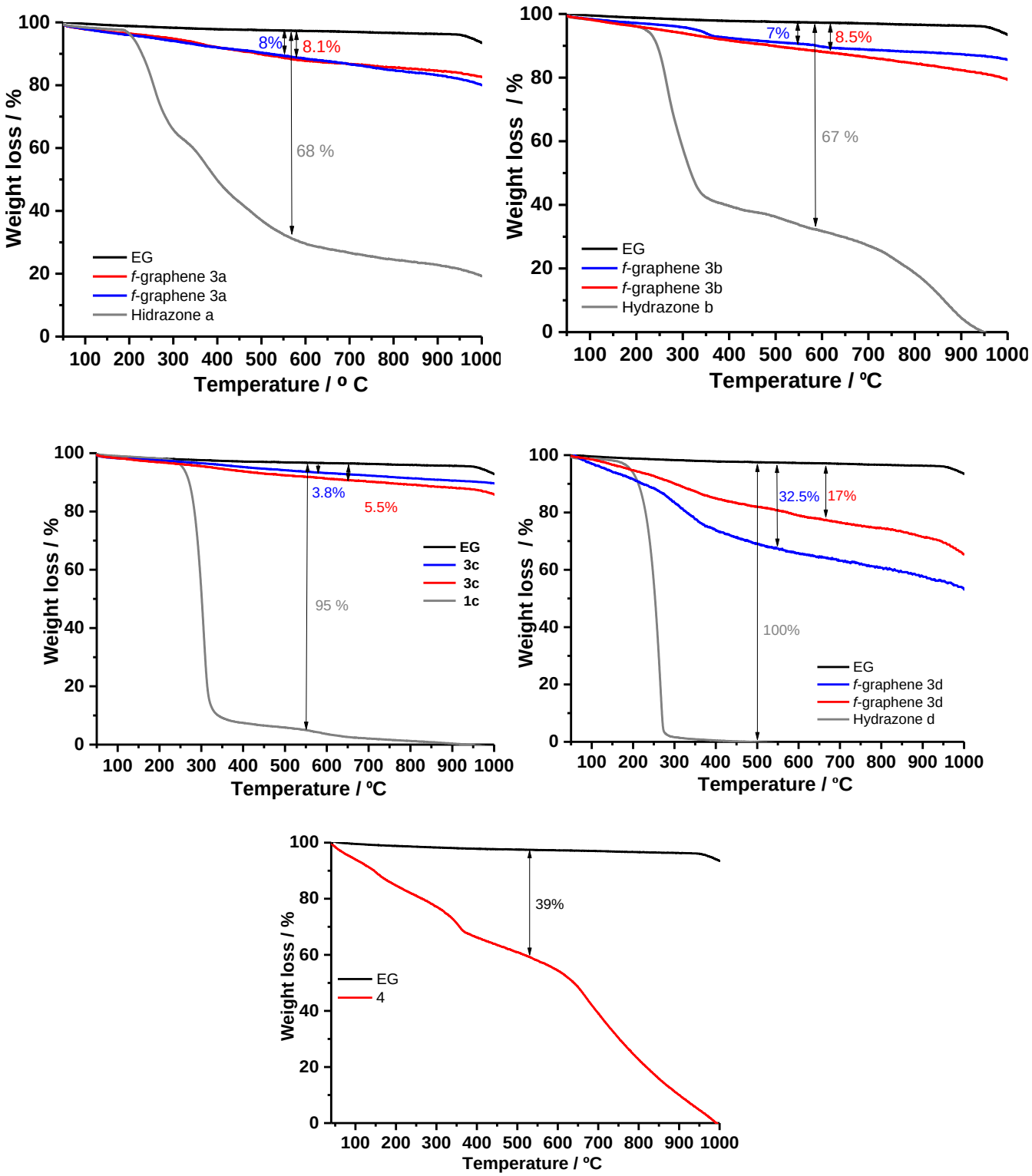


Figure S11. TGA curves recorded at 10º C/min under N_2 of **EG** and functionalized graphene materials **3a**-**d** and **4.** The curves *in blue* represents the hybrids prepared under classical heating and *in red* under microwave irradiation. Also *in grey* are depicted the corresponding hydrazones **1a-d**.

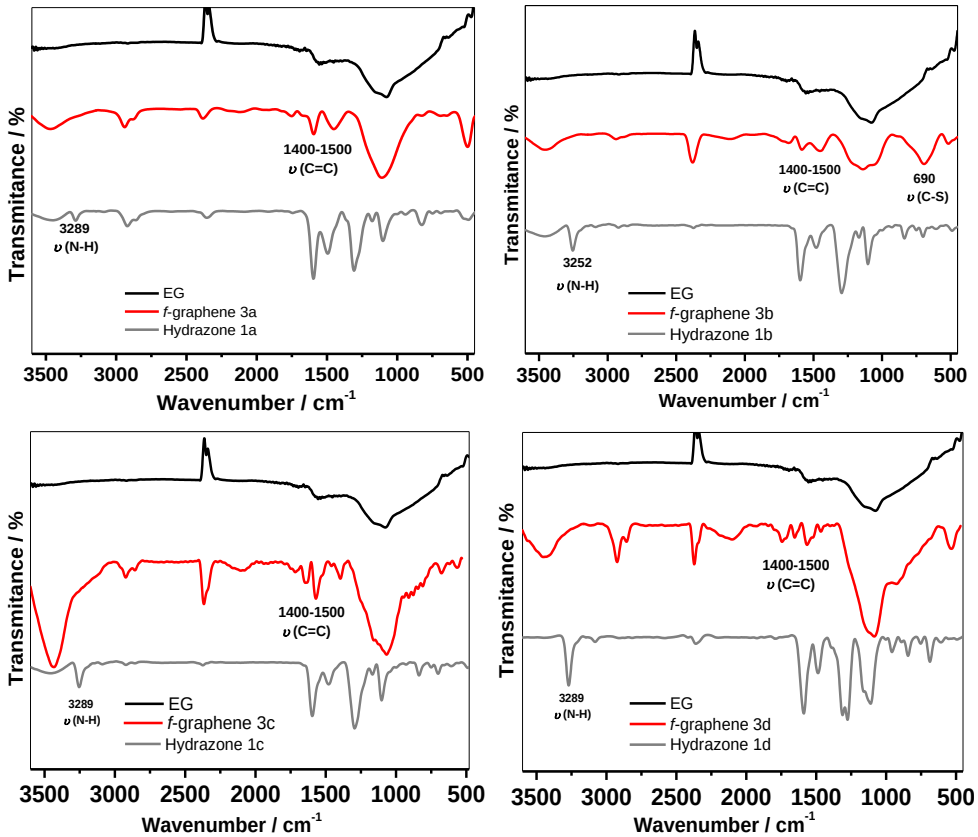


Fig S12. FTIR spectra of *functionalized* graphene samples **3a-d** compared with their corresponding hydrazones **1a-d** and the starting EG.

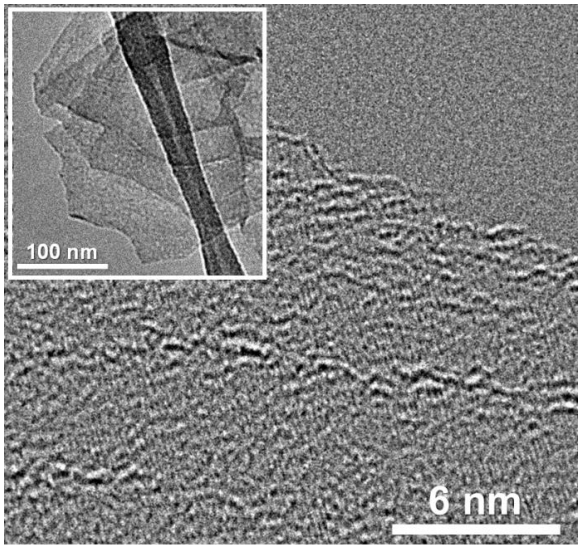


Figure S13. HRTEM image of the edge of a flake of sample **3d**, in which one can clearly distinguish the terraces composed of different numbers of graphene layers. Moreover, it is possible to observe the crystal lattice in addition to some amorphous areas, probably related with the presence of organic addends.

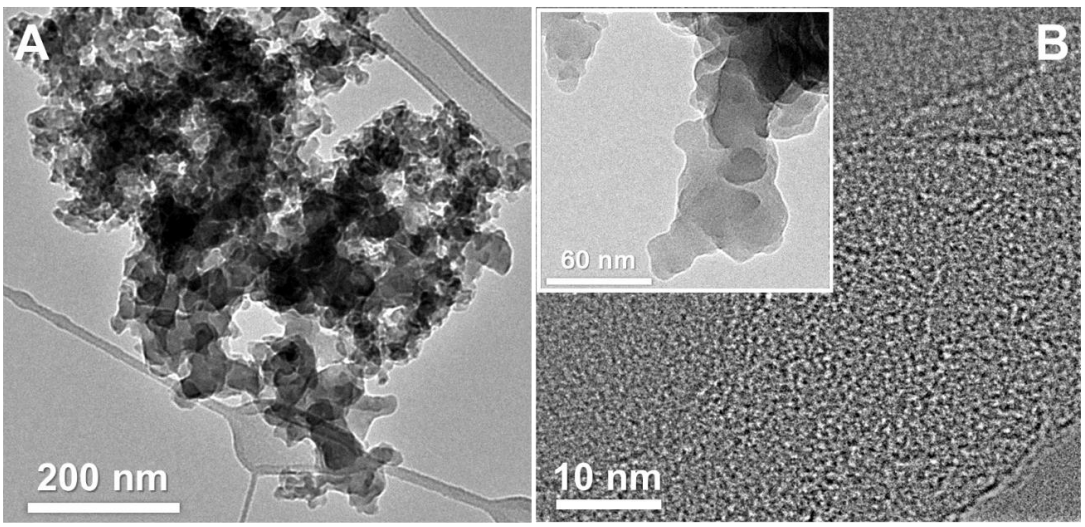


Figure S14. (A) TEM image of an agglomerate of graphitic flakes of sample **3c** on a holey carbon grid; the sample seems to consist on aggregates of few-layer graphene terraces with scrolled edges. (B) HRTEM image showing some of the thinnest flakes with the presence of an amorphous contribution in the same way that sample **3d**.

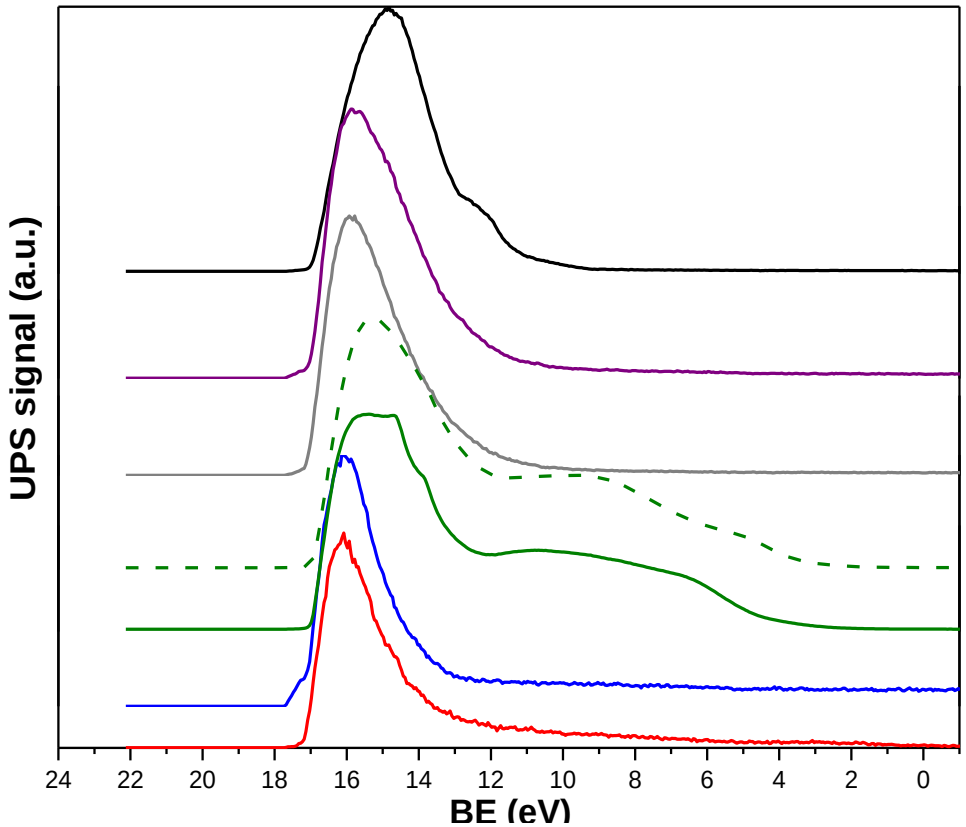


Figure S15. Valence band spectra of the graphene-based nanohybrids. From top to bottom: EG (black line); **4** (purple line); **3d** (gray line); **3c**, green lines: solid and dashed lines corresponding to higher and lower functionalization degree, respectively; **3b** (blue line); **3a** (red line).

Table S1. Energy values (eV) of nitrile imines frontier molecular orbitals and energy band gap (eV) in gas-phase computed at (U)M06-2X/6-31G(d). Energy band gap is related to graphene model 2 ((HOMO=-4.55 eV, LUMO=-3.04 eV).

Nitrile imine	**HOMO (eV)**	**LUMO (eV)**	**Band gap ($LUMO_{graphene}$-$HOMO_{dipole}$)**	**Band gap ($LUMO_{dipole}$-$HOMO_{graphene}$)**
2a	-6.49	-0.91	3.45	3.64
2b	-7.00	-1.60	3.96	2.95
2c	-7.27	-2.09	4.23	2.46
2d	-6.75	-0.72	3.71	3.83

Table S2. Comparative of I_D/I_G ratio for *functionalized* graphene samples **3a-d** and **4.**

samples	I_D/I_G[a]	
	classical Heating	**microwave irradiation**
3a	0.22	0.18
3b	0.17	0.24
3c	0.15	0.21
3d	0.32	0.20
4	-	0.31

[a] Raman D/G ratio for **EG** = 0.05

Table S3. Comparative study of the degree of functionalization of nanohybrids **3a-d** and **4**.

Sample	TGA wt loss (%)[a]		C atom/ organic group	
	classical heating	microwave irradiation	classical heating	microwave irradiation
3a	8.6	8.1	261	279
3b	7	8.5	290	231
3c	3.8	5.5	803	551[b]
3d	32.5	17	55	102
4	-	39	-	34

[a] TGA results show relative weight loss.

[b] TGA weight loss corresponding to the sample **3c*** (derivative **3c** prepared under microwave irradiation).

Table S4. Binding energy (eV) of the core-level atoms of **3a-d** and **4** and its precursors (top) prepared under classical heating and (bottom) prepared under microwave irradiation. The peak percentages are indicated in brackets.

Sample	C 1s							O1s		N1s		F1s	S2p
	C sp^2	C sp^3	C-O	C=O	COO	C-F	C-N	O=C	O-C	C=N C-N	NO_2	F-C	S-C
EG	284.8 (65)	-	286.2 (20)	287.8 (12)	289.3 (3)	-	-	531.3 (38)	532.4 (62)	-	-		
1a	284.8 (66)	285.2 (16)	-	-	-	-	286.1 (18)	-	532.1	399.4 (50) 400.4 (24)	405.9 (26)		
1b	284.8 (90)	-	286.2 (10)	-	-	-	-		532.0	399.9 (66)	406.1 (34)		164.0
1c	284.8 (58)	-	-	287.8 (12)	-	292.7 (5)	286.2 (25)		532.0	400.3(67)	406.5 (33)	688.4	
1d	284.8 (68)	285.3 (13)	-	-	-		286.2 (19)		532.0	400.1 (67)	406.2 (33)		
3a	284.8 (81)	285.3 (2)	286.3 (14)	287.7 (2)	289.3 (1)		-	531.8 (33)	533.2 (67)	399.4 (25) 400.4 (50)	407.1 (25)		
3b	284.8 (75)		286.3 (16)	287.7 (6)	289.3 (3)			531.9 (34)	533.2 (66)	400.4 (67)	407.1 (33)		164.0
3c	284.8 (71)	285.3 (2)	286.3 (18)	287.7 (7)	289.3 (2)			531.8 (33)	533.1 (67)	400.4 (67)	407.0 (33)	688.4	
3d	284.8 (75)	285.2 (6)	286.3 (12)	287.7 (4)	289.2 (3)			531.6 (20)	532.9 (80)	400.0 (67)	406.0 (33)		

Sample	C1s							O1s		N1s		F1s	S2p
	C sp^2	C sp^3	C-O	C=O	COO	C-F	C-N	O=C	O-C	C=N C-N	NO_2	F-C	S-C
EG	284.8 (65)	-	286.2 (20)	287.8 (12)	289.3 (3)	-	-	531.3 (38)	532.4 (62)	-	-		
1a	284.8 (66)	285.2 (16)	-	-	-	-	286.1 18)	-	532.1	399.4 (50) 400.4 (24)	405.9 (26)		
1b	284.8 (90)	-	286.2 (10)	-	-	-	-		532.0	399.9 (66)	406.1 (34)		164.0
1c	284.8 (58)	-	-	287.8 (12)	-	292.7 (5)	286.2 (25)		532.0	400.3(67)	406.5 (33)	688.4	
1d	284.8 (68)	285.3 (13)	-	-	-		286.2 (19)		532.0	400.1 (67)	406.2 (33)		
3a	284.8 (62)	285.3 (3)	286.3 (24)	287.7 (8)	289.2 (3)		-	531.7 (46)	533.9 (54)	399.9 (69)	407.5 (31)		

3b	284.8 (70)		286.2 (23)	287.7 (7)				531.3 (25)	532.7 (75)	400.0 (75)	407.4 (25)		164.1
3c	284.8 (64)		286.3 (25)	287.7 (9)	289.3 (2)			531.9 (36)	533.4 (64)	399.9 (67)	407.0 (33)	688.4	
3d	284.8 (68)	285.2 (2)	286.2 (21)	287.7 (9)				531.7 (36)	533.2 (64)	400.0 (67)	407.4 (33)		
4	284.8 (73)		286.2 (31)	288.1 (6)				531.9 (37)	533.2 (63)	400.1			16

Table S5. Elemental content of graphite and EG.

Sample	Carbon (%at)	Oxigen (%at)
graphite	97.6	2.4
EG	97.3	2.8

Table S6. Total Electronic Energies[a] (E, in a.u.), Zero-point correction of Energies (ZPE, in a.u.), and number of imaginary frequencies[b] (NIMAG, cm^{-1}) of all stationary points discussed in the main text.

	Structure	E	ΔZPE	NIMAG(ν)
	Nitril_tBu	-740.974215	0.233494	0
	Graphene 1	-2679.393886	0.686541	0
	Graphene 2	-2679.439574	0.686241	0
Cycloadducts structures	A1-r1c1	-3420.351857	0.920244	0
	A1-r1c2	-3420.362489	0.920713	0
	A2-r2c1	-3420.351859	0.921082	0
	A2-r2c2	-3420.361947	0.920715	0
	B1-r1c1	-3420.344534	0.920427	0
	B1-r1c2	-3420.352691	0.919334	0
	B2-r2c1	-3420.344340	0.919714	0
	B2-r2c2	-3420.352907	0.922182	0
	C	-3420.324296	0.921199	0
	D1-r1c1	-3420.396911	0.920530	0
	D1-r1c2	-3420.406515	0.921418	0
	D2-r2c1	-3420.394871	0.921173	0
	D2-r2c2	-3420.404642	0.921386	0
	E1-r1c1	-3420.383888	0.921022	0
	E1-r1c2	-3420.399239	0.920762	0
	E2-r2c1	-3420.384393	0.921021	0
	E2-r2c2	-3420.399244	0.920470	0
	f	-3420.352035	0.921022	0
TS structur	TsA1-r1c1	-3420.443740	0.916660	-440.7946
	TsA1-r1c2	-3420.435229	0.917337	-441.8965

	TsA2-r2c1	-3420.443740	0.916660	-439.4977
	TsA2-r2c2	-3420.428931	0.916057	-440.3970
	TsB1-r1c1	-3420.416811	0.914087	-439.5710
	TsB1-r1c2	-3420.405574	0.914547	-431.8550
	TsB2-r2c1	-3420.416555	0.922182	-453.6869
	TsB2-r2c2	-3420.405786	0.917702	-474.6346
	TsC	-3420.340738	0.915672	-276.4484
	TsD1-r1c1	-3420.484114	0.915123	-424.4990
	TsD1-r1c2	-3420.467161	0.915798	-440.3134
	TsD2-r2c1	-3420.484202	0.916799	-437.3954
	TsD2-r2c2	-3420.460988	0.916848	-447.5270
	TsE1-r1c1	-3420.4317	0.916436	-445.1605
	TsE1-r1c2	-3420.433853	0.916848	-460.4905
	TsE2-r2c1	-3420.445967	0.915808	-463.7708
	TsE2-r2c2	-3420.428275	0.916853	-460.5372
	TsF	-3420.357415	0.920079	-330.8347

Cartesian coordinates optimized at the (U)M06-2X/6-31G(d) of all the stationary points discussed in the main text.

Nitrilimini 2d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.745123	0.372505	0.000378
2	6	0	-4.009220	-0.393053	-0.000010

3	7	0	-1.753127	0.973716	0.000259
4	7	0	-0.727418	1.731335	0.000194
5	6	0	0.485507	1.056833	0.000146
6	6	0	0.633702	-0.343433	0.000243
7	6	0	1.641353	1.863383	-0.000008
8	6	0	1.894071	-0.916825	0.000179
9	1	0	-0.242579	-0.984128	0.000371
10	6	0	2.898750	1.295295	-0.000078
11	1	0	1.512588	2.940188	-0.000080
12	6	0	3.014321	-0.094435	0.000017
13	1	0	2.026346	-1.992149	0.000251
14	1	0	3.795873	1.902308	-0.000204
15	7	0	4.338605	-0.700055	-0.000071
16	8	0	5.305331	0.044579	-0.000203
17	8	0	4.407987	-1.919108	-0.000008
18	6	0	-5.171870	0.613592	-0.002984
19	1	0	-6.114837	0.058054	-0.003547
20	1	0	-5.144632	1.250600	0.885021
21	1	0	-5.142174	1.248178	-0.892636
22	6	0	-4.060832	-1.271650	-1.260942
23	1	0	-4.026028	-0.660599	-2.166584
24	1	0	-3.225026	-1.976742	-1.282347
25	1	0	-4.994691	-1.842635	-1.259927
26	6	0	-4.064021	-1.268066	1.263258
27	1	0	-3.228477	-1.973362	1.288538
28	1	0	-4.031104	-0.654519	2.167289
29	1	0	-4.998056	-1.838808	1.261677

Graphene 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000303	7.070923	0.000000
2	6	0	-0.000308	7.784472	1.238335
3	6	0	-0.000504	4.945163	1.231560
4	6	0	0.000252	5.669498	2.476137
5	6	0	-0.000862	2.820511	2.466328
6	6	0	-0.000308	7.784472	-1.238335
7	6	0	-0.000504	4.945163	-1.231560
8	6	0	0.000252	5.669498	-2.476137
9	6	0	-0.000862	2.820511	-2.466328
10	6	0	0.000124	5.655924	0.000000
11	6	0	-0.002303	2.824913	0.000000
12	6	0	0.001317	3.537624	1.234325
13	6	0	-0.003263	0.703606	1.233220
14	6	0	0.001317	3.537624	-1.234325
15	6	0	-0.003263	0.703606	-1.233220
16	6	0	0.003246	1.415710	0.000000
17	6	0	-0.003247	-1.415710	0.000000
18	6	0	0.000698	3.551185	3.713204
19	6	0	-0.000715	0.694245	3.704144
20	6	0	0.000441	1.433983	4.952651
21	6	0	-0.000441	-1.433983	4.952651
22	6	0	0.001986	1.420615	2.468144
23	6	0	-0.001986	-1.420615	2.468144
24	6	0	0.000716	-0.694245	3.704144

25	6	0	-0.000698	-3.551185	3.713204
26	6	0	0.003263	-0.703606	1.233220
27	6	0	-0.001317	-3.537624	1.234325
28	6	0	0.000862	-2.820511	2.466328
29	6	0	-0.000252	-5.669498	2.476137
30	6	0	0.000698	3.551185	-3.713204
31	6	0	-0.000715	0.694245	-3.704144
32	6	0	0.000441	1.433983	-4.952651
33	6	0	-0.000441	-1.433983	-4.952651
34	6	0	0.001986	1.420615	-2.468144
35	6	0	-0.001986	-1.420615	-2.468144
36	6	0	0.003263	-0.703606	-1.233220
37	6	0	-0.001317	-3.537624	-1.234325
38	6	0	0.000716	-0.694245	-3.704144
39	6	0	-0.000698	-3.551185	-3.713204
40	6	0	0.000862	-2.820511	-2.466328
41	6	0	-0.000252	-5.669498	-2.476137
42	6	0	0.002304	-2.824913	0.000000
43	6	0	-0.000124	-5.655924	0.000000
44	6	0	0.000505	-4.945163	1.231560
45	6	0	0.000308	-7.784472	1.238335
46	6	0	0.000505	-4.945163	-1.231560
47	6	0	0.000308	-7.784472	-1.238335
48	6	0	0.000303	-7.070923	0.000000
49	6	0	0.000354	0.673329	6.189681
50	1	0	0.000420	1.228023	7.124187
51	6	0	0.000944	2.798704	4.938138
52	1	0	0.001043	3.347818	5.877309
53	6	0	0.000723	4.927136	3.695589

54	1	0	0.000834	5.475380	4.635102
55	6	0	0.000074	7.056297	2.452740
56	1	0	0.000128	7.605378	3.391743
57	6	0	-0.000469	9.192694	1.208663
58	1	0	-0.000485	9.738513	2.148055
59	6	0	-0.000614	9.878383	0.000000
60	1	0	-0.000724	10.964026	0.000000
61	6	0	-0.000469	9.192694	-1.208663
62	1	0	-0.000485	9.738513	-2.148055
63	6	0	0.000074	7.056297	-2.452740
64	1	0	0.000128	7.605378	-3.391743
65	6	0	0.000723	4.927136	-3.695589
66	1	0	0.000834	5.475380	-4.635102
67	6	0	0.000944	2.798704	-4.938138
68	1	0	0.001043	3.347818	-5.877309
69	6	0	0.000354	0.673329	-6.189681
70	1	0	0.000420	1.228023	-7.124187
71	6	0	-0.000354	-0.673329	6.189681
72	1	0	-0.000420	-1.228023	7.124187
73	6	0	-0.000944	-2.798704	4.938138
74	1	0	-0.001043	-3.347818	5.877309
75	6	0	-0.000723	-4.927136	3.695589
76	1	0	-0.000834	-5.475380	4.635102
77	6	0	-0.000074	-7.056297	2.452740
78	1	0	-0.000128	-7.605378	3.391743
79	6	0	0.000469	-9.192694	1.208663
80	1	0	0.000485	-9.738513	2.148055
81	6	0	0.000614	-9.878383	0.000000
82	1	0	0.000724	-10.964026	0.000000

83	6	0	0.000469	-9.192694	-1.208663
84	1	0	0.000485	-9.738513	-2.148055
85	6	0	-0.000074	-7.056297	-2.452740
86	1	0	-0.000128	-7.605378	-3.391743
87	6	0	-0.000723	-4.927136	-3.695589
88	1	0	-0.000834	-5.475380	-4.635102
89	6	0	-0.000944	-2.798704	-4.938138
90	1	0	-0.001043	-3.347818	-5.877309
91	6	0	-0.000354	-0.673329	-6.189681
92	1	0	-0.000420	-1.228023	-7.124187

Graphene 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.039454	2.850910	0.000005
2	6	0	0.811148	3.554617	0.000006
3	6	0	0.807028	0.714563	0.000001
4	6	0	-0.416648	1.420207	0.000002
5	6	0	-0.416648	-1.420207	-0.000002
6	6	0	3.261372	3.558311	0.000007
7	6	0	3.266917	0.715376	0.000002
8	6	0	4.503270	1.426368	0.000003
9	6	0	4.503271	-1.426367	-0.000002
10	6	0	2.043107	1.418564	0.000003
11	6	0	2.043108	-1.418564	-0.000002
12	6	0	0.807028	-0.714563	-0.000001

13	6	0	0.811149	-3.554617	-0.000006
14	6	0	3.266918	-0.715375	-0.000001
15	6	0	3.261374	-3.558310	-0.000006
16	6	0	2.039455	-2.850910	-0.000005
17	6	0	-1.655296	-0.717080	-0.000002
18	6	0	-0.414769	-2.849747	-0.000005
19	6	0	0.813283	-4.994440	-0.000008
20	6	0	2.058871	-5.676601	-0.000009
21	1	0	2.056561	-6.764253	-0.000011
22	6	0	3.255825	-4.998516	-0.000008
23	6	0	4.491515	-2.852765	-0.000004
24	6	0	5.742489	-0.730331	0.000000
25	6	0	5.742488	0.730333	0.000002
26	6	0	4.491514	2.852766	0.000006
27	6	0	3.255823	4.998517	0.000009
28	6	0	2.058870	5.676601	0.000010
29	1	0	2.056559	6.764253	0.000012
30	6	0	0.813281	4.994439	0.000009
31	6	0	-0.414770	2.849747	0.000005
32	6	0	-1.655297	0.717080	0.000001
33	6	0	4.520963	5.693318	0.000011
34	6	0	5.716471	3.574166	0.000007
35	6	0	-0.395823	5.677370	0.000010
36	6	0	-1.642323	3.557904	0.000006
37	6	0	-1.642321	-3.557905	-0.000006
38	6	0	5.716472	-3.574165	-0.000005
39	6	0	4.520965	-5.693317	-0.000009
40	6	0	-0.395822	-5.677370	-0.000010
41	6	0	-1.630047	4.998394	0.000008

42	6	0	5.688945	5.014798	0.000010
43	6	0	5.688947	-5.014796	-0.000008
44	6	0	-1.630046	-4.998395	-0.000009
45	1	0	6.638383	5.543658	0.000011
46	1	0	4.506760	6.779789	0.000013
47	1	0	-0.394928	6.764826	0.000011
48	1	0	6.638385	-5.543656	-0.000008
49	1	0	4.506763	-6.779789	-0.000011
50	1	0	-0.394926	-6.764827	-0.000012
51	6	0	6.915972	-2.863206	-0.000004
52	6	0	6.927250	1.477858	0.000004
53	6	0	6.927251	-1.477856	-0.000001
54	6	0	6.915970	2.863208	0.000006
55	1	0	7.854939	-3.410348	-0.000004
56	1	0	7.887325	-0.975851	0.000000
57	1	0	7.887324	0.975853	0.000003
58	1	0	7.854938	3.410350	0.000007
59	6	0	-2.845552	-5.687379	-0.000010
60	6	0	-2.871092	-2.860194	-0.000005
61	6	0	-2.874359	-1.422401	-0.000003
62	6	0	-2.874360	1.422400	0.000002
63	6	0	-2.871093	2.860193	0.000004
64	6	0	-4.113205	0.714551	0.000000
65	6	0	-2.845552	5.687378	0.000009
66	6	0	-4.069891	5.013745	0.000007
67	6	0	-4.092407	3.579815	0.000005
68	6	0	-4.069890	-5.013746	-0.000009
69	6	0	-4.092405	-3.579816	-0.000007
70	6	0	-4.113204	-0.714552	-0.000002

71	6	0	-5.299090	5.726144	0.000008
72	6	0	-5.343666	2.893952	0.000004
73	6	0	-5.343940	1.427112	0.000001
74	6	0	-5.343938	-1.427115	-0.000003
75	6	0	-5.343664	-2.893952	-0.000006
76	6	0	-5.299091	-5.726143	-0.000010
77	6	0	-6.489775	-5.049300	-0.000009
78	1	0	-7.428682	-5.594052	-0.000010
79	6	0	-6.512948	-3.641792	-0.000007
80	1	0	-7.478912	-3.151154	-0.000006
81	6	0	-6.527242	-0.692810	-0.000002
82	1	0	-7.485257	-1.198856	-0.000003
83	6	0	-6.527243	0.692804	0.000000
84	6	0	-6.512949	3.641795	0.000004
85	6	0	-6.489774	5.049303	0.000006
86	1	0	-7.428680	5.594057	0.000007
87	1	0	-7.485259	1.198845	0.000001
88	1	0	-7.478914	3.151161	0.000003
89	1	0	-5.272361	6.812182	0.000010
90	1	0	-5.272363	-6.812181	-0.000012
91	1	0	-2.838691	-6.774846	-0.000012
92	1	0	-2.838691	6.774845	0.000011

A1-r1c1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-6.998942	-3.195232	-0.455842
2	6	0	-6.808419	-4.607659	-0.556611
3	6	0	-4.563906	-2.876263	-0.395625
4	6	0	-4.378953	-4.300651	-0.488366
5	6	0	-2.128273	-2.559613	-0.319796
6	6	0	-8.319766	-2.649755	-0.431406
7	6	0	-6.067551	-0.928522	-0.280156
8	6	0	-7.400793	-0.385101	-0.251542
9	6	0	-5.138669	1.340573	-0.113594
10	6	0	-5.878403	-2.334154	-0.378229
11	6	0	-3.636859	-0.611563	-0.237733
12	6	0	-3.447944	-2.021368	-0.316666
13	6	0	-1.202591	-0.295486	-0.212801
14	6	0	-4.954498	-0.069694	-0.208103
15	6	0	-2.709070	1.654574	-0.094981
16	6	0	-2.519606	0.245894	-0.175040
17	6	0	-0.277710	1.970648	-0.092208
18	6	0	-1.950241	-3.989384	-0.391631
19	6	0	0.314480	-2.247941	-0.263376
20	6	0	0.475845	-3.685697	-0.206432
21	6	0	2.771111	-1.922186	-0.432263
22	6	0	-1.015279	-1.710128	-0.260265
23	6	0	1.235002	0.021056	-0.239256
24	6	0	1.420944	-1.402633	-0.307548
25	6	0	3.674856	0.351029	-0.273169
26	6	0	-0.086973	0.560603	-0.170086
27	6	0	2.153274	2.293801	-0.111976
28	6	0	2.337704	0.883782	-0.208094

29	6	0	4.599404	2.614171	-0.132862
30	6	0	-6.478500	1.881243	-0.076070
31	6	0	-4.210330	3.612530	0.049968
32	6	0	-5.558313	4.148535	0.095016
33	6	0	-3.287000	5.894347	0.214788
34	6	0	-4.030921	2.193642	-0.048864
35	6	0	-1.780834	3.924310	0.056750
36	6	0	-1.594136	2.511107	-0.034956
37	6	0	0.647585	4.241577	0.050506
38	6	0	-3.110607	4.457958	0.108698
39	6	0	-0.854251	6.206641	0.214759
40	6	0	-0.671901	4.776835	0.110055
41	6	0	1.578323	6.521718	0.204073
42	6	0	0.836717	2.832457	-0.045578
43	6	0	3.078116	4.559056	0.034671
44	6	0	3.266931	3.153739	-0.068501
45	6	0	5.519154	4.879361	0.010407
46	6	0	1.764169	5.097798	0.097481
47	6	0	4.009026	6.833412	0.184031
48	6	0	4.199159	5.421371	0.076733
49	6	0	1.854400	-4.235215	0.017353
50	1	0	1.891100	-5.267061	-0.364538
51	6	0	-0.600786	-4.500703	-0.320648
52	1	0	-0.466959	-5.580768	-0.319452
53	6	0	-3.043741	-4.813733	-0.480782
54	1	0	-2.902783	-5.891049	-0.535560
55	6	0	-5.489325	-5.125557	-0.569977
56	1	0	-5.350542	-6.201995	-0.642367
57	6	0	-7.941315	-5.440623	-0.634095

58	1	0	-7.799692	-6.515048	-0.711449
59	6	0	-9.222318	-4.901660	-0.610924
60	1	0	-10.082161	-5.561785	-0.670117
61	6	0	-9.416899	-3.529457	-0.510566
62	1	0	-10.422527	-3.118775	-0.491948
63	6	0	-8.484677	-1.247014	-0.327309
64	1	0	-9.492907	-0.839436	-0.307260
65	6	0	-7.557350	1.030025	-0.145455
66	1	0	-8.565239	1.438305	-0.120421
67	6	0	-6.630411	3.306459	0.032042
68	1	0	-7.638660	3.713906	0.062911
69	6	0	-5.711139	5.588174	0.205290
70	1	0	-6.720876	5.988413	0.240090
71	6	0	2.970812	-3.422639	-0.646173
72	1	0	3.068843	-3.659923	-1.709164
73	6	0	3.829819	-1.078559	-0.395923
74	1	0	4.843773	-1.461770	-0.463869
75	6	0	4.754762	1.196949	-0.235717
76	1	0	5.761091	0.787266	-0.286199
77	6	0	5.683767	3.475991	-0.093784
78	1	0	6.691264	3.069160	-0.143077
79	6	0	6.617081	5.760038	0.051559
80	1	0	7.621972	5.350496	-0.000201
81	6	0	6.423785	7.132415	0.156402
82	1	0	7.283880	7.793922	0.186064
83	6	0	5.143110	7.668159	0.222412
84	1	0	5.002067	8.742376	0.304097
85	6	0	2.691284	7.348651	0.246302
86	1	0	2.553045	8.424487	0.327785

87	6	0	0.246073	7.031673	0.261398
88	1	0	0.106150	8.107343	0.342288
89	6	0	-2.197790	6.714880	0.266517
90	1	0	-2.337204	7.790777	0.347464
91	6	0	-4.644532	6.408014	0.262060
92	1	0	-4.776119	7.483632	0.344376
93	7	0	3.728197	-4.208927	1.402085
94	6	0	2.450398	-4.308438	1.440203
95	7	0	4.118222	-3.921484	0.109055
96	6	0	5.442944	-3.940500	-0.246076
97	6	0	6.417792	-4.368902	0.679618
98	6	0	5.848239	-3.556077	-1.541396
99	6	0	7.749127	-4.410956	0.315911
100	1	0	6.103333	-4.659651	1.673359
101	6	0	7.183559	-3.603851	-1.899676
102	1	0	5.117894	-3.203002	-2.261585
103	6	0	8.124759	-4.030853	-0.970223
104	1	0	8.510160	-4.736404	1.015176
105	1	0	7.509530	-3.308833	-2.889824
106	7	0	9.529806	-4.075913	-1.347161
107	8	0	9.827898	-3.723815	-2.477354
108	8	0	10.330138	-4.462966	-0.511259
109	6	0	1.725858	-4.592237	2.734485
110	6	0	2.737940	-4.706917	3.879165
111	1	0	2.205350	-4.916369	4.812467
112	1	0	3.454128	-5.512688	3.696037
113	1	0	3.301677	-3.777756	3.999399
114	6	0	0.747701	-3.444124	3.045611
115	1	0	-0.062457	-3.379376	2.314028

116	1	0	0.297822	-3.611372	4.030289
117	1	0	1.271664	-2.482689	3.068120
118	6	0	0.952907	-5.914847	2.608583
119	1	0	0.449600	-6.135561	3.555924
120	1	0	0.186788	-5.861565	1.830372
121	1	0	1.630743	-6.744503	2.380839

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.433549	0.637335	0.303308
2	6	0	7.756462	2.018930	0.135100
3	6	0	5.062220	1.148819	-0.084119
4	6	0	5.394984	2.538361	-0.257530
5	6	0	2.691578	1.661592	-0.479423
6	6	0	8.466210	-0.311038	0.579515
7	6	0	5.768825	-1.168232	0.360092
8	6	0	6.814070	-2.119592	0.635649
9	6	0	4.106701	-2.976573	0.416805
10	6	0	6.090267	0.206616	0.193378
11	6	0	3.401732	-0.653859	-0.020421
12	6	0	3.725442	0.721896	-0.197026
13	6	0	1.030883	-0.132354	-0.395693
14	6	0	4.433544	-1.599254	0.249570
15	6	0	1.741609	-2.457282	0.042034
16	6	0	2.063040	-1.080072	-0.132598

17	6	0	-0.625289	-1.942919	-0.327937
18	6	0	3.034036	3.048544	-0.665212
19	6	0	0.313675	2.197765	-0.862514
20	6	0	0.677673	3.584464	-1.115549
21	6	0	-2.093252	2.710635	-1.085054
22	6	0	1.357595	1.247903	-0.585323
23	6	0	-1.342834	0.382567	-0.743517
24	6	0	-1.011267	1.769869	-0.900788
25	6	0	-3.733001	0.896875	-1.093824
26	6	0	-0.303761	-0.565293	-0.499212
27	6	0	-2.997913	-1.428334	-0.684824
28	6	0	-2.673180	-0.049008	-0.840620
29	6	0	-5.385174	-0.908650	-1.037217
30	6	0	5.159234	-3.928515	0.690088
31	6	0	2.445205	-4.788597	0.472606
32	6	0	3.506923	-5.739380	0.745844
33	6	0	0.785600	-6.613090	0.531596
34	6	0	2.778790	-3.403664	0.306248
35	6	0	0.081605	-4.269276	0.099633
36	6	0	0.407177	-2.888657	-0.070905
37	6	0	-2.284377	-3.753108	-0.266545
38	6	0	1.127811	-5.212349	0.365901
39	6	0	-1.581652	-6.091609	0.160108
40	6	0	-1.247173	-4.695246	-0.006299
41	6	0	-3.950740	-5.571976	-0.203309
42	6	0	-1.963174	-2.374393	-0.432580
43	6	0	-4.653594	-3.235771	-0.623897
44	6	0	-4.334748	-1.859197	-0.783862
45	6	0	-7.035683	-2.716102	-0.970337

46	6	0	-3.621996	-4.179519	-0.367603
47	6	0	-6.318488	-5.048924	-0.556127
48	6	0	-5.998525	-3.665497	-0.718093
49	6	0	-0.397894	4.555660	-1.595215
50	1	0	-0.392928	4.593556	-2.689463
51	6	0	1.971190	3.965997	-0.998875
52	1	0	2.251217	4.998154	-1.178658
53	6	0	4.339133	3.456594	-0.550428
54	1	0	4.588910	4.506193	-0.691438
55	6	0	6.716331	2.939806	-0.143834
56	1	0	6.967769	3.990080	-0.273938
57	6	0	9.101435	2.419880	0.249131
58	1	0	9.349340	3.469958	0.121383
59	6	0	10.099571	1.491116	0.519393
60	1	0	11.130272	1.821703	0.602486
61	6	0	9.794629	0.145059	0.682680
62	1	0	10.582164	-0.573656	0.891334
63	6	0	8.123831	-1.675926	0.738940
64	1	0	8.914770	-2.393005	0.946912
65	6	0	6.460305	-3.493547	0.793078
66	1	0	7.250886	-4.211451	0.999735
67	6	0	4.798377	-5.310757	0.847005
68	1	0	5.590047	-6.028017	1.052649
69	6	0	3.142383	-7.135894	0.905069
70	1	0	3.938634	-7.846577	1.109833
71	6	0	-1.774277	4.168900	-1.062744
72	1	0	-2.546123	4.727935	-1.617560
73	6	0	-3.374562	2.289855	-1.202934
74	1	0	-4.173297	3.017543	-1.332724

75	6	0	-5.033132	0.468633	-1.185475
76	1	0	-5.825604	1.190839	-1.368208
77	6	0	-6.695661	-1.349481	-1.124307
78	1	0	-7.489223	-0.630016	-1.312655
79	6	0	-8.365693	-3.170386	-1.055358
80	1	0	-9.156097	-2.449460	-1.244068
81	6	0	-8.668036	-4.517851	-0.897825
82	1	0	-9.700046	-4.847673	-0.965576
83	6	0	-7.665559	-5.448454	-0.652031
84	1	0	-7.911429	-6.499482	-0.528260
85	6	0	-5.274968	-5.971899	-0.301858
86	1	0	-5.524446	-7.023325	-0.177792
87	6	0	-2.893308	-6.494300	0.058839
88	1	0	-3.141884	-7.545856	0.183739
89	6	0	-0.514199	-7.015549	0.428700
90	1	0	-0.763895	-8.067019	0.553433
91	6	0	1.863878	-7.546193	0.805007
92	1	0	1.607206	-8.595027	0.927496
93	7	0	-1.032210	6.001100	0.107780
94	6	0	-0.307090	5.939217	-0.945218
95	7	0	-1.678214	4.780671	0.298453
96	6	0	-2.859692	4.856468	1.071149
97	6	0	-3.549360	6.061710	1.249854
98	6	0	-3.341112	3.681821	1.665908
99	6	0	-4.720868	6.089358	1.993442
100	1	0	-3.153673	6.967969	0.807072
101	6	0	-4.520302	3.698638	2.393923
102	1	0	-2.772526	2.764347	1.564299
103	6	0	-5.195014	4.905014	2.542108

104	1	0	-5.276371	7.007091	2.143802
105	1	0	-4.913036	2.802772	2.859079
106	7	0	-6.445018	4.928745	3.307642
107	8	0	-6.844289	3.874552	3.769860
108	8	0	-7.012801	5.999785	3.431373
109	6	0	0.436875	7.174958	-1.433577
110	6	0	-0.584464	8.322877	-1.533869
111	1	0	-1.024429	8.528174	-0.554463
112	1	0	-0.093236	9.231804	-1.898057
113	1	0	-1.393464	8.067647	-2.226766
114	6	0	1.521471	7.588885	-0.425664
115	1	0	2.311259	6.838484	-0.327528
116	1	0	1.985708	8.527569	-0.747521
117	1	0	1.076137	7.738618	0.561665
118	6	0	1.042359	6.942319	-2.822500
119	1	0	1.749016	6.106608	-2.842176
120	1	0	0.261595	6.739664	-3.564062
121	1	0	1.578450	7.841326	-3.143189

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.199383	5.421164	0.076711
2	6	0	-5.519352	4.879095	0.010345
3	6	0	-3.267056	3.153559	-0.068294
4	6	0	-4.599504	2.613929	-0.132652

5	6	0	-2.337724	0.883642	-0.207784
6	6	0	-4.009313	6.833220	0.183913
7	6	0	-1.764379	5.097693	0.097571
8	6	0	-1.578598	6.521626	0.204079
9	6	0	0.671705	4.776838	0.110166
10	6	0	-3.078304	4.558892	0.034769
11	6	0	-0.836823	2.832386	-0.045373
12	6	0	-2.153359	2.293670	-0.111719
13	6	0	0.086969	0.560571	-0.169891
14	6	0	-0.647757	4.241518	0.050649
15	6	0	1.594042	2.511149	-0.034811
16	6	0	0.277639	1.970626	-0.092017
17	6	0	2.519615	0.245978	-0.174941
18	6	0	-3.674850	0.350823	-0.272781
19	6	0	-1.420861	-1.402729	-0.307364
20	6	0	-2.771005	-1.922349	-0.432044
21	6	0	-0.475651	-3.685764	-0.206426
22	6	0	-1.234984	0.020962	-0.239011
23	6	0	1.015377	-1.710116	-0.260181
24	6	0	-0.314358	-2.247999	-0.263281
25	6	0	1.950449	-3.989316	-0.391691
26	6	0	1.202623	-0.295466	-0.212671
27	6	0	3.448060	-2.021235	-0.316658
28	6	0	2.128411	-2.559543	-0.319785
29	6	0	4.379177	-4.300466	-0.488446
30	6	0	0.853990	6.206654	0.214820
31	6	0	3.110425	4.458072	0.108784
32	6	0	3.286752	5.894469	0.214850
33	6	0	5.558144	4.148766	0.095054

34	6	0	1.780676	3.924360	0.056870
35	6	0	4.030841	2.193798	-0.048788
36	6	0	2.709014	1.654666	-0.094868
37	6	0	4.954523	-0.069491	-0.208078
38	6	0	4.210187	3.612694	0.050039
39	6	0	6.478433	1.881519	-0.076061
40	6	0	5.138629	1.340782	-0.113553
41	6	0	7.400831	-0.384777	-0.251580
42	6	0	3.636908	-0.611424	-0.237685
43	6	0	5.878535	-2.333903	-0.378273
44	6	0	4.564061	-2.876073	-0.395662
45	6	0	6.808659	-4.607359	-0.556712
46	6	0	6.067616	-0.928264	-0.280173
47	6	0	8.319912	-2.649383	-0.431495
48	6	0	6.999113	-3.194925	-0.455919
49	6	0	-2.970619	-3.422785	-0.646214
50	1	0	-3.068608	-3.659879	-1.709247
51	6	0	-3.829750	-1.078768	-0.395540
52	1	0	-4.843693	-1.462004	-0.463448
53	6	0	-4.754799	1.196694	-0.235380
54	1	0	-5.761108	0.786962	-0.285847
55	6	0	-5.683903	3.475713	-0.093740
56	1	0	-6.691382	3.068841	-0.143064
57	6	0	-6.617318	5.759731	0.051362
58	1	0	-7.622190	5.350146	-0.000428
59	6	0	-6.424084	7.132123	0.156115
60	1	0	-7.284206	7.793598	0.185676
61	6	0	-5.143434	7.667924	0.222163
62	1	0	-5.002438	8.742153	0.303777

63	6	0	-2.691596	7.348516	0.246212
64	1	0	-2.553401	8.424363	0.327629
65	6	0	-0.246371	7.031640	0.261409
66	1	0	-0.106494	8.107320	0.342252
67	6	0	2.197505	6.714955	0.266567
68	1	0	2.336873	7.790859	0.347489
69	6	0	4.644261	6.408202	0.262102
70	1	0	4.775798	7.483826	0.344408
71	6	0	-1.854195	-4.235410	0.017218
72	1	0	-1.890824	-5.267200	-0.364822
73	6	0	0.601025	-4.500705	-0.320732
74	1	0	0.467244	-5.580776	-0.319648
75	6	0	3.043993	-4.813611	-0.480881
76	1	0	2.903078	-5.890930	-0.535702
77	6	0	5.489591	-5.125319	-0.570081
78	1	0	5.350854	-6.201762	-0.642493
79	6	0	7.941597	-5.440267	-0.634220
80	1	0	7.800023	-6.514697	-0.711586
81	6	0	9.222573	-4.901241	-0.611058
82	1	0	10.082449	-5.561321	-0.670269
83	6	0	9.417087	-3.529028	-0.510684
84	1	0	10.422695	-3.118298	-0.492075
85	6	0	8.484756	-1.246636	-0.327381
86	1	0	9.492967	-0.839010	-0.307348
87	6	0	7.557323	1.030354	-0.145480
88	1	0	8.565194	1.438681	-0.120471
89	6	0	6.630281	3.306741	0.032055
90	1	0	7.638512	3.714233	0.062897
91	6	0	5.710905	5.588411	0.205322

92	1	0	6.720626	5.988694	0.240103
93	6	0	-2.450277	-4.308863	1.440052
94	7	0	-3.728085	-4.209395	1.401875
95	7	0	-4.118047	-3.921788	0.108898
96	6	0	-1.725866	-4.592780	2.734372
97	6	0	-5.442769	-3.940765	-0.246269
98	6	0	-5.848034	-3.556135	-1.541534
99	6	0	-6.417617	-4.369282	0.679367
100	6	0	-7.183368	-3.603695	-1.899782
101	1	0	-5.117668	-3.203037	-2.261688
102	6	0	-7.748971	-4.411098	0.315698
103	1	0	-6.103157	-4.660210	1.673055
104	6	0	-8.124588	-4.030710	-0.970355
105	1	0	-7.509347	-3.308480	-2.889868
106	1	0	-8.510026	-4.736577	1.014923
107	7	0	-9.529661	-4.075469	-1.347243
108	8	0	-10.330006	-4.462596	-0.511388
109	8	0	-9.827741	-3.723049	-2.477338
110	6	0	-2.738073	-4.707793	3.878904
111	1	0	-3.454097	-5.513662	3.695558
112	1	0	-2.205568	-4.917303	4.812240
113	1	0	-3.301984	-3.778751	3.999211
114	6	0	-0.952643	-5.915242	2.608409
115	1	0	-0.449478	-6.136006	3.555809
116	1	0	-1.630277	-6.744997	2.380427
117	1	0	-0.186402	-5.861723	1.830345
118	6	0	-0.747932	-3.444531	3.045764
119	1	0	0.062301	-3.379594	2.314285
120	1	0	-1.272041	-2.483180	3.068301

121	1	0	-0.298141	-3.611816	4.030476

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.334294	0.241928	-0.527777
2	6	0	7.782657	1.590136	-0.675352
3	6	0	5.002932	1.010025	-0.634138
4	6	0	5.461981	2.366254	-0.778435
5	6	0	2.671329	1.781819	-0.730233
6	6	0	8.283731	-0.818169	-0.396972
7	6	0	5.501982	-1.385769	-0.358460
8	6	0	6.463337	-2.449260	-0.224026
9	6	0	3.671432	-3.015455	-0.183931
10	6	0	5.948239	-0.044646	-0.508002
11	6	0	3.175827	-0.617206	-0.471213
12	6	0	3.623384	0.727797	-0.611622
13	6	0	0.847685	0.153014	-0.593448
14	6	0	4.123720	-1.672725	-0.336310
15	6	0	1.348564	-2.244646	-0.304349
16	6	0	1.794931	-0.901249	-0.451316
17	6	0	-0.976594	-1.473605	-0.429037
18	6	0	3.139724	3.140142	-0.863732
19	6	0	0.336452	2.557642	-0.842530
20	6	0	0.821174	3.918840	-0.877902

21	6	0	-2.010947	3.327911	-1.140779
22	6	0	1.297888	1.501255	-0.718836
23	6	0	-1.482919	0.926174	-0.748194
24	6	0	-1.027183	2.280589	-0.906801
25	6	0	-3.820910	1.681840	-0.898263
26	6	0	-0.531010	-0.128415	-0.581192
27	6	0	-3.303948	-0.711310	-0.562067
28	6	0	-2.851747	0.629021	-0.734565
29	6	0	-5.644942	0.060601	-0.689761
30	6	0	4.639545	-4.079183	-0.043928
31	6	0	1.840665	-4.647218	0.000115
32	6	0	2.817767	-5.710359	0.143857
33	6	0	0.010563	-6.289578	0.193266
34	6	0	2.300883	-3.299242	-0.159722
35	6	0	-0.480595	-3.873519	-0.120300
36	6	0	-0.029871	-2.527314	-0.277871
37	6	0	-2.803088	-3.105696	-0.242736
38	6	0	0.481048	-4.927145	0.025093
39	6	0	-2.313208	-5.514981	0.073474
40	6	0	-1.851290	-4.156096	-0.095010
41	6	0	-4.638138	-4.743220	-0.047841
42	6	0	-2.356199	-1.762687	-0.406601
43	6	0	-5.127908	-2.337286	-0.366088
44	6	0	-4.682329	-0.998244	-0.537264
45	6	0	-7.464007	-1.567547	-0.491654
46	6	0	-4.182129	-3.388267	-0.218693
47	6	0	-6.960290	-3.970098	-0.171599
48	6	0	-6.513703	-2.623780	-0.342918
49	6	0	-0.179352	5.022362	-0.789915

50	1	0	0.244015	5.938787	-1.219566
51	6	0	2.147607	4.186887	-0.920423
52	1	0	2.490837	5.219752	-0.945857
53	6	0	4.486035	3.405087	-0.888532
54	1	0	4.831485	4.432005	-0.985798
55	6	0	6.823082	2.625295	-0.797679
56	1	0	7.170699	3.650201	-0.906185
57	6	0	9.167197	1.847009	-0.690670
58	1	0	9.511297	2.871413	-0.801920
59	6	0	10.083751	0.809972	-0.563820
60	1	0	11.146829	1.029540	-0.577095
61	6	0	9.656858	-0.504293	-0.418469
62	1	0	10.381374	-1.307552	-0.317882
63	6	0	7.816737	-2.146452	-0.247152
64	1	0	8.544512	-2.948267	-0.145161
65	6	0	5.983366	-3.784454	-0.068201
66	1	0	6.710334	-4.586647	0.036722
67	6	0	4.151117	-5.420983	0.118540
68	1	0	4.878880	-6.222279	0.226374
69	6	0	2.324054	-7.065386	0.312467
70	1	0	3.056573	-7.860568	0.421727
71	6	0	-1.522031	4.741059	-1.454626
72	1	0	-1.474257	4.895873	-2.537153
73	6	0	-3.330132	3.021975	-1.110928
74	1	0	-4.072959	3.797453	-1.264332
75	6	0	-5.162504	1.393991	-0.870519
76	1	0	-5.888385	2.195004	-0.994325
77	6	0	-6.997329	-0.240946	-0.663064
78	1	0	-7.725521	0.558849	-0.777665

79	6	0	-8.836799	-1.881050	-0.465490
80	1	0	-9.561939	-1.080033	-0.578606
81	6	0	-9.262653	-3.193308	-0.298134
82	1	0	-10.325511	-3.413633	-0.280609
83	6	0	-8.345138	-4.226896	-0.152992
84	1	0	-8.688764	-5.249278	-0.022871
85	6	0	-6.000715	-5.001585	-0.027562
86	1	0	-6.348184	-6.024052	0.102158
87	6	0	-3.663872	-5.776722	0.094843
88	1	0	-4.010328	-6.799650	0.223863
89	6	0	-1.328398	-6.552038	0.215147
90	1	0	-1.675787	-7.574926	0.343451
91	6	0	1.005595	-7.337376	0.335857
92	1	0	0.651147	-8.356650	0.463895
93	6	0	-2.344246	5.800331	-0.714837
94	7	0	-1.861762	6.045921	0.446423
95	7	0	-0.621487	5.406710	0.595610
96	6	0	-3.553971	6.578163	-1.215444
97	6	0	-0.535225	4.525375	1.690482
98	6	0	0.726695	4.125811	2.160428
99	6	0	-1.690275	4.070628	2.343311
100	6	0	0.831458	3.254440	3.230681
101	1	0	1.620729	4.515019	1.689176
102	6	0	-1.589524	3.219875	3.433443
103	1	0	-2.662167	4.380084	1.976717
104	6	0	-0.330389	2.814261	3.855224
105	1	0	1.794682	2.928359	3.603452
106	1	0	-2.469065	2.852390	3.947992
107	7	0	-0.221781	1.907007	4.998082

108	8	0	-1.254112	1.554660	5.542274
109	8	0	0.894894	1.557386	5.339711
110	6	0	-3.183948	8.072917	-1.176792
111	1	0	-2.942027	8.377872	-0.155817
112	1	0	-2.314270	8.278221	-1.810526
113	1	0	-4.023273	8.675299	-1.541402
114	6	0	-3.909596	6.206641	-2.659364
115	1	0	-4.130111	5.142439	-2.786470
116	1	0	-4.794299	6.770499	-2.971984
117	1	0	-3.094011	6.464316	-3.343921
118	6	0	-4.750544	6.352599	-0.277554
119	1	0	-5.589168	6.985956	-0.586376
120	1	0	-5.092939	5.312951	-0.284922
121	1	0	-4.475627	6.611856	0.748697

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.567304	-0.565741	0.079241
2	6	0	10.377592	0.607899	-0.000442
3	6	0	7.551339	0.822410	-0.082222
4	6	0	8.370092	2.002061	-0.161529
5	6	0	5.534620	2.212868	-0.244347
6	6	0	10.178694	-1.851426	0.201435
7	6	0	7.348915	-1.624528	0.120211
8	6	0	7.971438	-2.917998	0.245037

9	6	0	5.133326	-2.687640	0.162749
10	6	0	8.158252	-0.455010	0.039826
11	6	0	5.337143	-0.235920	-0.042966
12	6	0	6.145769	0.935538	-0.119597
13	6	0	3.325685	1.153001	-0.204865
14	6	0	5.949082	-1.517507	0.084400
15	6	0	3.122212	-1.297790	-0.002533
16	6	0	3.933766	-0.125366	-0.074332
17	6	0	1.111275	0.092598	-0.164692
18	6	0	6.359256	3.395080	-0.323415
19	6	0	3.513473	3.605570	-0.407567
20	6	0	4.347830	4.788739	-0.487963
21	6	0	1.488191	5.007977	-0.573543
22	6	0	4.134792	2.323975	-0.280136
23	6	0	1.309675	2.542046	-0.365287
24	6	0	2.126006	3.712764	-0.444931
25	6	0	-0.719280	3.939337	-0.528867
26	6	0	1.919040	1.263979	-0.235553
27	6	0	-0.897295	1.482919	-0.320734
28	6	0	-0.094134	2.649408	-0.399618
29	6	0	-2.920790	2.872710	-0.475486
30	6	0	5.762087	-3.983274	0.289517
31	6	0	2.916988	-3.753535	0.203393
32	6	0	3.554369	-5.050985	0.330592
33	6	0	0.698593	-4.830420	0.237076
34	6	0	3.740432	-2.580772	0.127673
35	6	0	0.906697	-2.361952	0.034987
36	6	0	1.724517	-1.188086	-0.034128
37	6	0	-1.107640	-0.971826	-0.135844

38	6	0	1.534127	-3.646393	0.162836
39	6	0	-1.311891	-3.437137	0.059769
40	6	0	-0.483649	-2.253314	-0.008213
41	6	0	-3.328374	-2.049666	-0.134140
42	6	0	-0.290429	0.203764	-0.198701
43	6	0	-3.117521	0.421887	-0.300856
44	6	0	-2.309456	1.592309	-0.355388
45	6	0	-5.117794	1.814990	-0.375870
46	6	0	-2.498403	-0.862626	-0.189451
47	6	0	-5.349857	-0.665938	-0.398514
48	6	0	-4.517772	0.539200	-0.345239
49	6	0	3.686648	6.075254	-0.613940
50	1	0	4.311948	6.961943	-0.674571
51	6	0	5.707791	4.669599	-0.445754
52	1	0	6.328931	5.560649	-0.505581
53	6	0	7.731292	3.270386	-0.281670
54	1	0	8.352568	4.161212	-0.340684
55	6	0	9.753788	1.869608	-0.119241
56	1	0	10.376072	2.759802	-0.177699
57	6	0	11.782120	0.467226	0.043142
58	1	0	12.400694	1.358471	-0.015392
59	6	0	12.366439	-0.784676	0.160363
60	1	0	13.447878	-0.872277	0.192517
61	6	0	11.581205	-1.933142	0.239363
62	1	0	12.049126	-2.909172	0.333197
63	6	0	9.353798	-3.002893	0.281585
64	1	0	9.826040	-3.978136	0.376200
65	6	0	7.134286	-4.072418	0.326491
66	1	0	7.605832	-5.047907	0.421658

67	6	0	4.915404	-5.142041	0.370472
68	1	0	5.387779	-6.117240	0.466167
69	6	0	2.698954	-6.221697	0.409237
70	1	0	3.177148	-7.192735	0.505439
71	6	0	2.344149	6.178037	-0.655611
72	1	0	1.866384	7.149298	-0.752178
73	6	0	0.125082	5.097623	-0.612161
74	1	0	-0.347217	6.072767	-0.709547
75	6	0	-2.099486	4.024279	-0.564254
76	1	0	-2.572670	4.999238	-0.658061
77	6	0	-4.331770	2.946979	-0.481172
78	1	0	-4.800913	3.925153	-0.562597
79	6	0	-6.618195	1.911365	-0.253504
80	1	0	-6.955009	2.857979	-0.701293
81	6	0	-7.376807	0.742313	-0.899011
82	1	0	-7.591928	0.926854	-1.958117
83	6	0	-6.678766	-0.571383	-0.678724
84	1	0	-7.278887	-1.474468	-0.759101
85	6	0	-4.696013	-1.934324	-0.234874
86	1	0	-5.311027	-2.830907	-0.227584
87	6	0	-2.679569	-3.317804	-0.000872
88	1	0	-3.298349	-4.211092	0.045095
89	6	0	-0.659751	-4.711800	0.186205
90	1	0	-1.281129	-5.603107	0.239831
91	6	0	1.357240	-6.117955	0.363756
92	1	0	0.730353	-7.003741	0.420934
93	6	0	-7.246079	1.859798	1.157716
94	6	0	-6.728836	2.510249	2.421694
95	7	0	-8.381779	1.269961	1.140626

96	7	0	-8.633483	0.787077	-0.127306
97	6	0	-9.685156	-0.086813	-0.315388
98	6	0	-10.658473	-0.268884	0.687153
99	6	0	-9.817783	-0.777128	-1.536002
100	6	0	-11.726435	-1.118731	0.471053
101	1	0	-10.550420	0.260668	1.624750
102	6	0	-10.888396	-1.627990	-1.747598
103	1	0	-9.079941	-0.649562	-2.320094
104	6	0	-11.833303	-1.793435	-0.742309
105	1	0	-12.482007	-1.273530	1.231858
106	1	0	-11.001202	-2.167613	-2.680110
107	7	0	-12.955855	-2.695840	-0.962273
108	8	0	-13.017289	-3.275997	-2.034260
109	8	0	-13.769524	-2.822023	-0.062067
110	6	0	-7.761448	2.346781	3.542627
111	1	0	-7.385429	2.824377	4.453248
112	1	0	-8.715230	2.808006	3.271842
113	1	0	-7.948433	1.290442	3.753884
114	6	0	-5.410523	1.846924	2.861406
115	1	0	-5.541488	0.766267	2.980712
116	1	0	-4.600509	2.019854	2.148501
117	1	0	-5.103325	2.262771	3.827378
118	6	0	-6.498053	4.008269	2.167552
119	1	0	-7.423275	4.498452	1.845714
120	1	0	-6.160417	4.489444	3.091753
121	1	0	-5.729543	4.175053	1.408190

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.373113	-0.048121	0.799771
2	6	0	10.054508	1.179564	1.060769
3	6	0	7.252413	1.172479	0.628627
4	6	0	7.941470	2.407182	0.891764
5	6	0	5.130869	2.395665	0.455986
6	6	0	10.101498	-1.276207	0.755354
7	6	0	7.295034	-1.271762	0.323955
8	6	0	8.035158	-2.507247	0.280631
9	6	0	5.220042	-2.499557	-0.152583
10	6	0	7.975489	-0.048201	0.585509
11	6	0	5.178190	-0.050293	0.153153
12	6	0	5.857690	1.174604	0.417024
13	6	0	3.061674	1.171286	-0.017289
14	6	0	5.906221	-1.275375	0.113098
15	6	0	3.103310	-1.276831	-0.321104
16	6	0	3.785058	-0.051868	-0.052303
17	6	0	0.986217	-0.054800	-0.485088
18	6	0	5.825552	3.633558	0.719829
19	6	0	3.004758	3.620789	0.279601
20	6	0	3.709164	4.860716	0.542965
21	6	0	0.874518	4.855915	0.097162
22	6	0	3.741841	2.395874	0.245876
23	6	0	0.940855	2.392356	-0.191166
24	6	0	1.628870	3.618408	0.067557
25	6	0	-1.191248	3.622334	-0.378013

26	6	0	1.665203	1.169378	-0.222090
27	6	0	-1.127694	1.166697	-0.653972
28	6	0	-0.451232	2.388197	-0.403790
29	6	0	-3.248735	2.388316	-0.852962
30	6	0	5.966781	-3.736857	-0.195426
31	6	0	3.143854	-3.729347	-0.630579
32	6	0	3.899886	-4.967382	-0.674208
33	6	0	1.067304	-4.969601	-1.112151
34	6	0	3.837616	-2.502919	-0.360551
35	6	0	1.026613	-2.504713	-0.794495
36	6	0	1.714952	-1.279036	-0.522354
37	6	0	-1.096969	-1.282896	-0.948211
38	6	0	1.771539	-3.730661	-0.838951
39	6	0	-1.050600	-3.742685	-1.272126
40	6	0	-0.354618	-2.505300	-0.998068
41	6	0	-3.176069	-2.522530	-1.417601
42	6	0	-0.406350	-0.056028	-0.685249
43	6	0	-3.219807	-0.057652	-1.098955
44	6	0	-2.528484	1.163181	-0.866328
45	6	0	-5.319915	1.177678	-1.329989
46	6	0	-2.481167	-1.282273	-1.143265
47	6	0	-5.321684	-1.315710	-1.486738
48	6	0	-4.616845	-0.048259	-1.295300
49	6	0	2.931994	6.087064	0.571265
50	1	0	3.459838	7.016405	0.767689
51	6	0	5.058899	4.848154	0.751909
52	1	0	5.582381	5.781291	0.948168
53	6	0	7.188027	3.616381	0.928199
54	1	0	7.711824	4.548909	1.125682

55	6	0	9.316340	2.383225	1.100240
56	1	0	9.841176	3.315017	1.298787
57	6	0	11.450643	1.149319	1.271545
58	1	0	11.971501	2.081923	1.469924
59	6	0	12.149459	-0.047455	1.226910
60	1	0	13.222237	-0.050091	1.391842
61	6	0	11.489950	-1.248042	0.972577
62	1	0	12.046965	-2.180328	0.940062
63	6	0	9.404189	-2.483398	0.494289
64	1	0	9.965761	-3.414413	0.462481
65	6	0	7.326109	-3.718333	0.016467
66	1	0	7.886999	-4.649646	-0.016166
67	6	0	5.248242	-4.952428	-0.463425
68	1	0	5.809670	-5.883547	-0.496908
69	6	0	3.174160	-6.195250	-0.946679
70	1	0	3.741344	-7.121595	-0.979024
71	6	0	1.601487	6.084771	0.360921
72	1	0	1.035563	7.012209	0.384385
73	6	0	-0.474578	4.839039	-0.119498
74	1	0	-1.035071	5.771167	-0.097173
75	6	0	-2.555334	3.598575	-0.602913
76	1	0	-3.116891	4.530442	-0.589271
77	6	0	-4.636203	2.357215	-1.104544
78	1	0	-5.166606	3.301315	-1.115676
79	6	0	-6.806386	1.187331	-1.691112
80	1	0	-6.909277	1.389258	-2.762670
81	6	0	-7.508624	-0.125496	-1.310484
82	1	0	-8.456785	-0.197577	-1.869427
83	6	0	-6.682985	-1.347400	-1.525668

84	1	0	-7.178562	-2.294737	-1.709202
85	6	0	-4.540980	-2.513362	-1.593500
86	1	0	-5.062705	-3.450358	-1.773516
87	6	0	-2.409849	-3.728778	-1.474758
88	1	0	-2.931184	-4.661547	-1.677799
89	6	0	-0.281598	-4.956169	-1.317937
90	1	0	-0.804996	-5.888050	-1.520828
91	6	0	1.843628	-6.195780	-1.153439
92	1	0	1.314592	-7.123131	-1.356105
93	6	0	-7.617604	2.152508	-0.824910
94	6	0	-7.933598	3.624726	-1.066987
95	7	0	-8.131128	1.551896	0.181407
96	7	0	-7.857521	0.195231	0.105322
97	6	0	-8.625446	-0.620921	0.927715
98	6	0	-9.002034	-0.148435	2.200340
99	6	0	-9.019626	-1.909484	0.535062
100	6	0	-9.734018	-0.947262	3.056326
101	1	0	-8.707408	0.851296	2.493277
102	6	0	-9.749782	-2.714617	1.396477
103	1	0	-8.778486	-2.283186	-0.450292
104	6	0	-10.096858	-2.228657	2.648014
105	1	0	-10.027400	-0.599250	4.039269
106	1	0	-10.065309	-3.708924	1.104783
107	7	0	-10.866450	-3.075821	3.552777
108	8	0	-11.171310	-4.191888	3.165449
109	8	0	-11.162035	-2.619324	4.644508
110	6	0	-9.465988	3.780188	-1.033716
111	1	0	-9.861719	3.472397	-0.062928
112	1	0	-9.739669	4.825414	-1.215034

113	1	0	-9.937469	3.162309	-1.805244
114	6	0	-7.345756	4.501561	0.051156
115	1	0	-6.252771	4.478516	0.075998
116	1	0	-7.658938	5.541625	-0.092078
117	1	0	-7.710103	4.158743	1.023554
118	6	0	-7.440802	4.082530	-2.445191
119	1	0	-7.677167	5.142637	-2.582223
120	1	0	-6.361910	3.961506	-2.580119
121	1	0	-7.942488	3.526232	-3.244659

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.230946	-1.253239	0.233910
2	6	0	-9.666802	-2.605764	0.375456
3	6	0	-6.897781	-2.011051	0.250944
4	6	0	-7.340143	-3.371633	0.395988
5	6	0	-4.563404	-2.771476	0.263775
6	6	0	-10.189116	-0.196385	0.152917
7	6	0	-7.412373	0.387781	0.028957
8	6	0	-8.383405	1.449398	-0.050436
9	6	0	-5.597617	2.031550	-0.182194
10	6	0	-7.848845	-0.960099	0.172706
11	6	0	-5.083064	-0.372333	0.039922
12	6	0	-5.518407	-1.721187	0.188856
13	6	0	-2.754444	-1.133316	0.046776

14	6	0	-6.040154	0.681951	-0.033438
15	6	0	-3.268514	1.269376	-0.176493
16	6	0	-3.706729	-0.080096	-0.021014
17	6	0	-0.939977	0.506442	-0.173951
18	6	0	-5.010764	-4.135864	0.412685
19	6	0	-2.224179	-3.533239	0.272547
20	6	0	-2.680558	-4.901170	0.424611
21	6	0	0.121453	-4.303989	0.276954
22	6	0	-3.190310	-2.481419	0.199559
23	6	0	-0.421763	-1.893313	0.049222
24	6	0	-0.864416	-3.243636	0.202875
25	6	0	1.924673	-2.659569	0.042942
26	6	0	-1.374994	-0.840704	-0.017672
27	6	0	1.385352	-0.257622	-0.180789
28	6	0	0.953525	-1.599612	-0.026499
29	6	0	3.721222	-1.020578	-0.208230
30	6	0	-6.575290	3.093887	-0.259552
31	6	0	-3.782302	3.677214	-0.399683
32	6	0	-4.768937	4.738902	-0.476242
33	6	0	-1.968331	5.333123	-0.624124
34	6	0	-4.231936	2.323632	-0.246569
35	6	0	-1.453136	2.912350	-0.397328
36	6	0	-1.897586	1.560467	-0.239339
37	6	0	0.880062	2.149219	-0.397102
38	6	0	-2.426116	3.965030	-0.469157
39	6	0	0.361736	4.565283	-0.624075
40	6	0	-0.088785	3.200258	-0.467541
41	6	0	2.696559	3.803268	-0.622206
42	6	0	0.435122	0.796335	-0.242786

43	6	0	3.210550	1.379601	-0.409787
44	6	0	2.769362	0.035095	-0.267128
45	6	0	5.520666	0.596138	-0.501863
46	6	0	2.246235	2.434968	-0.468662
47	6	0	5.042085	3.048918	-0.567469
48	6	0	4.589997	1.657138	-0.498448
49	6	0	-1.674674	-5.945730	0.501561
50	1	0	-2.017676	-6.970394	0.616601
51	6	0	-4.017707	-5.171202	0.489878
52	1	0	-4.355605	-6.199079	0.601993
53	6	0	-6.361220	-4.404412	0.474228
54	1	0	-6.699459	-5.432260	0.584073
55	6	0	-8.704194	-3.636367	0.454215
56	1	0	-9.043655	-4.664052	0.562254
57	6	0	-11.053273	-2.868963	0.431873
58	1	0	-11.388562	-3.896826	0.538786
59	6	0	-11.975901	-1.837010	0.352178
60	1	0	-13.037229	-2.060111	0.397080
61	6	0	-11.556739	-0.515610	0.214463
62	1	0	-12.287752	0.285779	0.151653
63	6	0	-9.732591	1.139024	0.012332
64	1	0	-10.467484	1.938657	-0.049550
65	6	0	-7.915846	2.791030	-0.193955
66	1	0	-8.649999	3.591330	-0.255127
67	6	0	-6.099280	4.441964	-0.407162
68	1	0	-6.833902	5.242078	-0.467615
69	6	0	-4.287960	6.100552	-0.628424
70	1	0	-5.027233	6.894960	-0.687244
71	6	0	-0.359115	-5.665155	0.432246

72	1	0	0.380403	-6.459212	0.492090
73	6	0	1.452488	-4.005876	0.199407
74	1	0	2.187885	-4.805509	0.256295
75	6	0	3.269833	-2.353597	-0.046193
76	1	0	4.006171	-3.152639	0.003544
77	6	0	5.090735	-0.706342	-0.336661
78	1	0	5.809839	-1.519316	-0.298166
79	6	0	6.995639	0.892913	-0.763678
80	6	0	7.413978	2.291178	-0.288141
81	1	0	8.324207	2.591598	-0.830981
82	6	0	6.369911	3.341434	-0.471974
83	1	0	6.689315	4.379377	-0.511588
84	6	0	4.045619	4.075266	-0.670878
85	1	0	4.380248	5.106643	-0.757289
86	6	0	1.707911	4.834248	-0.696959
87	1	0	2.043718	5.862526	-0.811600
88	6	0	-0.632210	5.601423	-0.696434
89	1	0	-0.294067	6.629017	-0.811897
90	6	0	-2.972445	6.379450	-0.698263
91	1	0	-2.627790	7.403730	-0.812600
92	7	0	8.221559	0.697516	1.222198
93	7	0	7.879186	0.054536	0.048692
94	6	0	7.909352	1.934818	1.131178
95	6	0	8.149114	2.905492	2.259860
96	6	0	8.418170	-1.167319	-0.258670
97	6	0	9.323828	-1.784787	0.631702
98	6	0	8.085889	-1.824805	-1.462613
99	6	0	9.872998	-3.013011	0.324353
100	1	0	9.576215	-1.278452	1.554007

101	6	0	8.644755	-3.053579	-1.765732
102	1	0	7.377776	-1.379861	-2.153505
103	6	0	9.533629	-3.640075	-0.872500
104	1	0	10.568336	-3.498841	0.998466
105	1	0	8.398535	-3.569783	-2.685899
106	7	0	10.115348	-4.934477	-1.193224
107	8	0	9.787986	-5.461871	-2.244600
108	8	0	10.897771	-5.420389	-0.392400
109	6	0	8.968085	4.091984	1.727431
110	1	0	9.145744	4.810579	2.534299
111	1	0	9.939988	3.759170	1.347470
112	1	0	8.444453	4.618932	0.923106
113	6	0	8.921375	2.218139	3.389489
114	1	0	8.360000	1.368955	3.788011
115	1	0	9.886840	1.845550	3.035368
116	1	0	9.096293	2.934217	4.199024
117	6	0	6.797425	3.406435	2.799638
118	1	0	6.969885	4.084241	3.643053
119	1	0	6.229163	3.944938	2.036004
120	1	0	6.188047	2.567581	3.150777
121	1	0	7.218311	0.752273	-1.826265

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.052952	0.112825	0.263356

2	6	0	-9.784933	-1.113319	0.302008
3	6	0	-6.961118	-1.149700	0.041343
4	6	0	-7.701348	-2.382190	0.081683
5	6	0	-4.868304	-2.414307	-0.180188
6	6	0	-9.741454	1.361479	0.356442
7	6	0	-6.913555	1.312666	0.094478
8	6	0	-7.613707	2.568300	0.189979
9	6	0	-4.777396	2.516803	-0.075159
10	6	0	-7.644600	0.090888	0.133589
11	6	0	-4.826129	0.049509	-0.129261
12	6	0	-5.556194	-1.174003	-0.086338
13	6	0	-2.738690	-1.213850	-0.350885
14	6	0	-5.514668	1.294165	-0.032870
15	6	0	-2.690732	1.252355	-0.301158
16	6	0	-3.423129	0.028072	-0.252640
17	6	0	-0.603811	-0.012430	-0.523239
18	6	0	-5.614185	-3.649633	-0.138426
19	6	0	-2.771070	-3.681069	-0.401187
20	6	0	-3.526568	-4.918162	-0.359042
21	6	0	-0.669537	-4.957911	-0.622322
22	6	0	-3.469353	-2.436852	-0.305887
23	6	0	-0.646620	-2.477132	-0.570005
24	6	0	-1.384871	-3.700703	-0.527133
25	6	0	1.457775	-3.748905	-0.790065
26	6	0	-1.332534	-1.235442	-0.473628
27	6	0	1.481396	-1.276938	-0.739432
28	6	0	0.755951	-2.495623	-0.695935
29	6	0	3.579355	-2.542046	-0.954181
30	6	0	-5.483896	3.774316	0.022268

31	6	0	-2.641030	3.723882	-0.247610
32	6	0	-3.356325	4.982749	-0.148857
33	6	0	-0.503734	4.941795	-0.426479
34	6	0	-3.385578	2.498105	-0.202057
35	6	0	-0.555372	2.457572	-0.477148
36	6	0	-1.293495	1.231420	-0.425001
37	6	0	1.534086	1.192882	-0.707423
38	6	0	-1.259689	3.704017	-0.378965
39	6	0	1.581555	3.673315	-0.667200
40	6	0	0.833535	2.436549	-0.611889
41	6	0	3.671374	2.409936	-0.923618
42	6	0	0.797503	-0.034625	-0.649231
43	6	0	3.620172	-0.074633	-0.927559
44	6	0	2.892777	-1.296754	-0.866157
45	6	0	5.694680	-1.338978	-1.071637
46	6	0	2.923349	1.170724	-0.850128
47	6	0	5.763622	1.146565	-1.241088
48	6	0	5.021005	-0.102704	-1.058438
49	6	0	-2.788256	-6.164804	-0.455285
50	1	0	-3.354595	-7.091759	-0.424690
51	6	0	-4.886015	-4.884449	-0.233051
52	1	0	-5.447711	-5.815564	-0.202532
53	6	0	-6.986016	-3.611395	-0.011470
54	1	0	-7.547811	-4.542265	0.019198
55	6	0	-9.085289	-2.336883	0.209948
56	1	0	-9.648301	-3.267035	0.240606
57	6	0	-11.190265	-1.060776	0.432678
58	1	0	-11.749713	-1.991630	0.462568
59	6	0	-11.849407	0.155663	0.521737

60	1	0	-12.930081	0.174933	0.622151
61	6	0	-11.141246	1.354845	0.485391
62	1	0	-11.667578	2.302589	0.557431
63	6	0	-8.993398	2.566103	0.317254
64	1	0	-9.523994	3.512866	0.390040
65	6	0	-6.853579	3.776882	0.149790
66	1	0	-7.383501	4.723977	0.222947
67	6	0	-4.714804	4.987969	-0.019782
68	1	0	-5.245575	5.934703	0.054097
69	6	0	-2.579366	6.208725	-0.192899
70	1	0	-3.115672	7.150850	-0.116901
71	6	0	-1.447183	-6.183444	-0.579199
72	1	0	-0.910816	-7.125996	-0.649677
73	6	0	0.691046	-4.961995	-0.747644
74	1	0	1.222112	-5.908879	-0.818003
75	6	0	2.834897	-3.747382	-0.915469
76	1	0	3.366835	-4.693826	-0.983731
77	6	0	4.987059	-2.525621	-1.051949
78	1	0	5.525372	-3.471586	-1.081852
79	6	0	7.195526	-1.339976	-1.044954
80	1	0	7.573755	-2.274993	-1.474960
81	6	0	7.854684	-0.155957	-1.762763
82	1	0	8.055362	-0.383889	-2.817277
83	6	0	7.075435	1.119363	-1.613712
84	1	0	7.583508	2.056644	-1.828510
85	6	0	5.034311	2.376735	-1.115212
86	1	0	5.583486	3.311249	-1.203325
87	6	0	2.947152	3.639028	-0.818005
88	1	0	3.504836	4.571787	-0.863533

89	6	0	0.853211	4.908291	-0.565095
90	1	0	1.414654	5.839430	-0.600396
91	6	0	-1.239494	6.189276	-0.323862
92	1	0	-0.671740	7.115352	-0.354876
93	7	0	9.027157	-0.577737	0.214261
94	7	0	7.805715	-1.242779	0.329610
95	6	0	9.137235	-0.041684	-0.939538
96	6	0	10.385558	0.731026	-1.326547
97	6	0	7.078464	-0.922822	1.487636
98	6	0	6.059852	-1.779462	1.935646
99	6	0	7.387985	0.223862	2.235513
100	6	0	5.341026	-1.479432	3.079933
101	1	0	5.851163	-2.692625	1.392676
102	6	0	6.688838	0.515656	3.396032
103	1	0	8.175427	0.883661	1.891933
104	6	0	5.666822	-0.334101	3.798201
105	1	0	4.550835	-2.128318	3.437109
106	1	0	6.912016	1.398278	3.982849
107	7	0	4.921248	-0.023665	5.017006
108	8	0	5.235755	0.979564	5.634611
109	8	0	4.028276	-0.785932	5.345405
110	6	0	10.390059	1.038310	-2.827785
111	1	0	11.289969	1.605723	-3.085493
112	1	0	10.392307	0.118482	-3.422578
113	1	0	9.522173	1.636444	-3.127140
114	6	0	11.623850	-0.103820	-0.970486
115	1	0	11.631380	-0.342742	0.095589
116	1	0	11.634798	-1.044243	-1.530830
117	1	0	12.533392	0.454702	-1.217036

118	6	0	10.418105	2.043962	-0.524624
119	1	0	11.316316	2.617660	-0.778661
120	1	0	9.543857	2.667774	-0.738419
121	1	0	10.432324	1.830446	0.548315

c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.412451	-0.112462	-0.753188
2	6	0	-7.985915	-1.361685	-1.151027
3	6	0	-5.163319	-1.131287	-0.785061
4	6	0	-5.756697	-2.380524	-1.218533
5	6	0	-2.930868	-2.168068	-0.805885
6	6	0	-8.254280	1.020996	-0.538504
7	6	0	-5.447271	1.246873	-0.221845
8	6	0	-6.295492	2.391395	-0.025097
9	6	0	-3.474142	2.622122	0.244880
10	6	0	-6.014179	0.003602	-0.579600
11	6	0	-3.206380	0.217757	-0.183615
12	6	0	-3.790714	-1.033444	-0.575049
13	6	0	-1.033074	-0.952444	0.291566
14	6	0	-4.045142	1.367703	-0.064792
15	6	0	-1.251426	1.588235	0.219080
16	6	0	-1.835068	0.317222	0.082464
17	6	0	1.001055	0.657572	-0.155254
18	6	0	-3.531317	-3.403805	-1.277747

19	6	0	-0.734337	-3.204488	-0.853929
20	6	0	-1.331473	-4.452253	-1.286375
21	6	0	1.494701	-4.159492	-1.316891
22	6	0	-1.580932	-2.108469	-0.525463
23	6	0	1.261883	-1.788448	-0.646696
24	6	0	0.659332	-3.053419	-0.888607
25	6	0	3.427153	-2.675695	-1.404780
26	6	0	0.538407	-0.744025	0.173258
27	6	0	3.166850	-0.256788	-0.902922
28	6	0	2.582165	-1.569834	-0.996028
29	6	0	5.366855	-1.186529	-1.513392
30	6	0	-4.328167	3.777376	0.419484
31	6	0	-1.487929	4.046049	0.475364
32	6	0	-2.350816	5.194480	0.690726
33	6	0	0.482681	5.525061	0.486155
34	6	0	-2.077984	2.746047	0.319506
35	6	0	0.725225	3.074177	0.113568
36	6	0	0.174706	1.759344	0.099951
37	6	0	2.906042	2.161135	-0.479673
38	6	0	-0.116566	4.206845	0.375057
39	6	0	2.681376	4.586472	-0.042244
40	6	0	2.095796	3.264859	-0.127477
41	6	0	4.867856	3.658842	-0.632608
42	6	0	2.337098	0.851528	-0.524447
43	6	0	5.100129	1.240890	-1.068294
44	6	0	4.518076	-0.064315	-1.169762
45	6	0	7.311036	0.302839	-1.618783
46	6	0	4.286870	2.347240	-0.733300
47	6	0	7.057711	2.726376	-1.193404

48	6	0	6.482974	1.423248	-1.295334
49	6	0	-0.463494	-5.585200	-1.548226
50	1	0	-0.930742	-6.539904	-1.773857
51	6	0	-2.681364	-4.535754	-1.467329
52	1	0	-3.129165	-5.474725	-1.785065
53	6	0	-4.890835	-3.486897	-1.457810
54	1	0	-5.329434	-4.428866	-1.779505
55	6	0	-7.123051	-2.468650	-1.384295
56	1	0	-7.560319	-3.411038	-1.706660
57	6	0	-9.372865	-1.450773	-1.309891
58	1	0	-9.809030	-2.398415	-1.613742
59	6	0	-10.192379	-0.340960	-1.085474
60	1	0	-11.266328	-0.435774	-1.213383
61	6	0	-9.651213	0.873884	-0.708884
62	1	0	-10.292834	1.734394	-0.540721
63	6	0	-7.668847	2.251546	-0.174537
64	1	0	-8.312666	3.114134	-0.017279
65	6	0	-5.689930	3.640276	0.303903
66	1	0	-6.331428	4.508027	0.440702
67	6	0	-3.705960	5.044833	0.682017
68	1	0	-4.346588	5.910129	0.838179
69	6	0	-1.723747	6.489483	0.881787
70	1	0	-2.369579	7.338766	1.088128
71	6	0	0.873652	-5.448978	-1.554089
72	1	0	1.521885	-6.289887	-1.785112
73	6	0	2.830964	-3.969314	-1.519096
74	1	0	3.459162	-4.807067	-1.813420
75	6	0	4.768556	-2.475322	-1.626063
76	1	0	5.399513	-3.320474	-1.891395

77	6	0	6.716376	-0.985458	-1.718483
78	1	0	7.350130	-1.834335	-1.964308
79	6	0	8.678766	0.508846	-1.829502
80	1	0	9.308485	-0.342480	-2.072068
81	6	0	9.235286	1.787113	-1.730335
82	1	0	10.299274	1.921885	-1.897565
83	6	0	8.445674	2.878760	-1.419590
84	1	0	8.883077	3.870133	-1.340271
85	6	0	6.227807	3.818680	-0.864934
86	1	0	6.668868	4.809667	-0.783714
87	6	0	4.022913	4.754355	-0.286027
88	1	0	4.461602	5.746994	-0.214003
89	6	0	1.822782	5.686880	0.295634
90	1	0	2.264286	6.677530	0.378856
91	6	0	-0.390659	6.645466	0.783644
92	1	0	0.065539	7.623666	0.909194
93	6	0	-1.168586	-1.408833	1.814063
94	7	0	-0.039426	-1.419962	2.397364
95	7	0	0.978838	-0.925658	1.647289
96	6	0	2.235806	-1.537961	1.936322
97	6	0	3.375286	-0.739463	2.023965
98	6	0	2.337125	-2.926575	2.079538
99	6	0	4.630331	-1.325136	2.139840
100	1	0	3.271738	0.338773	1.962572
101	6	0	3.580693	-3.523439	2.213415
102	1	0	1.434301	-3.528483	2.041589
103	6	0	4.708332	-2.708378	2.209544
104	1	0	5.537066	-0.732689	2.161862
105	1	0	3.695730	-4.597785	2.287577

106	7	0	6.033296	-3.337571	2.267279
107	8	0	6.078609	-4.551459	2.364352
108	8	0	7.008186	-2.610463	2.203835
109	6	0	-2.384877	-1.813606	2.670369
110	6	0	-1.850709	-2.186496	4.069465
111	1	0	-1.154991	-3.028291	4.021668
112	1	0	-1.329752	-1.349234	4.538482
113	1	0	-2.700940	-2.470061	4.697408
114	6	0	-3.376671	-0.649849	2.870189
115	1	0	-2.852706	0.285297	3.097534
116	1	0	-4.017960	-0.488504	2.003361
117	1	0	-4.028528	-0.887555	3.717650
118	6	0	-3.137775	-3.051872	2.141213
119	1	0	-3.853129	-2.808889	1.355260
120	1	0	-2.447009	-3.813311	1.761399
121	1	0	-3.705381	-3.494066	2.966839

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.121548	-1.126424	-0.184920
2	6	0	0.413427	-2.358420	-0.248874
3	6	0	-1.031448	0.081228	-0.121023
4	6	0	-1.726699	-1.145836	-0.192913
5	6	0	-3.171425	1.292269	-0.042799
6	6	0	2.528063	-1.116975	-0.180410

7	6	0	1.088790	1.330974	-0.062610
8	6	0	2.515253	1.349316	-0.106738
9	6	0	1.055217	3.803951	0.085542
10	6	0	0.392520	0.106112	-0.128463
11	6	0	-1.052845	2.542276	0.028819
12	6	0	-1.759467	1.308363	-0.047196
13	6	0	-3.203491	3.749077	0.112317
14	6	0	0.356997	2.561665	0.016858
15	6	0	-1.099071	4.999527	0.187413
16	6	0	-1.787446	3.770132	0.109008
17	6	0	-3.880390	0.058940	-0.120369
18	6	0	-3.898860	2.521202	0.034532
19	6	0	-3.935166	4.986031	0.192805
20	6	0	-3.212065	6.206692	0.272767
21	1	0	-3.769208	7.138745	0.335050
22	6	0	-1.838015	6.233758	0.272367
23	6	0	0.318480	5.020955	0.177752
24	6	0	2.474286	3.841496	0.058439
25	6	0	3.221965	2.587824	-0.065397
26	6	0	3.238274	0.123385	-0.206037
27	6	0	3.243925	-2.362410	-0.148154
28	6	0	2.573235	-3.539217	-0.265617
29	1	0	3.121416	-4.478606	-0.292638
30	6	0	1.142276	-3.592395	-0.322327
31	6	0	-0.997028	-2.373829	-0.261660
32	6	0	-3.150342	-1.172277	-0.195482
33	6	0	4.734899	-2.344413	0.031084
34	6	0	4.647741	0.148315	-0.353614
35	6	0	0.461304	-4.790193	-0.411756

36	6	0	-1.693823	-3.607629	-0.345924
37	6	0	-5.315761	2.505389	0.034660
38	6	0	1.004363	6.264614	0.258209
39	6	0	-1.104287	7.475030	0.353895
40	6	0	-5.322735	4.958730	0.190924
41	6	0	-0.951839	-4.837174	-0.424983
42	6	0	5.421595	-1.140656	-0.613729
43	6	0	0.245546	7.487667	0.348311
44	6	0	-6.038894	3.747861	0.113085
45	1	0	1.017683	-5.723110	-0.464832
46	1	0	0.793276	8.424199	0.409574
47	1	0	-1.671039	8.399753	0.418981
48	1	0	-5.875681	5.893236	0.251260
49	6	0	2.396586	6.266163	0.246971
50	6	0	4.607827	2.558734	-0.152661
51	6	0	3.112311	5.081760	0.147494
52	6	0	5.306490	1.360060	-0.307737
53	1	0	6.387983	1.394675	-0.388842
54	6	0	-7.435838	3.723331	0.110818
55	6	0	-6.018494	1.281814	-0.042102
56	6	0	-5.289181	0.045018	-0.119710
57	6	0	-3.841081	-2.398007	-0.273868
58	6	0	-3.106442	-3.631729	-0.351921
59	6	0	-5.266878	-2.419505	-0.275200
60	6	0	-1.643388	-6.045156	-0.507107
61	6	0	-3.041750	-6.089457	-0.513059
62	6	0	-3.790803	-4.870411	-0.433978
63	6	0	-8.146582	2.522758	0.035773
64	6	0	-7.435363	1.279983	-0.041443

65	6	0	-5.994730	-1.192066	-0.196796
66	6	0	-3.735840	-7.325685	-0.595772
67	6	0	-5.217451	-4.917010	-0.437999
68	6	0	-5.964126	-3.657526	-0.353430
69	6	0	-7.417437	-1.205798	-0.194996
70	6	0	-8.163601	0.054392	-0.116203
71	6	0	-9.567611	2.511040	0.035422
72	6	0	-10.247411	1.324783	-0.036739
73	1	0	-11.332762	1.314800	-0.036567
74	6	0	-9.550074	0.103853	-0.111842
75	6	0	-8.061545	-2.437445	-0.268965
76	6	0	-7.355778	-3.627867	-0.346033
77	6	0	-5.842493	-6.152918	-0.521385
78	6	0	-5.105507	-7.349466	-0.599800
79	1	0	-5.636105	-8.294287	-0.663941
80	1	0	-7.923080	-4.549265	-0.400428
81	1	0	-10.097220	3.457740	0.094435
82	1	0	-7.983198	4.661228	0.169659
83	1	0	-1.083508	-6.975501	-0.566925
84	1	0	5.181368	3.477102	-0.123968
85	1	0	-10.132094	-0.808296	-0.166451
86	1	0	-9.143646	-2.490318	-0.268076
87	1	0	-3.159805	-8.244843	-0.654835
88	1	0	-6.923566	-6.222867	-0.528672
89	1	0	5.149820	-3.268614	-0.399431
90	1	0	5.586419	-1.291511	-1.684710
91	6	0	5.363131	-2.241025	1.438539
92	1	0	2.926811	7.212246	0.314722
93	1	0	4.194121	5.139819	0.143376

94	7	0	6.496027	-1.642503	1.387530
95	7	0	6.690922	-1.156209	0.110718
96	6	0	4.858441	-2.854488	2.723218
97	6	0	7.919397	-0.704176	-0.295024
98	6	0	8.094658	-0.152977	-1.581972
99	6	0	9.031348	-0.799804	0.568651
100	6	0	9.342214	0.281143	-1.992917
101	1	0	7.250254	-0.052807	-2.255269
102	6	0	10.272402	-0.359897	0.152998
103	1	0	8.892279	-1.222055	1.555367
104	6	0	10.422081	0.174835	-1.124593
105	1	0	9.491236	0.707041	-2.977833
106	1	0	11.136282	-0.424768	0.803684
107	7	0	11.732984	0.635139	-1.557726
108	8	0	12.661155	0.528929	-0.772476
109	8	0	11.829987	1.101032	-2.681832
110	6	0	5.884210	-2.633839	3.839810
111	1	0	5.507561	-3.074147	4.768694
112	1	0	6.842100	-3.100997	3.594142
113	1	0	6.063655	-1.568160	4.005208
114	6	0	3.527036	-2.193762	3.124397
115	1	0	3.646948	-1.110240	3.227651
116	1	0	2.735691	-2.386693	2.394954
117	1	0	3.200108	-2.595218	4.089893
118	6	0	4.648705	-4.364060	2.523189
119	1	0	5.578017	-4.851548	2.209178
120	1	0	4.328772	-4.816374	3.467983
121	1	0	3.874210	-4.568209	1.779489

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.147368	-0.761508	-0.860070
2	6	0	1.640987	-2.087781	-0.827012
3	6	0	-0.159680	0.089630	-0.602517
4	6	0	-0.647706	-1.233583	-0.545607
5	6	0	-2.438253	0.946985	-0.254730
6	6	0	3.537227	-0.526944	-0.911528
7	6	0	1.705924	1.663221	-0.883810
8	6	0	3.100915	1.907659	-1.038143
9	6	0	1.278513	4.101152	-0.891784
10	6	0	1.230652	0.338993	-0.782762
11	6	0	-0.572691	2.520408	-0.549722
12	6	0	-1.064084	1.187274	-0.466785
13	6	0	-2.855295	3.372079	-0.176651
14	6	0	0.795676	2.763440	-0.779389
15	6	0	-1.007202	4.942766	-0.515059
16	6	0	-1.480886	3.617765	-0.408871
17	6	0	-2.938670	-0.385780	-0.196162
18	6	0	-3.339370	2.046465	-0.100813
19	6	0	-3.762159	4.479424	-0.028549
20	6	0	-3.252653	5.802163	-0.132363
21	1	0	-3.942944	6.635582	-0.022820
22	6	0	-1.922116	6.046614	-0.375643
23	6	0	0.365698	5.188104	-0.769563

24	6	0	2.653882	4.361186	-1.128855
25	6	0	3.598191	3.241690	-1.160886
26	6	0	4.011635	0.818539	-0.975183
27	6	0	4.452826	-1.643153	-0.899678
28	6	0	3.954078	-2.906988	-0.971395
29	1	0	4.625752	-3.756519	-1.010602
30	6	0	2.550579	-3.189708	-0.936498
31	6	0	0.257806	-2.329738	-0.686563
32	6	0	-2.035850	-1.486677	-0.357672
33	6	0	5.957565	-1.411481	-0.760037
34	6	0	5.398057	1.085116	-0.896953
35	6	0	2.068282	-4.484485	-0.943256
36	6	0	-0.232306	-3.661453	-0.662648
37	6	0	-4.717386	1.805057	0.121630
38	6	0	0.829333	6.526201	-0.902948
39	6	0	-1.409552	7.390744	-0.504151
40	6	0	-5.108232	4.231409	0.201572
41	6	0	0.686573	-4.758476	-0.812746
42	6	0	6.291613	0.021797	-0.355906
43	6	0	-0.103605	7.616522	-0.760229
44	6	0	-5.615223	2.918930	0.282329
45	1	0	2.762932	-5.317161	-1.030661
46	1	0	0.276800	8.629362	-0.861457
47	1	0	-2.108175	8.215521	-0.393377
48	1	0	-5.794316	5.067171	0.318008
49	6	0	2.177963	6.747006	-1.171583
50	6	0	4.972607	3.434496	-1.249787
51	6	0	3.067233	5.687908	-1.280473
52	6	0	5.861729	2.369092	-1.086403

53	1	0	6.930223	2.564545	-1.033043
54	6	0	-6.971324	2.671686	0.510297
55	6	0	-5.212527	0.482747	0.183288
56	6	0	-4.310586	-0.624197	0.014789
57	6	0	-2.521167	-2.808689	-0.323528
58	6	0	-1.612467	-3.910734	-0.489064
59	6	0	-3.910714	-3.057567	-0.121519
60	6	0	0.192359	-6.062478	-0.807629
61	6	0	-1.172052	-6.329161	-0.646235
62	6	0	-2.092530	-5.244426	-0.473577
63	6	0	-7.476842	1.370688	0.579725
64	6	0	-6.592279	0.254924	0.409568
65	6	0	-4.808349	-1.960382	0.060262
66	6	0	-1.664924	-7.661196	-0.645192
67	6	0	-3.481818	-5.518035	-0.290127
68	6	0	-4.402196	-4.392651	-0.092953
69	6	0	-6.192768	-2.200872	0.282631
70	6	0	-7.112115	-1.073503	0.472455
71	6	0	-8.857721	1.132460	0.815838
72	6	0	-9.335314	-0.149206	0.880464
73	1	0	-10.389304	-0.332552	1.063930
74	6	0	-8.468212	-1.245376	0.709507
75	6	0	-6.632458	-3.521503	0.312416
76	6	0	-5.762964	-4.585475	0.129576
77	6	0	-3.907173	-6.838714	-0.303344
78	6	0	-3.003380	-7.902830	-0.480799
79	1	0	-3.379528	-8.921108	-0.484732
80	1	0	-6.173964	-5.587233	0.168711
81	1	0	-9.520059	1.983956	0.944496

82	1	0	-7.650682	3.511581	0.636174
83	1	0	0.884133	-6.893040	-0.927066
84	1	0	5.383181	4.430567	-1.363088
85	1	0	-8.892873	-2.240340	0.770176
86	1	0	-7.678888	-3.746170	0.480892
87	1	0	-0.960617	-8.477458	-0.778801
88	1	0	-4.955962	-7.079192	-0.177077
89	1	0	6.481110	-1.696612	-1.677622
90	1	0	7.339059	0.234176	-0.597401
91	6	0	6.509789	-2.130102	0.487147
92	1	0	2.536138	7.766160	-1.289127
93	1	0	4.106819	5.914012	-1.486947
94	7	0	6.534453	-1.370590	1.516602
95	7	0	6.239905	-0.045281	1.169225
96	6	0	7.021812	-3.562591	0.609598
97	6	0	5.073308	0.481409	1.791943
98	6	0	3.979566	-0.326149	2.123020
99	6	0	4.971799	1.872185	1.919249
100	6	0	2.747436	0.255119	2.392032
101	1	0	4.069512	-1.406202	2.053242
102	6	0	3.745712	2.464817	2.180842
103	1	0	5.848630	2.479089	1.725297
104	6	0	2.640560	1.640328	2.360337
105	1	0	1.859036	-0.346742	2.545864
106	1	0	3.620725	3.541086	2.193592
107	7	0	1.307252	2.247766	2.414464
108	8	0	1.237284	3.464758	2.404582
109	8	0	0.344236	1.499889	2.429496
110	6	0	8.330970	-3.528763	1.419088

111	1	0	9.086580	-2.917616	0.914639
112	1	0	8.159783	-3.104984	2.410552
113	1	0	8.725162	-4.545066	1.527003
114	6	0	7.336083	-4.168571	-0.763973
115	1	0	7.729687	-5.181710	-0.632263
116	1	0	6.465423	-4.236609	-1.422233
117	1	0	8.101397	-3.580564	-1.283255
118	6	0	6.011280	-4.426791	1.385139
119	1	0	5.047919	-4.515633	0.876318
120	1	0	6.418555	-5.434417	1.524394
121	1	0	5.832587	-3.987205	2.371127

D2-r2c1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.538410	0.374720	-0.222685
2	6	0	1.512035	-1.044056	-0.138775
3	6	0	-0.931198	0.399125	-0.156433
4	6	0	-0.946552	-1.009699	-0.059175
5	6	0	-3.391304	0.430572	-0.117592
6	6	0	2.768311	1.057268	-0.300523
7	6	0	0.317454	2.512756	-0.315299
8	6	0	1.557941	3.214021	-0.354076
9	6	0	-0.906659	4.662715	-0.444051
10	6	0	0.304245	1.105032	-0.222513
11	6	0	-2.142863	2.543901	-0.287806

12	6	0	-2.162899	1.123497	-0.183015
13	6	0	-4.609495	2.566072	-0.258716
14	6	0	-0.917977	3.238825	-0.348490
15	6	0	-3.372303	4.673251	-0.427073
16	6	0	-3.380187	3.265622	-0.323702
17	6	0	-3.414945	-0.990299	-0.011251
18	6	0	-4.623211	1.156508	-0.152961
19	6	0	-5.848906	3.296856	-0.298643
20	6	0	-5.806563	4.713500	-0.406128
21	1	0	-6.745610	5.261415	-0.437902
22	6	0	-4.616718	5.398157	-0.468801
23	6	0	-2.141372	5.373828	-0.485904
24	6	0	0.318919	5.378656	-0.492546
25	6	0	1.582457	4.639802	-0.438209
26	6	0	2.781233	2.486364	-0.303450
27	6	0	3.994506	0.307052	-0.392532
28	6	0	3.972586	-1.047694	-0.288246
29	1	0	4.894389	-1.620828	-0.322971
30	6	0	2.746141	-1.774428	-0.139262
31	6	0	0.285559	-1.734720	-0.046855
32	6	0	-2.179983	-1.717145	0.016957
33	6	0	5.303749	1.045446	-0.663203
34	6	0	4.010082	3.186149	-0.241177
35	6	0	2.730924	-3.150976	-0.027212
36	6	0	0.273451	-3.149957	0.060317
37	6	0	-5.855928	0.461128	-0.085105
38	6	0	-2.142991	6.793263	-0.585568
39	6	0	-4.575386	6.837993	-0.575639
40	6	0	-7.050193	2.605499	-0.232042

41	6	0	1.517919	-3.870088	0.077983
42	6	0	5.293233	2.437417	-0.033165
43	6	0	-3.399696	7.498889	-0.630611
44	6	0	-7.090660	1.200984	-0.124575
45	1	0	3.669158	-3.700648	-0.025596
46	1	0	-3.373672	8.582349	-0.709792
47	1	0	-5.519588	7.374607	-0.609719
48	1	0	-7.986775	3.157275	-0.262870
49	6	0	-0.924756	7.465184	-0.634480
50	6	0	2.815887	5.278310	-0.474013
51	6	0	0.276300	6.772603	-0.586048
52	6	0	4.009104	4.559997	-0.371076
53	1	0	4.953990	5.097372	-0.384226
54	6	0	-8.301338	0.507294	-0.055596
55	6	0	-5.878552	-0.948218	0.021508
56	6	0	-4.641217	-1.679968	0.057821
57	6	0	-2.190835	-3.122566	0.122028
58	6	0	-0.950593	-3.849609	0.147299
59	6	0	-3.428296	-3.826849	0.198470
60	6	0	1.498644	-5.259990	0.192086
61	6	0	0.296652	-5.970140	0.284203
62	6	0	-0.949183	-5.262870	0.258059
63	6	0	-8.342063	-0.885356	0.050985
64	6	0	-7.117808	-1.631330	0.090040
65	6	0	-4.659743	-3.102408	0.164584
66	6	0	0.288633	-7.385681	0.401630
67	6	0	-2.175073	-5.989147	0.343591
68	6	0	-3.438909	-5.245978	0.306098
69	6	0	-5.898505	-3.798646	0.234479

70	6	0	-7.161932	-3.054427	0.198023
71	6	0	-9.580167	-1.579304	0.121553
72	6	0	-9.600845	-2.944387	0.225388
73	1	0	-10.546150	-3.475124	0.280049
74	6	0	-8.399338	-3.677949	0.263099
75	6	0	-5.865814	-5.186776	0.334991
76	6	0	-4.671444	-5.889314	0.369701
77	6	0	-2.122565	-7.370993	0.458030
78	6	0	-0.898127	-8.064261	0.487265
79	1	0	-0.904533	-9.145845	0.578269
80	1	0	-4.721832	-6.968803	0.447134
81	1	0	-10.502100	-1.005529	0.092039
82	1	0	-9.234581	1.064744	-0.085282
83	1	0	2.439230	-5.805432	0.208757
84	1	0	2.877139	6.355515	-0.569431
85	1	0	-8.467448	-4.756059	0.346082
86	1	0	-6.787525	-5.753793	0.387538
87	1	0	1.237969	-7.913375	0.422285
88	1	0	-3.034785	-7.951320	0.527884
89	1	0	6.117157	3.028932	-0.462003
90	1	0	-0.919545	8.549223	-0.709303
91	1	0	1.195278	7.345348	-0.621780
92	7	0	6.475779	0.972005	1.340551
93	6	0	5.777394	2.046897	1.380923
94	7	0	6.420239	0.449331	0.063714
95	6	0	5.613970	2.829736	2.661640
96	6	0	7.251842	-0.568170	-0.325260
97	6	0	7.116021	-1.158081	-1.599622
98	6	0	8.269231	-1.025090	0.538864

99	6	0	7.976302	-2.164244	-1.999999
100	1	0	6.325551	-0.838027	-2.269772
101	6	0	9.121353	-2.033628	0.133927
102	1	0	8.368314	-0.572745	1.517140
103	6	0	8.973963	-2.594381	-1.132717
104	1	0	7.882043	-2.625577	-2.975657
105	1	0	9.907946	-2.395893	0.784998
106	7	0	9.877831	-3.653557	-1.555238
107	8	0	10.739929	-4.013285	-0.770009
108	8	0	9.722643	-4.122786	-2.671489
109	6	0	6.182412	4.245310	2.473968
110	1	0	6.091407	4.802292	3.412490
111	1	0	7.242031	4.209680	2.199185
112	1	0	5.638032	4.800082	1.705240
113	6	0	6.368539	2.129445	3.796270
114	1	0	5.988175	1.116641	3.954053
115	1	0	7.436764	2.056033	3.574164
116	1	0	6.241132	2.699962	4.722027
117	6	0	4.120199	2.913651	3.026587
118	1	0	3.550187	3.497380	2.298513
119	1	0	3.678955	1.913308	3.089691
120	1	0	4.013713	3.396934	4.003879
121	1	0	5.515018	1.087170	-1.735609

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.003029	-0.860585	-1.087866
2	6	0	1.249975	-2.050224	-1.267618
3	6	0	-0.079914	0.381498	-0.663681
4	6	0	-0.808159	-0.824776	-0.710976
5	6	0	-2.143871	1.623510	-0.190961
6	6	0	3.404415	-0.910771	-1.075319
7	6	0	2.068481	1.571621	-0.779092
8	6	0	3.489356	1.541574	-0.882881
9	6	0	2.119421	4.038970	-0.635554
10	6	0	1.330345	0.374053	-0.837144
11	6	0	-0.011842	2.830971	-0.420898
12	6	0	-0.752139	1.615295	-0.417617
13	6	0	-2.094792	4.076513	0.012481
14	6	0	1.384670	2.818084	-0.612842
15	6	0	0.024032	5.283722	-0.248955
16	6	0	-0.697013	4.071203	-0.218257
17	6	0	-2.879924	0.403771	-0.184212
18	6	0	-2.818748	2.862234	0.040034
19	6	0	-2.777551	5.325515	0.224629
20	6	0	-2.024540	6.531760	0.175306
21	1	0	-2.543623	7.475577	0.326517
22	6	0	-0.668556	6.532108	-0.055343
23	6	0	1.426403	5.273016	-0.465944
24	6	0	3.528335	4.036053	-0.827904
25	6	0	4.232967	2.755855	-0.948641
26	6	0	4.164795	0.286182	-0.916858
27	6	0	4.065631	-2.166840	-1.274870
28	6	0	3.355566	-3.262140	-1.656585

29	1	0	3.865565	-4.212406	-1.804630
30	6	0	1.919492	-3.264511	-1.634307
31	6	0	-0.140513	-2.045835	-1.039138
32	6	0	-2.206560	-0.831313	-0.457071
33	6	0	5.444729	-2.334474	-0.712342
34	6	0	5.581635	0.242062	-0.904405
35	6	0	1.190645	-4.432366	-1.755260
36	6	0	-0.873534	-3.257101	-1.106202
37	6	0	-4.213504	2.867790	0.287991
38	6	0	2.144172	6.500382	-0.505785
39	6	0	0.096324	7.757018	-0.108197
40	6	0	-4.144509	5.319559	0.469969
41	6	0	-0.195835	-4.473521	-1.465498
42	6	0	6.316328	-1.057974	-0.615918
43	6	0	1.429316	7.740368	-0.324948
44	6	0	-4.886386	4.120537	0.514480
45	1	0	1.699333	-5.360184	-2.008690
46	1	0	1.996900	8.666346	-0.362718
47	1	0	-0.432558	8.695786	0.032235
48	1	0	-4.661146	6.262315	0.634213
49	6	0	3.521629	6.466750	-0.710906
50	6	0	5.606847	2.661526	-1.137293
51	6	0	4.196629	5.262540	-0.861631
52	6	0	6.263829	1.426655	-1.106878
53	1	0	7.344660	1.415412	-1.207469
54	6	0	-6.260368	4.113685	0.770789
55	6	0	-4.940714	1.654933	0.315502
56	6	0	-4.264260	0.409799	0.069212
57	6	0	-2.924929	-2.042021	-0.474511

58	6	0	-2.251418	-3.271340	-0.795658
59	6	0	-4.321715	-2.046926	-0.193169
60	6	0	-0.916395	-5.667503	-1.479621
61	6	0	-2.275904	-5.706820	-1.147905
62	6	0	-2.962246	-4.494959	-0.810797
63	6	0	-6.993067	2.923642	0.810961
64	6	0	-6.332445	1.671998	0.577202
65	6	0	-4.994999	-0.815072	0.079751
66	6	0	-2.994182	-6.931685	-1.142924
67	6	0	-4.354304	-4.531901	-0.495011
68	6	0	-5.044664	-3.272511	-0.192024
69	6	0	-6.391207	-0.810840	0.351205
70	6	0	-7.083942	0.457078	0.610282
71	6	0	-8.389137	2.929697	1.078242
72	6	0	-9.090516	1.754213	1.111578
73	1	0	-10.156317	1.758999	1.317495
74	6	0	-8.443137	0.525404	0.878150
75	6	0	-7.060723	-2.031576	0.352076
76	6	0	-6.407617	-3.226325	0.087673
77	6	0	-5.002264	-5.758209	-0.500527
78	6	0	-4.325312	-6.950508	-0.820164
79	1	0	-4.872844	-7.887708	-0.810434
80	1	0	-6.995143	-4.136656	0.097793
81	1	0	-8.882255	3.881589	1.254027
82	1	0	-6.772318	5.057327	0.944210
83	1	0	-0.408329	-6.593094	-1.740390
84	1	0	6.206634	3.554365	-1.272935
85	1	0	-9.041722	-0.377050	0.911507
86	1	0	-8.123937	-2.071813	0.557181

87	1	0	-2.466623	-7.847229	-1.394954
88	1	0	-6.055874	-5.823399	-0.255848
89	1	0	5.982887	-3.125635	-1.242361
90	1	0	7.182738	-1.138697	-1.280917
91	1	0	4.075290	7.401325	-0.742150
92	1	0	5.271503	5.291746	-0.998861
93	7	0	6.131864	-2.002101	1.540721
94	6	0	6.765398	-1.123992	0.864189
95	7	0	5.328681	-2.791225	0.744550
96	6	0	7.859891	-0.312281	1.546988
97	6	0	4.036614	-3.056383	1.289806
98	6	0	3.501773	-4.338788	1.147830
99	6	0	3.255331	-2.034060	1.839752
100	6	0	2.160352	-4.576737	1.419384
101	1	0	4.139644	-5.128357	0.763937
102	6	0	1.909206	-2.252794	2.101822
103	1	0	3.689695	-1.047636	1.974727
104	6	0	1.376909	-3.511212	1.843990
105	1	0	1.703092	-5.545650	1.258716
106	1	0	1.257200	-1.454321	2.436693
107	7	0	-0.075400	-3.702782	1.952242
108	8	0	-0.757222	-2.724986	2.205188
109	8	0	-0.515237	-4.821229	1.750841
110	6	0	8.345289	-1.080731	2.786443
111	1	0	9.152759	-0.518485	3.267810
112	1	0	7.535725	-1.220508	3.505469
113	1	0	8.722737	-2.070471	2.512826
114	6	0	7.335625	1.054969	2.022364
115	1	0	7.022941	1.700558	1.200750

116	1	0	6.479617	0.915473	2.690578
117	1	0	8.124431	1.571186	2.581218
118	6	0	9.058023	-0.137523	0.602786
119	1	0	9.864027	0.386457	1.126878
120	1	0	9.444530	-1.110181	0.278100
121	1	0	8.814137	0.443593	-0.289915

E1-r1c1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.651857	-3.073575	0.084722
2	6	0	2.362643	-3.646507	0.038918
3	6	0	2.654973	-0.822081	-0.087926
4	6	0	1.359557	-1.395703	-0.112318
5	6	0	1.665479	1.425433	-0.260368
6	6	0	4.791730	-3.903405	0.190375
7	6	0	5.098191	-1.080185	0.019095
8	6	0	6.251370	-1.915435	0.122713
9	6	0	6.559259	0.912225	-0.086903
10	6	0	3.806294	-1.649892	0.006004
11	6	0	4.111544	1.163216	-0.177004
12	6	0	2.809310	0.594544	-0.175223
13	6	0	3.124127	3.413254	-0.375015
14	6	0	5.252596	0.336887	-0.080732
15	6	0	5.557043	3.156522	-0.301757
16	6	0	4.264380	2.585390	-0.285783

17	6	0	0.361906	0.861124	-0.257144
18	6	0	1.824366	2.844009	-0.351945
19	6	0	3.278858	4.838108	-0.485782
20	6	0	4.589099	5.381397	-0.509364
21	1	0	4.705411	6.459312	-0.596357
22	6	0	5.706988	4.581555	-0.419171
23	6	0	6.702731	2.326561	-0.203235
24	6	0	7.714262	0.092085	0.014249
25	6	0	7.555840	-1.354042	0.132412
26	6	0	6.088401	-3.329392	0.216929
27	6	0	4.633955	-5.330559	0.264138
28	6	0	3.372289	-5.881585	0.209500
29	1	0	3.254395	-6.961873	0.253805
30	6	0	2.212304	-5.074998	0.085241
31	6	0	1.215025	-2.816710	-0.063713
32	6	0	0.203075	-0.571727	-0.191666
33	6	0	5.814826	-6.151300	0.382287
34	6	0	7.227650	-4.171749	0.327812
35	6	0	0.939110	-5.629797	-0.013490
36	6	0	-0.067622	-3.394480	-0.149777
37	6	0	0.688257	3.677481	-0.414823
38	6	0	7.998018	2.911140	-0.221248
39	6	0	7.039158	5.136109	-0.436834
40	6	0	2.147301	5.645211	-0.562079
41	6	0	-0.207404	-4.826546	-0.151747
42	6	0	7.047275	-5.597646	0.413955
43	6	0	8.127038	4.340172	-0.342071
44	6	0	0.848907	5.104756	-0.521598
45	1	0	0.825705	-6.711222	-0.000239

46	1	0	9.128049	4.763058	-0.355054
47	1	0	7.143187	6.213909	-0.527385
48	1	0	2.266571	6.722757	-0.646448
49	6	0	9.113575	2.078568	-0.123319
50	6	0	8.653623	-2.217853	0.251584
51	6	0	8.974187	0.706341	-0.008715
52	6	0	8.495633	-3.589401	0.347284
53	1	0	9.370094	-4.228664	0.435122
54	6	0	-0.291568	5.913881	-0.579477
55	6	0	-0.611909	3.112083	-0.365281
56	6	0	-0.768678	1.693931	-0.307909
57	6	0	-1.079877	-1.149420	-0.236508
58	6	0	-1.216715	-2.568670	-0.254280
59	6	0	-2.266026	-0.324812	-0.277239
60	6	0	-1.480570	-5.381752	-0.319560
61	6	0	-2.616062	-4.581388	-0.484342
62	6	0	-2.494219	-3.153762	-0.421630
63	6	0	-1.580789	5.374704	-0.509572
64	6	0	-1.749252	3.955122	-0.388624
65	6	0	-2.092309	1.137705	-0.245375
66	6	0	-3.887148	-5.156232	-0.733858
67	6	0	-3.651402	-2.331567	-0.566123
68	6	0	-3.513465	-0.901443	-0.418855
69	6	0	-3.184158	1.968006	-0.139482
70	6	0	-3.059033	3.399136	-0.274747
71	6	0	-2.732351	6.201720	-0.546074
72	6	0	-3.989080	5.650389	-0.456033
73	1	0	-4.866269	6.288946	-0.488783
74	6	0	-4.158255	4.266576	-0.315320

75	6	0	-4.498592	1.338545	0.184204
76	6	0	-4.750966	-0.011433	-0.479917
77	6	0	-4.871318	-2.956435	-0.853638
78	6	0	-4.981556	-4.350544	-0.938696
79	1	0	-2.601428	7.275576	-0.644755
80	1	0	-0.172254	6.991011	-0.668676
81	1	0	-1.588171	-6.463591	-0.346367
82	1	0	9.660206	-1.818000	0.271741
83	1	0	-5.169042	3.883041	-0.243202
84	1	0	-5.332206	1.997200	-0.085715
85	1	0	-3.973157	-6.238189	-0.780322
86	1	0	10.106478	2.520146	-0.139692
87	1	0	9.873829	0.106461	0.058143
88	1	0	5.684862	-7.228360	0.442474
89	1	0	7.933775	-6.220359	0.499923
90	1	0	-5.950104	-4.789101	-1.156893
91	1	0	-5.764587	-2.374512	-1.017660
92	7	0	-5.592704	-0.064427	1.693879
93	6	0	-4.780904	0.922461	1.650577
94	7	0	-5.834863	-0.520660	0.386640
95	6	0	-4.328703	1.605726	2.923451
96	6	0	-7.168654	-0.581287	0.005223
97	6	0	-8.179795	-0.548994	0.989442
98	6	0	-7.546130	-0.728508	-1.345267
99	6	0	-9.510358	-0.655685	0.633551
100	1	0	-7.897060	-0.438741	2.027922
101	6	0	-8.881786	-0.829922	-1.698491
102	1	0	-6.801293	-0.762063	-2.132034
103	6	0	-9.853113	-0.791103	-0.708442

104	1	0	-10.293803	-0.628301	1.381673
105	1	0	-9.179956	-0.935305	-2.734697
106	7	0	-11.258496	-0.890091	-1.083788
107	8	0	-11.521882	-1.015516	-2.268423
108	8	0	-12.088233	-0.841118	-0.191412
109	6	0	-2.792133	1.661589	3.008241
110	1	0	-2.347394	0.673708	2.844615
111	1	0	-2.363290	2.358767	2.283859
112	1	0	-2.506538	2.001869	4.009293
113	6	0	-4.895440	3.034907	2.944243
114	1	0	-5.989248	3.022771	2.883665
115	1	0	-4.611013	3.524035	3.882040
116	1	0	-4.503107	3.639095	2.121465
117	6	0	-4.866720	0.832852	4.133130
118	1	0	-5.958626	0.782808	4.118903
119	1	0	-4.485195	-0.191858	4.147355
120	1	0	-4.550875	1.338310	5.051331
121	1	0	-5.104282	0.083296	-1.510216

E1-r1c2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.693865	-2.966198	-0.198638
2	6	0	1.383847	-3.431475	-0.448543
3	6	0	1.895638	-0.635962	-0.312020
4	6	0	0.579021	-1.104631	-0.527553

5	6	0	1.091267	1.689491	-0.421503
6	6	0	3.747135	-3.888310	-0.014029
7	6	0	4.277766	-1.091452	0.057903
8	6	0	5.344488	-2.020577	0.241886
9	6	0	5.875448	0.784605	0.263754
10	6	0	2.961926	-1.557234	-0.149856
11	6	0	3.483681	1.232702	-0.096596
12	6	0	2.155491	0.767802	-0.276213
13	6	0	2.685602	3.561891	-0.271462
14	6	0	4.542011	0.313693	0.075772
15	6	0	5.067140	3.111740	0.071231
16	6	0	3.745405	2.643729	-0.097672
17	6	0	-0.240705	1.227614	-0.569101
18	6	0	1.355053	3.093770	-0.416443
19	6	0	2.950108	4.975160	-0.298016
20	6	0	4.289752	5.414029	-0.131103
21	1	0	4.494607	6.482101	-0.147485
22	6	0	5.328418	4.526058	0.054593
23	6	0	6.129705	2.189428	0.256414
24	6	0	6.947010	-0.129280	0.451341
25	6	0	6.673269	-1.564937	0.451386
26	6	0	5.067384	-3.420922	0.215505
27	6	0	3.474855	-5.300025	-0.064403
28	6	0	2.194523	-5.744066	-0.321008
29	1	0	1.996955	-6.812452	-0.368844
30	6	0	1.119162	-4.842155	-0.534694
31	6	0	0.324171	-2.507476	-0.620530
32	6	0	-0.495264	-0.187811	-0.646754
33	6	0	4.568902	-6.217008	0.147400

34	6	0	6.117989	-4.357085	0.410277
35	6	0	-0.167471	-5.281416	-0.847324
36	6	0	-0.973796	-2.968851	-0.920733
37	6	0	0.293449	4.009648	-0.572528
38	6	0	7.454229	2.671470	0.433464
39	6	0	6.688464	4.973805	0.234944
40	6	0	1.893932	5.865575	-0.489215
41	6	0	-1.223730	-4.377210	-1.079338
42	6	0	5.822972	-5.766708	0.374955
43	6	0	7.696149	4.091302	0.416455
44	6	0	0.564054	5.422374	-0.632059
45	1	0	-0.360522	-6.348059	-0.930987
46	1	0	8.717397	4.437148	0.552632
47	1	0	6.880567	6.043191	0.222057
48	1	0	2.099311	6.932809	-0.525982
49	6	0	8.486674	1.749852	0.615789
50	6	0	7.680453	-2.521169	0.646607
51	6	0	8.239022	0.387466	0.624401
52	6	0	7.411434	-3.879479	0.628608
53	1	0	8.218094	-4.591046	0.783043
54	6	0	-0.507032	6.302382	-0.839975
55	6	0	-1.040996	3.540322	-0.666350
56	6	0	-1.302803	2.140946	-0.651218
57	6	0	-1.797145	-0.654650	-0.871894
58	6	0	-2.033218	-2.043792	-1.073952
59	6	0	-2.914940	0.246090	-0.833356
60	6	0	-2.496577	-4.794656	-1.496151
61	6	0	-3.528816	-3.876999	-1.747587
62	6	0	-3.313229	-2.486738	-1.476858

63	6	0	-1.829535	5.849908	-0.951906
64	6	0	-2.111748	4.449158	-0.831296
65	6	0	-2.664425	1.681079	-0.653722
66	6	0	-4.794647	-4.280300	-2.245993
67	6	0	-4.387897	-1.556572	-1.588759
68	6	0	-4.185802	-0.218619	-1.077015
69	6	0	-3.709164	2.575579	-0.609256
70	6	0	-3.462895	3.978856	-0.853696
71	6	0	-2.909431	6.742410	-1.177926
72	6	0	-4.197341	6.267850	-1.276959
73	1	0	-5.013412	6.955482	-1.476808
74	6	0	-4.480290	4.903926	-1.108261
75	6	0	-5.068996	2.058432	-0.200000
76	6	0	-5.361411	0.567071	-0.568619
77	6	0	-5.600517	-2.001678	-2.123058
78	6	0	-5.784757	-3.347984	-2.470161
79	1	0	-6.214681	0.504665	-1.245756
80	1	0	-2.699868	7.803196	-1.282167
81	1	0	-0.308213	7.368971	-0.914145
82	1	0	-2.687351	-5.855712	-1.637952
83	1	0	8.703020	-2.206641	0.818252
84	1	0	-5.509880	4.574037	-1.190941
85	1	0	-5.863146	2.688230	-0.612515
86	1	0	-4.962572	-5.332219	-2.458901
87	1	0	9.501692	2.114208	0.750188
88	1	0	9.078202	-0.283148	0.765172
89	1	0	4.356477	-7.282139	0.117713
90	1	0	6.641433	-6.463963	0.532828
91	1	0	-6.738333	-3.663153	-2.882978

92	1	0	-6.427283	-1.309225	-2.245793
93	7	0	-5.603837	0.891484	1.776619
94	6	0	-5.233386	2.029806	1.345295
95	7	0	-5.823175	-0.025464	0.772602
96	6	0	-5.094970	3.174419	2.340420
97	6	0	-5.329733	-1.319131	1.148818
98	6	0	-4.077999	-1.464072	1.756592
99	6	0	-6.080831	-2.445796	0.820648
100	6	0	-3.529121	-2.727191	1.931140
101	1	0	-3.520042	-0.576390	2.037738
102	6	0	-5.543072	-3.716101	0.980455
103	1	0	-7.064099	-2.309838	0.383495
104	6	0	-4.260472	-3.828489	1.501944
105	1	0	-2.535501	-2.868916	2.339501
106	1	0	-6.080520	-4.605869	0.677292
107	7	0	-3.629690	-5.152072	1.533947
108	8	0	-4.229064	-6.074632	1.005890
109	8	0	-2.536292	-5.249782	2.060334
110	6	0	-6.049770	4.315843	1.958611
111	1	0	-7.085243	3.960293	1.917229
112	1	0	-5.992091	5.107794	2.713271
113	1	0	-5.789232	4.760882	0.995474
114	6	0	-5.486262	2.667449	3.736712
115	1	0	-6.505952	2.275164	3.748516
116	1	0	-4.819040	1.867649	4.068925
117	1	0	-5.417738	3.498017	4.446911
118	6	0	-3.649613	3.699733	2.418992
119	1	0	-3.555782	4.346503	3.298120
120	1	0	-2.937039	2.874686	2.527989

121	1	0	-3.366827	4.289844	1.546861

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.264174	2.585549	-0.285556
2	6	0	-3.123858	3.413302	-0.374948
3	6	0	-2.809276	0.594559	-0.175262
4	6	0	-1.665370	1.425345	-0.260498
5	6	0	-1.359699	-1.395822	-0.112479
6	6	0	-5.556787	3.156813	-0.301283
7	6	0	-5.252582	0.337130	-0.080540
8	6	0	-6.559191	0.912600	-0.086479
9	6	0	-6.251562	-1.915119	0.122711
10	6	0	-4.111459	1.163355	-0.176888
11	6	0	-3.806464	-1.649794	0.005875
12	6	0	-2.655066	-0.822082	-0.088051
13	6	0	-2.363003	-3.646545	0.038604
14	6	0	-5.098308	-1.079964	0.019106
15	6	0	-4.792116	-3.903238	0.189980
16	6	0	-3.652165	-3.073498	0.084428
17	6	0	-0.203137	-0.571948	-0.191804
18	6	0	-1.215301	-2.816844	-0.063906
19	6	0	-2.212806	-5.075050	0.084819
20	6	0	-3.372869	-5.881550	0.208883
21	1	0	-3.255071	-6.961853	0.253051

22	6	0	-4.634484	-5.330415	0.263533
23	6	0	-6.088731	-3.329104	0.216667
24	6	0	-7.555974	-1.353596	0.132628
25	6	0	-7.714260	0.092563	0.014748
26	6	0	-6.702540	2.326961	-0.202626
27	6	0	-5.706611	4.581865	-0.418579
28	6	0	-4.588658	5.381596	-0.508968
29	1	0	-4.704877	6.459526	-0.595903
30	6	0	-3.278472	4.838171	-0.485671
31	6	0	-1.824144	2.843932	-0.352080
32	6	0	-0.361844	0.860916	-0.257364
33	6	0	-7.038726	5.136561	-0.435927
34	6	0	-7.997772	2.911674	-0.220337
35	6	0	-2.146852	5.645162	-0.562212
36	6	0	-0.687969	3.677297	-0.415164
37	6	0	0.067302	-3.394728	-0.149847
38	6	0	-7.228058	-4.171371	0.327453
39	6	0	-5.815433	-6.151066	0.381522
40	6	0	-0.939652	-5.629959	-0.013779
41	6	0	-0.848507	5.104583	-0.521990
42	6	0	-8.126670	4.340729	-0.341002
43	6	0	-7.047826	-5.597300	0.413308
44	6	0	0.206950	-4.826805	-0.151804
45	1	0	-2.266035	6.722717	-0.646584
46	1	0	-7.934388	-6.219941	0.499159
47	1	0	-5.685569	-7.228150	0.441497
48	1	0	-0.826346	-6.711394	-0.000574
49	6	0	-8.495982	-3.588901	0.347118
50	6	0	-8.974126	0.706953	-0.007881

51	6	0	-8.653838	-2.217319	0.251711
52	6	0	-9.113396	2.079207	-0.122277
53	1	0	-10.106256	2.520892	-0.138387
54	6	0	1.480095	-5.382143	-0.319335
55	6	0	1.216489	-2.569021	-0.254196
56	6	0	1.079774	-1.149754	-0.236533
57	6	0	0.768814	1.693621	-0.308284
58	6	0	0.612154	3.111783	-0.365797
59	6	0	2.092411	1.137291	-0.245750
60	6	0	0.292024	5.913603	-0.580180
61	6	0	1.581208	5.374315	-0.510529
62	6	0	1.749561	3.954731	-0.389450
63	6	0	2.615699	-4.581898	-0.483852
64	6	0	2.493969	-3.154255	-0.421265
65	6	0	2.266003	-0.325249	-0.277251
66	6	0	2.732838	6.201218	-0.547414
67	6	0	3.059310	3.398650	-0.275762
68	6	0	3.184333	1.967544	-0.140160
69	6	0	3.513415	-0.902032	-0.418573
70	6	0	3.651265	-2.332187	-0.565547
71	6	0	3.886802	-5.156893	-0.732942
72	6	0	4.981360	-4.351336	-0.937465
73	1	0	5.949951	-4.790011	-1.155239
74	6	0	4.871226	-2.957209	-0.852583
75	6	0	4.750984	-0.012157	-0.479764
76	6	0	4.498705	1.338111	0.183801
77	6	0	4.158613	4.265970	-0.316785
78	6	0	3.989538	5.649779	-0.457657
79	1	0	5.332402	1.996559	-0.086376

80	1	0	3.972706	-6.238864	-0.779275
81	1	0	1.587586	-6.463994	-0.346086
82	1	0	0.172784	6.990736	-0.669442
83	1	0	-9.873817	0.107160	0.059093
84	1	0	5.764627	-2.375394	-1.016266
85	1	0	5.104456	0.082197	-1.510049
86	1	0	2.601989	7.275075	-0.646178
87	1	0	-9.370503	-4.228092	0.434875
88	1	0	-9.660380	-1.817367	0.272012
89	1	0	-7.142660	6.214379	-0.526377
90	1	0	-9.127639	4.763723	-0.353744
91	1	0	4.866780	6.288248	-0.490737
92	1	0	5.169382	3.882337	-0.244919
93	6	0	4.780931	0.922660	1.650364
94	7	0	5.592591	-0.064320	1.694127
95	7	0	5.834778	-0.521147	0.387091
96	6	0	4.328857	1.606564	2.922952
97	6	0	7.168604	-0.581692	0.005732
98	6	0	7.546117	-0.729657	-1.344669
99	6	0	8.179752	-0.548554	0.989907
100	6	0	8.881803	-0.830853	-1.697865
101	1	0	6.801264	-0.764054	-2.131391
102	6	0	9.510349	-0.655030	0.634060
103	1	0	7.897029	-0.437783	2.028336
104	6	0	9.853144	-0.791098	-0.707857
105	1	0	9.179957	-0.936801	-2.734018
106	1	0	10.293762	-0.626940	1.382188
107	7	0	11.258551	-0.889892	-1.083165
108	8	0	12.088304	-0.840001	-0.190855

109	8	0	11.521944	-1.016048	-2.267716
110	6	0	4.866466	0.833948	4.132981
111	1	0	5.958345	0.783301	4.118769
112	1	0	4.550909	1.340018	5.050945
113	1	0	4.484375	-0.190545	4.147709
114	6	0	4.896207	3.035506	2.943270
115	1	0	4.504334	3.639539	2.120155
116	1	0	4.611787	3.525142	3.880805
117	1	0	5.990028	3.022853	2.882933
118	6	0	2.792298	1.663119	3.007591
119	1	0	2.363811	2.360203	2.282908
120	1	0	2.347148	0.675363	2.844319
121	1	0	2.506767	2.003915	4.008487

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.553553	2.852861	0.334443
2	6	0	-2.396417	3.643035	0.156158
3	6	0	-2.250438	0.823037	-0.180872
4	6	0	-1.081070	1.609902	-0.305013
5	6	0	-0.963415	-1.192223	-0.763515
6	6	0	-4.781863	3.463618	0.669260
7	6	0	-4.654422	0.646012	0.285006
8	6	0	-5.893555	1.258207	0.639066
9	6	0	-5.775248	-1.555836	0.174695

10	6	0	-3.489082	1.431476	0.150486
11	6	0	-3.371480	-1.366311	-0.310008
12	6	0	-2.191783	-0.584579	-0.412830
13	6	0	-2.094220	-3.371034	-0.973019
14	6	0	-4.595121	-0.763393	0.052893
15	6	0	-4.483715	-3.557686	-0.478415
16	6	0	-3.313928	-2.773194	-0.584815
17	6	0	0.223444	-0.419597	-0.830252
18	6	0	-0.913466	-2.590611	-1.053735
19	6	0	-2.044202	-4.773699	-1.284451
20	6	0	-3.235761	-5.536065	-1.165112
21	1	0	-3.200364	-6.599162	-1.392049
22	6	0	-4.426457	-4.965295	-0.768363
23	6	0	-5.708870	-2.956915	-0.088872
24	6	0	-7.010355	-0.963037	0.549962
25	6	0	-7.070731	0.477271	0.788803
26	6	0	-5.946700	2.670788	0.836582
27	6	0	-4.846330	4.891408	0.831369
28	6	0	-3.717630	5.657005	0.627709
29	1	0	-3.776961	6.737931	0.733242
30	6	0	-2.472311	5.074266	0.274054
31	6	0	-1.157951	3.028551	-0.153830
32	6	0	0.166481	1.000066	-0.596821
33	6	0	-6.111403	5.483628	1.194568
34	6	0	-7.173724	3.293016	1.190704
35	6	0	-1.339400	5.843545	0.009643
36	6	0	-0.011291	3.819340	-0.372564
37	6	0	0.305211	-3.188265	-1.437529
38	6	0	-6.876498	-3.757947	0.028769

39	6	0	-5.635041	-5.743111	-0.637039
40	6	0	-0.839287	-5.340989	-1.696983
41	6	0	-0.109167	5.255329	-0.346633
42	6	0	-7.214418	4.721777	1.369334
43	6	0	-6.796892	-5.167974	-0.254489
44	6	0	0.344963	-4.582933	-1.790459
45	1	0	-1.410812	6.927650	0.056757
46	1	0	-7.703150	-5.759818	-0.156930
47	1	0	-5.585011	-6.806642	-0.853674
48	1	0	-0.809114	-6.398103	-1.950314
49	6	0	-8.072892	-3.149762	0.411969
50	6	0	-8.258668	1.127851	1.151074
51	6	0	-8.136973	-1.789732	0.664346
52	6	0	-8.309624	2.497521	1.348427
53	1	0	-9.249908	2.967458	1.624454
54	6	0	1.559133	-5.135539	-2.220697
55	6	0	1.493378	-2.417323	-1.469455
56	6	0	1.445538	-1.030384	-1.146390
57	6	0	1.327088	1.780814	-0.711884
58	6	0	1.229028	3.200423	-0.658553
59	6	0	2.617842	1.166039	-0.884262
60	6	0	1.006541	6.012253	-0.732768
61	6	0	2.209779	5.406875	-1.124203
62	6	0	2.347436	3.984650	-1.017974
63	6	0	2.739266	-4.379827	-2.274896
64	6	0	2.717244	-3.007841	-1.860642
65	6	0	2.670117	-0.287524	-1.074047
66	6	0	3.285804	6.151390	-1.675365
67	6	0	3.582401	3.353518	-1.350908

68	6	0	3.745580	1.944216	-1.067436
69	6	0	3.875713	-0.919178	-1.267394
70	6	0	3.927857	-2.250329	-1.817632
71	6	0	3.967245	-4.936732	-2.717101
72	6	0	5.113097	-4.172876	-2.737862
73	1	0	6.042855	-4.602764	-3.097401
74	6	0	5.104649	-2.845399	-2.285250
75	6	0	5.073672	-0.202333	-0.715410
76	6	0	5.129977	1.329768	-0.973803
77	6	0	4.559938	4.120592	-1.986172
78	6	0	4.406598	5.506221	-2.148409
79	1	0	5.739547	1.568534	-1.851885
80	1	0	3.986089	-5.972961	-3.042269
81	1	0	1.589459	-6.182433	-2.513490
82	1	0	0.921841	7.095600	-0.775403
83	1	0	-9.172520	0.560312	1.280088
84	1	0	6.030875	-2.279913	-2.302897
85	1	0	6.024628	-0.655033	-1.028880
86	1	0	3.185676	7.229260	-1.766468
87	1	0	-8.968667	-3.757914	0.506248
88	1	0	-9.093122	-1.369539	0.952856
89	1	0	-6.153033	6.561669	1.323900
90	1	0	-8.163310	5.175084	1.643715
91	1	0	5.194047	6.072113	-2.636822
92	1	0	5.448783	3.641271	-2.375776
93	6	0	5.831882	1.769242	0.352578
94	7	0	5.672455	0.887737	1.261306
95	7	0	5.013314	-0.207079	0.772006
96	6	0	6.670507	2.999637	0.700246

97	6	0	4.964616	-1.314364	1.617625
98	6	0	5.078370	-2.630986	1.153690
99	6	0	4.782131	-1.085004	2.995789
100	6	0	4.982479	-3.696717	2.037486
101	1	0	5.269708	-2.836371	0.110712
102	6	0	4.698702	-2.143796	3.878173
103	1	0	4.705909	-0.064605	3.350304
104	6	0	4.790648	-3.444010	3.387044
105	1	0	5.070624	-4.719267	1.690982
106	1	0	4.551481	-1.983555	4.939285
107	7	0	4.693116	-4.566131	4.316018
108	8	0	4.529727	-4.311899	5.497545
109	8	0	4.781780	-5.693159	3.857837
110	6	0	7.580063	2.636003	1.889315
111	1	0	6.995017	2.372639	2.772182
112	1	0	8.224860	1.785761	1.648132
113	1	0	8.211769	3.497253	2.130637
114	6	0	7.586467	3.386858	-0.468611
115	1	0	7.037748	3.779365	-1.324869
116	1	0	8.278439	4.169729	-0.141080
117	1	0	8.184151	2.529013	-0.797499
118	6	0	5.797598	4.187465	1.144575
119	1	0	6.446876	5.000831	1.488030
120	1	0	5.164136	4.578232	0.348538
121	1	0	5.158420	3.886399	1.980678

F

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.477473	1.501413	-0.895994
2	6	0	-1.684416	2.676088	-0.941033
3	6	0	-0.561343	0.257520	0.140060
4	6	0	0.332623	1.381245	-0.327416
5	6	0	1.605577	-1.172988	-0.041001
6	6	0	-3.873466	1.592896	-1.068235
7	6	0	-2.629654	-0.916513	-0.681008
8	6	0	-4.042761	-0.850471	-0.937375
9	6	0	-2.752015	-3.394501	-0.895156
10	6	0	-1.887969	0.240490	-0.572253
11	6	0	-0.626207	-2.307842	-0.339944
12	6	0	0.131984	-1.161005	0.302650
13	6	0	1.470463	-3.610329	-0.437152
14	6	0	-1.981756	-2.218877	-0.590470
15	6	0	-0.681424	-4.710311	-0.847257
16	6	0	0.055882	-3.542074	-0.551648
17	6	0	2.363736	-0.002382	-0.068800
18	6	0	2.240735	-2.425885	-0.240084
19	6	0	2.127408	-4.876339	-0.556410
20	6	0	1.350888	-6.041433	-0.791557
21	1	0	1.859775	-6.999749	-0.865061
22	6	0	-0.012836	-5.978593	-0.953275
23	6	0	-2.091592	-4.645860	-0.989808
24	6	0	-4.155926	-3.326941	-1.076559
25	6	0	-4.827531	-2.025218	-1.012896
26	6	0	-4.668769	0.418234	-1.028666

27	6	0	-4.503177	2.876818	-1.215821
28	6	0	-3.723080	4.006807	-1.290685
29	1	0	-4.193192	4.980125	-1.410075
30	6	0	-2.308367	3.939544	-1.182606
31	6	0	-0.279448	2.603911	-0.708892
32	6	0	1.716075	1.296390	-0.216062
33	6	0	-5.946332	2.943549	-1.225849
34	6	0	-6.085492	0.518342	-1.078670
35	6	0	-1.526350	5.093090	-1.246665
36	6	0	0.503144	3.780499	-0.808223
37	6	0	3.655328	-2.510108	-0.215658
38	6	0	-2.834519	-5.829723	-1.258130
39	6	0	-0.800300	-7.160608	-1.216652
40	6	0	3.515821	-4.949314	-0.438689
41	6	0	-0.133726	5.047359	-1.075354
42	6	0	-6.696800	1.822876	-1.140265
43	6	0	-2.140700	-7.088237	-1.361877
44	6	0	4.300693	-3.798684	-0.271874
45	1	0	-2.005725	6.053038	-1.422632
46	1	0	-2.726709	-7.980594	-1.565059
47	1	0	-0.280671	-8.111495	-1.296585
48	1	0	4.004493	-5.918610	-0.499120
49	6	0	-4.212864	-5.732579	-1.429795
50	6	0	-6.220421	-1.897172	-1.042911
51	6	0	-4.856308	-4.506450	-1.347042
52	6	0	-6.838147	-0.654559	-1.056002
53	1	0	-7.922658	-0.589798	-1.064459
54	6	0	5.692165	-3.871165	-0.146538
55	6	0	4.433751	-1.340671	-0.086779

56	6	0	3.787489	-0.069430	-0.085281
57	6	0	2.521759	2.465215	-0.358677
58	6	0	1.899394	3.724394	-0.606253
59	6	0	3.937697	2.391855	-0.238365
60	6	0	0.645298	6.208071	-1.119282
61	6	0	2.029214	6.172733	-0.915340
62	6	0	2.675285	4.918230	-0.668169
63	6	0	6.477693	-2.723454	0.004631
64	6	0	5.852086	-1.435147	0.004967
65	6	0	4.573841	1.117079	-0.096570
66	6	0	2.805798	7.358893	-0.942851
67	6	0	4.081934	4.876331	-0.478594
68	6	0	4.724821	3.576409	-0.288795
69	6	0	5.991234	1.038092	0.000109
70	6	0	6.648875	-0.264304	0.103626
71	6	0	7.885802	-2.806850	0.152340
72	6	0	8.636219	-1.665307	0.293989
73	1	0	9.712326	-1.731760	0.420569
74	6	0	8.026174	-0.402343	0.266398
75	6	0	6.723400	2.223717	-0.039344
76	6	0	6.109173	3.455018	-0.179260
77	6	0	4.796270	6.073314	-0.501759
78	6	0	4.161527	7.302813	-0.730915
79	1	0	8.353780	-3.787231	0.157065
80	1	0	6.174388	-4.845563	-0.166235
81	1	0	0.160776	7.163472	-1.306098
82	1	0	-6.845803	-2.782421	-1.041604
83	1	0	8.656691	0.471965	0.375400
84	1	0	2.307428	8.306135	-1.128379

85	1	0	-4.785285	-6.630330	-1.647103
86	1	0	-5.925558	-4.474179	-1.520121
87	1	0	-6.411711	3.923558	-1.277653
88	1	0	-7.781376	1.881745	-1.124549
89	1	0	4.754356	8.211945	-0.742463
90	1	0	5.867408	6.076191	-0.340558
91	1	0	6.739958	4.334635	-0.222739
92	1	0	7.805080	2.198833	0.015202
93	6	0	0.005965	-1.388228	1.893311
94	6	0	0.453663	-2.535738	2.824518
95	7	0	-0.578059	-0.410562	2.448893
96	7	0	-0.864308	0.641428	1.641870
97	6	0	-2.137252	1.222245	1.955983
98	6	0	-3.259641	0.416081	2.170895
99	6	0	-2.261785	2.611667	1.960207
100	6	0	-4.521490	0.987555	2.254890
101	1	0	-3.140541	-0.662603	2.207194
102	6	0	-3.519185	3.197564	2.032592
103	1	0	-1.370463	3.219775	1.843830
104	6	0	-4.628877	2.368346	2.138788
105	1	0	-5.417604	0.384935	2.344749
106	1	0	-3.652362	4.270858	1.974128
107	7	0	-5.966713	2.966440	2.069687
108	8	0	-6.039333	4.156863	1.816745
109	8	0	-6.925273	2.235885	2.245019
110	6	0	0.030651	-2.140512	4.256088
111	1	0	-1.051866	-2.013157	4.334391
112	1	0	0.340437	-2.939095	4.937095
113	1	0	0.501799	-1.206806	4.570879

114	6	0	-0.240382	-3.878980	2.515502
115	1	0	-1.294064	-3.735627	2.249415
116	1	0	0.247952	-4.434309	1.714874
117	1	0	-0.203749	-4.506663	3.412048
118	6	0	1.983903	-2.728500	2.853256
119	1	0	2.348857	-3.333530	2.023371
120	1	0	2.511017	-1.767812	2.844219
121	1	0	2.253290	-3.251393	3.776971

TS

TSA1-r1c1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.415959	-1.678507	-0.257773
2	6	0	-7.539070	-3.069700	-0.559707
3	6	0	-4.976640	-1.848453	-0.497879
4	6	0	-5.107263	-3.249177	-0.804920
5	6	0	-2.534350	-2.025247	-0.710762
6	6	0	-8.581571	-0.898581	0.016663
7	6	0	-6.014532	0.313389	0.064122
8	6	0	-7.192872	1.094816	0.336405
9	6	0	-4.617685	2.312663	0.363108
10	6	0	-6.137403	-1.072284	-0.229535
11	6	0	-3.580863	0.141345	-0.176452

12	6	0	-3.703290	-1.249326	-0.459282
13	6	0	-1.144137	-0.034050	-0.418432
14	6	0	-4.744693	0.919813	0.088407
15	6	0	-2.188882	2.142645	0.091106
16	6	0	-2.307640	0.745594	-0.157918
17	6	0	0.237578	1.981449	-0.213319
18	6	0	-2.671229	-3.426100	-1.028110
19	6	0	-0.082699	-2.222827	-0.878683
20	6	0	-0.223742	-3.648184	-1.130757
21	6	0	2.358931	-2.379564	-1.193236
22	6	0	-1.265289	-1.436846	-0.661560
23	6	0	1.286429	-0.193245	-0.725079
24	6	0	1.163621	-1.608637	-0.912739
25	6	0	3.712811	-0.336973	-1.151376
26	6	0	0.121597	0.580020	-0.437066
27	6	0	2.659703	1.831797	-0.579383
28	6	0	2.537658	0.430956	-0.810109
29	6	0	5.090005	1.685063	-0.976620
30	6	0	-5.802507	3.092989	0.637542
31	6	0	-3.223866	4.321618	0.628690
32	6	0	-4.416510	5.097856	0.912379
33	6	0	-1.835429	6.346250	0.872809
34	6	0	-3.355941	2.918134	0.367674
35	6	0	-0.799706	4.156346	0.321292
36	6	0	-0.921894	2.754531	0.077899
37	6	0	1.621039	4.000164	-0.020764
38	6	0	-1.973910	4.925731	0.611906
39	6	0	0.589423	6.183983	0.538331
40	6	0	0.459037	4.767339	0.284843

41	6	0	3.010882	6.028702	0.177575
42	6	0	1.502871	2.600668	-0.261313
43	6	0	4.038807	3.849998	-0.395979
44	6	0	3.919674	2.456206	-0.648171
45	6	0	6.465913	3.703001	-0.781826
46	6	0	2.884934	4.617277	-0.077621
47	6	0	5.427248	5.873677	-0.200479
48	6	0	5.307395	4.473832	-0.458970
49	6	0	0.998123	-4.463724	-1.257183
50	1	0	0.902384	-5.414112	-1.776208
51	6	0	-1.469588	-4.183959	-1.257078
52	1	0	-1.584600	-5.235813	-1.507795
53	6	0	-3.920722	-3.998839	-1.072208
54	1	0	-4.019483	-5.055603	-1.312057
55	6	0	-6.369444	-3.822124	-0.829970
56	1	0	-6.470898	-4.879902	-1.062445
57	6	0	-8.823525	-3.647088	-0.578920
58	1	0	-8.921297	-4.704567	-0.808279
59	6	0	-9.951796	-2.881433	-0.309468
60	1	0	-10.932456	-3.346985	-0.329864
61	6	0	-9.841141	-1.527761	-0.015250
62	1	0	-10.729031	-0.938072	0.194955
63	6	0	-8.435219	0.479249	0.309669
64	1	0	-9.326401	1.067265	0.517402
65	6	0	-7.036665	2.484657	0.622453
66	1	0	-7.927407	3.073631	0.829598
67	6	0	-5.640624	4.494054	0.913712
68	1	0	-6.531375	5.081757	1.125171
69	6	0	-4.253253	6.514906	1.183171

70	1	0	-5.146219	7.094495	1.401479
71	6	0	2.234394	-3.822226	-1.257025
72	1	0	3.121271	-4.384263	-1.542700
73	6	0	3.559753	-1.752429	-1.356210
74	1	0	4.445007	-2.334824	-1.600349
75	6	0	4.936600	0.287068	-1.226510
76	1	0	5.820825	-0.295383	-1.477234
77	6	0	6.323023	2.316773	-1.035670
78	1	0	7.208815	1.736162	-1.283230
79	6	0	7.716211	4.348765	-0.838176
80	1	0	8.598840	3.765271	-1.084446
81	6	0	7.824693	5.711009	-0.584592
82	1	0	8.797892	6.189485	-0.634405
83	6	0	6.702331	6.468248	-0.270165
84	1	0	6.797483	7.532737	-0.074657
85	6	0	4.264549	6.618837	0.114242
86	1	0	4.363047	7.684574	0.308166
87	6	0	1.832109	6.772822	0.486170
88	1	0	1.929076	7.838890	0.679201
89	6	0	-0.602317	6.930377	0.836664
90	1	0	-0.504559	7.996010	1.032653
91	6	0	-3.040936	7.101377	1.164577
92	1	0	-2.935792	8.163962	1.366778
93	7	0	2.043555	-5.059210	1.160880
94	6	0	1.134380	-5.621159	0.595024
95	7	0	2.780268	-4.021210	1.011819
96	6	0	4.156114	-4.233416	1.027073
97	6	0	4.764493	-5.499411	0.938012
98	6	0	4.959412	-3.080307	1.078441

99	6	0	6.142745	-5.607466	0.878708
100	1	0	4.145712	-6.390990	0.920354
101	6	0	6.338468	-3.183484	1.005332
102	1	0	4.474881	-2.116585	1.187447
103	6	0	6.911557	-4.446877	0.901635
104	1	0	6.635581	-6.569720	0.809076
105	1	0	6.976169	-2.308366	1.041203
106	7	0	8.367055	-4.561976	0.823676
107	8	0	9.017953	-3.531084	0.826923
108	8	0	8.843939	-5.682045	0.754844
109	6	0	0.172905	-6.707697	0.985042
110	6	0	0.888845	-7.588317	2.026293
111	1	0	0.223623	-8.405397	2.324364
112	1	0	1.804458	-8.021686	1.612154
113	1	0	1.150453	-7.004860	2.912659
114	6	0	-1.085198	-6.093428	1.619863
115	1	0	-1.628253	-5.455916	0.919139
116	1	0	-1.749889	-6.902160	1.942440
117	1	0	-0.819103	-5.494115	2.495203
118	6	0	-0.186139	-7.567448	-0.232105
119	1	0	-0.835463	-8.389327	0.084786
120	1	0	-0.717500	-6.995051	-0.995033
121	1	0	0.712211	-7.996959	-0.687163

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-7.604992	0.162122	-0.408852
2	6	0	-8.148877	-1.120887	-0.727455
3	6	0	-5.337196	-0.758215	-0.619053
4	6	0	-5.889751	-2.050095	-0.936197
5	6	0	-3.070024	-1.686581	-0.796399
6	6	0	-8.474002	1.264823	-0.139589
7	6	0	-5.658670	1.617771	-0.047765
8	6	0	-6.538486	2.724992	0.222898
9	6	0	-3.712096	3.082940	0.284310
10	6	0	-6.201988	0.340566	-0.358533
11	6	0	-3.397521	0.700822	-0.271214
12	6	0	-3.942321	-0.584192	-0.560879
13	6	0	-1.135085	-0.212211	-0.515208
14	6	0	-4.263729	1.800485	-0.006572
15	6	0	-1.455156	2.174058	0.009452
16	6	0	-2.000631	0.884956	-0.247522
17	6	0	0.799851	1.277000	-0.331432
18	6	0	-3.625228	-2.984664	-1.104171
19	6	0	-0.799120	-2.618825	-0.940770
20	6	0	-1.364331	-3.943360	-1.094948
21	6	0	1.456378	-3.520480	-1.398603
22	6	0	-1.682945	-1.509812	-0.742455
23	6	0	1.121329	-1.106671	-0.887813
24	6	0	0.572607	-2.421671	-1.041142
25	6	0	3.355729	-1.960303	-1.480920
26	6	0	0.256814	-0.019095	-0.556743
27	6	0	3.045470	0.403752	-0.791370
28	6	0	2.493799	-0.885864	-1.044377

29	6	0	5.293551	-0.459602	-1.315599
30	6	0	-4.597837	4.189720	0.563458
31	6	0	-1.763055	4.557887	0.576382
32	6	0	-2.657129	5.661608	0.871863
33	6	0	0.187510	6.046707	0.844358
34	6	0	-2.324764	3.268513	0.297816
35	6	0	0.490636	3.654737	0.250047
36	6	0	-0.061091	2.363959	-0.010001
37	6	0	2.739849	2.765710	-0.140021
38	6	0	-0.386772	4.744244	0.562618
39	6	0	2.442844	5.145921	0.486455
40	6	0	1.876735	3.846002	0.206148
41	6	0	4.693787	4.253262	0.085693
42	6	0	2.191838	1.478414	-0.407595
43	6	0	4.982980	1.887546	-0.589173
44	6	0	4.432062	0.614126	-0.895683
45	6	0	7.234778	1.007502	-1.045134
46	6	0	4.131720	2.961281	-0.211359
47	6	0	6.936570	3.361604	-0.341065
48	6	0	6.381329	2.084688	-0.658394
49	6	0	-0.421691	-5.074706	-1.026481
50	1	0	-0.841385	-6.061707	-1.218569
51	6	0	-2.708940	-4.089841	-1.255476
52	1	0	-3.130458	-5.073762	-1.449077
53	6	0	-4.990220	-3.136079	-1.175937
54	1	0	-5.411167	-4.112750	-1.405589
55	6	0	-7.267098	-2.199993	-0.985815
56	1	0	-7.689801	-3.173060	-1.226303
57	6	0	-9.548713	-1.268962	-0.771008

58	1	0	-9.967173	-2.241943	-1.013441
59	6	0	-10.386484	-0.191346	-0.508164
60	1	0	-11.462815	-0.329042	-0.547058
61	6	0	-9.866347	1.058649	-0.195726
62	1	0	-10.530565	1.893614	0.009150
63	6	0	-7.910319	2.526152	0.173561
64	1	0	-8.577915	3.360273	0.378039
65	6	0	-5.960052	3.994500	0.530365
66	1	0	-6.626277	4.828987	0.738241
67	6	0	-4.008705	5.467587	0.861348
68	1	0	-4.673875	6.300736	1.078612
69	6	0	-2.060367	6.953214	1.163928
70	1	0	-2.728656	7.779540	1.391435
71	6	0	0.921180	-4.861117	-1.371120
72	1	0	1.536140	-5.675852	-1.733808
73	6	0	2.776049	-3.259192	-1.670204
74	1	0	3.430637	-4.071778	-1.975886
75	6	0	4.708971	-1.728517	-1.613255
76	1	0	5.364901	-2.539094	-1.925197
77	6	0	6.662409	-0.243653	-1.380757
78	1	0	7.318974	-1.057975	-1.675429
79	6	0	8.624673	1.225429	-1.088872
80	1	0	9.275509	0.403204	-1.371772
81	6	0	9.159664	2.468108	-0.769747
82	1	0	10.234388	2.615604	-0.807332
83	6	0	8.334284	3.524993	-0.404941
84	1	0	8.761435	4.494298	-0.162307
85	6	0	6.069438	4.421405	0.021151
86	1	0	6.499560	5.393874	0.250787

87	6	0	3.807502	5.318525	0.431670
88	1	0	4.233454	6.295840	0.648010
89	6	0	1.541568	6.219030	0.809528
90	1	0	1.965514	7.198293	1.021758
91	6	0	-0.725505	7.133632	1.151944
92	1	0	-0.296463	8.108292	1.369126
93	7	0	0.851237	-5.455583	1.330490
94	6	0	-0.327721	-5.300668	1.089711
95	7	0	1.960068	-5.636218	0.707031
96	6	0	2.981212	-4.750929	0.996908
97	6	0	2.805082	-3.509177	1.640232
98	6	0	4.249686	-5.091656	0.494325
99	6	0	3.861801	-2.622153	1.746032
100	1	0	1.824056	-3.239095	2.019998
101	6	0	5.311635	-4.214226	0.605005
102	1	0	4.367170	-6.056836	0.012137
103	6	0	5.097739	-2.979640	1.212541
104	1	0	3.740476	-1.644315	2.197637
105	1	0	6.293591	-4.452912	0.214538
106	7	0	6.188222	-2.010552	1.236542
107	8	0	7.245977	-2.335440	0.716634
108	8	0	5.977073	-0.922794	1.741848
109	6	0	-1.538525	-5.432422	1.981465
110	6	0	-1.068194	-5.995269	3.333853
111	1	0	-1.930448	-6.096280	4.001259
112	1	0	-0.602207	-6.976737	3.209402
113	1	0	-0.340870	-5.325468	3.800863
114	6	0	-2.174068	-4.051114	2.206262
115	1	0	-2.573523	-3.625987	1.284683

116	1	0	-2.995278	-4.151661	2.923795
117	1	0	-1.440596	-3.352816	2.621857
118	6	0	-2.542738	-6.408081	1.355842
119	1	0	-3.382289	-6.542550	2.045343
120	1	0	-2.937628	-6.028435	0.413010
121	1	0	-2.082935	-7.386214	1.181827

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.311590	4.469605	-0.460489
2	6	0	-6.469519	3.697742	-0.782991
3	6	0	-3.922224	2.453072	-0.649306
4	6	0	-5.091974	1.680877	-0.977357
5	6	0	-2.538538	0.428925	-0.810942
6	6	0	-5.432579	5.869385	-0.202208
7	6	0	-2.889228	4.615106	-0.079263
8	6	0	-3.016336	6.026450	0.175783
9	6	0	-0.463509	4.767143	0.283585
10	6	0	-4.042477	3.846827	-0.397472
11	6	0	-1.505520	2.599584	-0.262546
12	6	0	-2.661729	1.829706	-0.580463
13	6	0	-0.122564	0.580060	-0.438067
14	6	0	-1.624837	3.999016	-0.022202
15	6	0	0.919057	2.755408	0.077169
16	6	0	-0.239727	1.981390	-0.214320

17	6	0	2.306467	0.747569	-0.158195
18	6	0	-3.713134	-0.340072	-1.151731
19	6	0	-1.162675	-1.609429	-0.914085
20	6	0	-2.357363	-2.381414	-1.194300
21	6	0	0.226571	-3.647559	-1.133548
22	6	0	-1.286741	-0.194193	-0.726097
23	6	0	1.266067	-1.435586	-0.662775
24	6	0	0.084202	-2.222506	-0.880444
25	6	0	2.673810	-3.423481	-1.029751
26	6	0	1.143681	-0.032968	-0.419250
27	6	0	3.703830	-1.246185	-0.459280
28	6	0	2.535639	-2.022919	-0.711711
29	6	0	5.109541	-3.244836	-0.804749
30	6	0	-0.595077	6.183685	0.537012
31	6	0	1.969185	4.927415	0.611620
32	6	0	1.829502	6.347812	0.872525
33	6	0	4.411480	5.101330	0.913556
34	6	0	0.795700	4.157131	0.320478
35	6	0	3.352850	2.920863	0.368098
36	6	0	2.186520	2.144502	0.090895
37	6	0	4.743261	0.923605	0.089534
38	6	0	3.219587	4.324234	0.629073
39	6	0	5.799121	3.097486	0.639571
40	6	0	4.615052	2.316326	0.364281
41	6	0	7.191148	1.100350	0.339256
42	6	0	3.580175	0.144310	-0.176160
43	6	0	6.137660	-1.067393	-0.227852
44	6	0	4.977661	-1.844338	-0.497244
45	6	0	7.541029	-3.063664	-0.557662

46	6	0	6.013569	0.318118	0.066017
47	6	0	8.581531	-0.891968	0.020125
48	6	0	7.416685	-1.672669	-0.255349
49	6	0	-2.231374	-3.823883	-1.259010
50	1	0	-3.117951	-4.386692	-1.544127
51	6	0	-3.558905	-1.755426	-1.356412
52	1	0	-4.443761	-2.338639	-1.600061
53	6	0	-4.937466	0.282921	-1.226765
54	1	0	-5.821261	-0.300338	-1.477121
55	6	0	-6.325523	2.311560	-1.036443
56	1	0	-7.210881	1.730141	-1.283664
57	6	0	-7.720375	4.342442	-0.839239
58	1	0	-8.602570	3.758152	-1.085182
59	6	0	-7.829959	5.704632	-0.585854
60	1	0	-8.803584	6.182260	-0.635483
61	6	0	-6.708178	6.462866	-0.271756
62	1	0	-6.804219	7.527282	-0.076287
63	6	0	-4.270487	6.615547	0.112377
64	1	0	-4.369888	7.681201	0.306295
65	6	0	-1.838219	6.771535	0.484538
66	1	0	-1.936104	7.837510	0.677616
67	6	0	0.595961	6.930997	0.835838
68	1	0	0.497272	7.996527	1.031921
69	6	0	3.034269	7.103813	1.165067
70	1	0	2.928193	8.166284	1.367385
71	6	0	-0.994511	-4.464139	-1.260709
72	1	0	-0.898107	-5.413870	-1.780800
73	6	0	1.472927	-4.182121	-1.259981
74	1	0	1.588971	-5.233619	-1.511686

75	6	0	3.923772	-3.995242	-1.073320
76	1	0	4.023520	-5.051786	-1.313733
77	6	0	6.372163	-3.816841	-0.829100
78	1	0	6.474587	-4.874435	-1.061981
79	6	0	8.825925	-3.640095	-0.576180
80	1	0	8.924655	-4.697405	-0.805893
81	6	0	9.953445	-2.873701	-0.305677
82	1	0	10.934469	-3.338505	-0.325577
83	6	0	9.841590	-1.520209	-0.011087
84	1	0	10.728894	-0.929914	0.199891
85	6	0	8.433965	0.485686	0.313321
86	1	0	9.324562	1.074323	0.521806
87	6	0	7.033732	2.490043	0.625330
88	1	0	7.923889	3.079648	0.833191
89	6	0	5.636033	4.498415	0.915697
90	1	0	6.526200	5.086751	1.127852
91	6	0	4.247006	6.518233	1.184368
92	1	0	5.139391	7.098451	1.403379
93	6	0	-1.128518	-5.624134	0.590075
94	7	0	-2.036767	-5.062690	1.157880
95	7	0	-2.773639	-4.024482	1.010972
96	6	0	-0.166543	-6.711273	0.977165
97	6	0	-4.149432	-4.236621	1.028536
98	6	0	-4.952613	-3.083484	1.081346
99	6	0	-4.758021	-5.502605	0.940597
100	6	0	-6.331806	-3.186648	1.010885
101	1	0	-4.467889	-2.119747	1.189383
102	6	0	-6.136390	-5.610639	0.884014
103	1	0	-4.139292	-6.394199	0.921794

104	6	0	-6.905140	-4.450037	0.908423
105	1	0	-6.969418	-2.311512	1.047883
106	1	0	-6.629366	-6.572899	0.815382
107	7	0	-8.360787	-4.565117	0.833464
108	8	0	-8.837852	-5.685205	0.766087
109	8	0	-9.011649	-3.534201	0.837592
110	6	0	-0.881783	-7.594384	2.016788
111	1	0	-1.143293	-7.012916	2.904489
112	1	0	-1.797358	-8.027225	1.602001
113	1	0	-0.216143	-8.411859	2.312849
114	6	0	0.192082	-7.568334	-0.242012
115	1	0	0.723363	-6.994355	-1.003800
116	1	0	0.841343	-8.391029	0.072851
117	1	0	-0.706427	-7.996687	-0.697835
118	6	0	1.091731	-6.098135	1.612712
119	1	0	1.756886	-6.907427	1.932969
120	1	0	1.634163	-5.458726	0.913200
121	1	0	0.825941	-5.500997	2.489630

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.997640	-0.390847	-0.745559
2	6	0	7.600507	0.858402	-1.085718
3	6	0	4.775800	0.628008	-0.971002
4	6	0	5.387426	1.889509	-1.297624

5	6	0	2.554706	1.663257	-1.145887
6	6	0	7.815270	-1.526744	-0.459212
7	6	0	4.988831	-1.745690	-0.350385
8	6	0	5.816752	-2.886989	-0.060986
9	6	0	2.980263	-3.106367	0.034581
10	6	0	5.589014	-0.502753	-0.688417
11	6	0	2.772672	-0.728734	-0.582892
12	6	0	3.374082	0.521203	-0.909622
13	6	0	0.556607	0.306821	-0.745315
14	6	0	3.588037	-1.860225	-0.293069
15	6	0	0.766594	-2.088252	-0.201459
16	6	0	1.370051	-0.835212	-0.503371
17	6	0	-1.449092	-1.065363	-0.427340
18	6	0	3.172957	2.938446	-1.429099
19	6	0	0.339459	2.733978	-1.128224
20	6	0	0.977301	4.027576	-1.281997
21	6	0	-1.889133	3.808676	-1.154596
22	6	0	1.163991	1.567750	-1.022948
23	6	0	-1.662809	1.349126	-0.888157
24	6	0	-1.043587	2.633284	-1.045087
25	6	0	-3.883903	2.372824	-1.173642
26	6	0	-0.844308	0.199419	-0.673860
27	6	0	-3.666224	-0.047859	-0.691650
28	6	0	-3.055393	1.220881	-0.909954
29	6	0	-5.891160	0.971804	-0.999636
30	6	0	3.814300	-4.251191	0.319448
31	6	0	0.968005	-4.480646	0.376156
32	6	0	1.811320	-5.626481	0.660681
33	6	0	-1.046966	-5.874089	0.677283

34	6	0	1.586066	-3.222353	0.078330
35	6	0	-1.244753	-3.464338	0.110640
36	6	0	-0.634940	-2.202588	-0.162049
37	6	0	-3.458470	-2.450746	-0.166912
38	6	0	-0.415671	-4.599493	0.391223
39	6	0	-3.262212	-4.859207	0.383405
40	6	0	-2.639573	-3.583678	0.113494
41	6	0	-5.477453	-3.846675	0.077613
42	6	0	-2.853285	-1.185688	-0.418366
43	6	0	-5.671310	-1.438272	-0.468263
44	6	0	-5.067328	-0.175271	-0.717725
45	6	0	-7.893701	-0.424354	-0.780679
46	6	0	-4.860790	-2.571958	-0.183733
47	6	0	-7.687469	-2.832852	-0.235279
48	6	0	-7.080753	-1.564704	-0.494294
49	6	0	0.153056	5.201336	-1.104521
50	1	0	0.632661	6.170229	-1.206165
51	6	0	2.327554	4.101343	-1.477100
52	1	0	2.800436	5.074832	-1.591065
53	6	0	4.542768	3.021014	-1.520667
54	1	0	5.009894	3.981324	-1.729041
55	6	0	6.770429	1.975153	-1.353013
56	1	0	7.237299	2.925955	-1.601141
57	6	0	9.005358	0.941510	-1.136742
58	1	0	9.467215	1.890384	-1.395577
59	6	0	9.794393	-0.168907	-0.859565
60	1	0	10.875675	-0.083027	-0.904139
61	6	0	9.215346	-1.386893	-0.524146
62	1	0	9.839854	-2.248700	-0.305373

63	6	0	7.196244	-2.754483	-0.120758
64	1	0	7.824746	-3.614859	0.098333
65	6	0	5.183539	-4.122609	0.270984
66	1	0	5.811046	-4.984447	0.487235
67	6	0	3.169933	-5.497174	0.634235
68	1	0	3.797343	-6.359449	0.849892
69	6	0	1.158334	-6.888572	0.960196
70	1	0	1.789692	-7.745752	1.178793
71	6	0	-1.241082	5.131407	-1.035724
72	1	0	-1.810864	5.994829	-1.373623
73	6	0	-3.234148	3.654197	-1.295531
74	1	0	-3.870695	4.524245	-1.442087
75	6	0	-5.250762	2.231101	-1.222630
76	1	0	-5.874795	3.100196	-1.421805
77	6	0	-7.268949	0.823562	-1.028129
78	1	0	-7.894364	1.687248	-1.243190
79	6	0	-9.293137	-0.579525	-0.802807
80	1	0	-9.914387	0.284374	-1.022235
81	6	0	-9.874939	-1.816197	-0.549386
82	1	0	-10.956117	-1.913783	-0.571564
83	6	0	-9.092423	-2.929897	-0.269354
84	1	0	-9.558017	-3.891871	-0.074090
85	6	0	-6.860541	-3.947856	0.047178
86	1	0	-7.329420	-4.909426	0.243729
87	6	0	-4.634526	-4.964217	0.361557
88	1	0	-5.101723	-5.925642	0.563237
89	6	0	-2.408068	-5.980435	0.667772
90	1	0	-2.874992	-6.940131	0.879095
91	6	0	-0.183452	-7.005657	0.965097

92	1	0	-0.655953	-7.959048	1.186318
93	6	0	-1.683084	5.579785	0.959076
94	7	0	-0.645518	5.383401	1.556749
95	7	0	0.598812	5.191437	1.314417
96	6	0	-3.008181	6.138069	1.421307
97	6	0	1.115906	3.965202	1.728788
98	6	0	2.508583	3.817703	1.622964
99	6	0	0.332100	2.863825	2.126385
100	6	0	3.108362	2.592196	1.860445
101	1	0	3.097394	4.679036	1.326898
102	6	0	0.924557	1.634420	2.360989
103	1	0	-0.745413	2.972386	2.208930
104	6	0	2.303946	1.512085	2.206594
105	1	0	4.176536	2.447525	1.742856
106	1	0	0.338648	0.762244	2.626943
107	7	0	2.922695	0.195131	2.361624
108	8	0	2.194844	-0.750662	2.613466
109	8	0	4.129920	0.114673	2.205609
110	6	0	-2.745198	7.028793	2.647621
111	1	0	-2.289437	6.449204	3.454700
112	1	0	-2.073775	7.855037	2.396021
113	1	0	-3.692481	7.445773	3.005546
114	6	0	-3.653190	6.986841	0.319864
115	1	0	-3.917796	6.392100	-0.556843
116	1	0	-4.572498	7.434019	0.710470
117	1	0	-2.988921	7.797699	0.003128
118	6	0	-3.933233	4.977952	1.824541
119	1	0	-4.874371	5.387946	2.206398
120	1	0	-4.156389	4.318332	0.983059

121	1	0	-3.473206	4.380892	2.618040

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.75148800	-0.07933700	0.51195200
2	6	0	9.49713600	1.13617100	0.59255700
3	6	0	6.68430100	1.21479200	0.23453600
4	6	0	7.43884800	2.43692300	0.31503000
5	6	0	4.61728500	2.51244500	-0.03608900
6	6	0	9.41953500	-1.33799200	0.61324500
7	6	0	6.60690600	-1.24779000	0.25269200
8	6	0	7.28435600	-2.51397300	0.35406600
9	6	0	4.46291500	-2.41871100	-0.00496000
10	6	0	7.34985400	-0.03742300	0.33196900
11	6	0	4.54254400	0.04720700	-0.01997300
12	6	0	5.28770300	1.25986100	0.05618700
13	6	0	2.47818900	1.34394100	-0.28453900
14	6	0	5.21117700	-1.20861500	0.07239700
15	6	0	2.40133100	-1.12231700	-0.27574400
16	6	0	3.14683400	0.08949500	-0.20165400
17	6	0	0.33703600	0.17452300	-0.53622500
18	6	0	5.37786400	3.73709200	0.04307000
19	6	0	2.54477200	3.81191200	-0.29890800
20	6	0	3.31527100	5.03778800	-0.22091700
21	6	0	0.46643300	5.12088500	-0.55159800

22	6	0	3.22554400	2.55615800	-0.21040900
23	6	0	0.40861600	2.64028200	-0.53798300
24	6	0	1.16349500	3.85259600	-0.46323500
25	6	0	-1.67473600	3.94453000	-0.77251900
26	6	0	1.08120500	1.38620400	-0.46024400
27	6	0	-1.73083300	1.47145700	-0.77014100
28	6	0	-0.98699200	2.67997100	-0.69579400
29	6	0	-3.81489300	2.76802300	-0.95931600
30	6	0	5.14600100	-3.68728700	0.09712100
31	6	0	2.31476200	-3.59045200	-0.26273500
32	6	0	3.00635100	-4.86050300	-0.15361600
33	6	0	0.16263800	-4.77170200	-0.51917200
34	6	0	3.07280700	-2.37838800	-0.18610100
35	6	0	0.25819700	-2.29129600	-0.54111200
36	6	0	1.00690800	-1.08009900	-0.45932200
37	6	0	-1.80441700	-0.99566000	-0.80115000
38	6	0	0.93593100	-3.54791700	-0.44384800
39	6	0	-1.88836600	-3.46856500	-0.83068300
40	6	0	-1.13114100	-2.24730800	-0.72911500
41	6	0	-3.94619500	-2.17126100	-1.09410700
42	6	0	-1.05939300	0.21679100	-0.70710200
43	6	0	-3.87932100	0.30191300	-0.99546500
44	6	0	-3.13457400	1.50969000	-0.90595600
45	6	0	-5.96585500	1.59749500	-1.04380200
46	6	0	-3.20162400	-0.95104800	-0.96893800
47	6	0	-6.02300700	-0.88682100	-1.18558300
48	6	0	-5.29031200	0.34326500	-1.07740800
49	6	0	2.59695300	6.29596700	-0.32023100
50	1	0	3.17482600	7.21467700	-0.26487000

51	6	0	4.67017000	4.98344500	-0.05724100
52	1	0	5.24328600	5.90621400	0.00154100
53	6	0	6.74420500	3.67780000	0.21361000
54	1	0	7.31732100	4.60026400	0.27440900
55	6	0	8.81597400	2.37132000	0.49074700
56	1	0	9.38955600	3.29351600	0.55239600
57	6	0	10.89392800	1.06502700	0.77289600
58	1	0	11.46320000	1.98837200	0.83430300
59	6	0	11.53670300	-0.16260100	0.87081200
60	1	0	12.61266500	-0.19606700	1.00971700
61	6	0	10.81685100	-1.34975700	0.79309200
62	1	0	11.32825600	-2.30521000	0.87158600
63	6	0	8.66211200	-2.53040400	0.53107600
64	1	0	9.17769800	-3.48488500	0.61033500
65	6	0	6.51284300	-3.71005800	0.27151700
66	1	0	7.02694300	-4.66514700	0.35167900
67	6	0	4.36124400	-4.88777000	0.01750900
68	1	0	4.87446500	-5.84314700	0.10173100
69	6	0	2.21026700	-6.07278200	-0.22595400
70	1	0	2.72768500	-7.02399400	-0.13471800
71	6	0	1.25942900	6.33468200	-0.47512900
72	1	0	0.73786800	7.28540600	-0.54709500
73	6	0	-0.89158200	5.14581500	-0.70063500
74	1	0	-1.40802900	6.10117500	-0.76602400
75	6	0	-3.04970000	3.96392100	-0.90498900
76	1	0	-3.56825700	4.91933100	-0.95849300
77	6	0	-5.21192200	2.77295000	-1.03877400
78	1	0	-5.73380000	3.72484400	-1.09575500
79	6	0	-7.41836500	1.60974400	-0.94277000

80	1	0	-7.95090800	2.45754500	-1.36597400
81	6	0	-8.10215800	0.33785200	-0.93830800
82	1	0	-9.17207300	0.37642800	-1.16127800
83	6	0	-7.44431700	-0.82765800	-1.21890000
84	1	0	-7.99772300	-1.75827600	-1.31005000
85	6	0	-5.33570600	-2.10301700	-1.23010300
86	1	0	-5.90434100	-3.02668100	-1.30964400
87	6	0	-3.25160900	-3.40896600	-1.03881800
88	1	0	-3.82290200	-4.33179900	-1.10637300
89	6	0	-1.18966600	-4.71513100	-0.70359100
90	1	0	-1.76944800	-5.63426500	-0.74475600
91	6	0	0.87452400	-6.03037200	-0.39417700
92	1	0	0.29265800	-6.94692100	-0.44057200
93	7	0	-7.35514700	2.14089800	1.03621500
94	7	0	-7.22469100	3.51871500	1.53874000
95	6	0	-7.68095500	1.08087500	1.51987000
96	6	0	-8.16240300	-0.03886900	1.05789200
97	6	0	-9.30418731	-0.63391991	0.67110850
98	6	0	10.60889243	-0.11566207	0.89182601
99	6	0	-9.18228704	-1.96138114	0.18106213
100	6	0	11.72525445	-0.89064937	0.66469253
101	1	0	10.71699447	0.89946622	1.26429557
102	6	0	10.29812168	-2.73984222	-0.03083414
103	1	0	-8.18425429	-2.34595374	-0.00169024
104	6	0	11.56615284	-2.20693646	0.22541572
105	1	0	12.72429864	-0.51301733	0.85101672
106	1	0	10.21736673	-3.76102384	-0.38442511
107	7	0	12.73469309	-3.04555125	0.08280950
108	8	0	12.56625630	-4.22805592	-0.19240983

109	8	0	13.83338536	-2.54289964	0.27262052
110	6	0	-7.88802200	3.53209300	2.93196700
111	1	0	-7.36590100	2.85822500	3.60856500
112	1	0	-7.85430700	4.54193800	3.34257200
113	1	0	-8.92729400	3.21425200	2.85963400
114	6	0	-5.70744000	3.76942100	1.65496700
115	1	0	-5.30751600	3.44522000	0.70222800
116	1	0	-5.48234200	4.82301400	1.82827500
117	1	0	-5.27436500	3.19222600	2.47285400
118	6	0	-7.90576300	4.59948700	0.69267700
119	1	0	-7.73589300	5.56376100	1.16883700
120	1	0	-7.50843600	4.64900000	-0.31984300
121	1	0	-8.97915600	4.42068100	0.63370400

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.75148800	-0.07933700	0.51195200
2	6	0	9.49713600	1.13617100	0.59255700
3	6	0	6.68430100	1.21479200	0.23453600
4	6	0	7.43884800	2.43692300	0.31503000
5	6	0	4.61728500	2.51244500	-0.03608900
6	6	0	9.41953500	-1.33799200	0.61324500
7	6	0	6.60690600	-1.24779000	0.25269200
8	6	0	7.28435600	-2.51397300	0.35406600

9	6	0	4.46291500	-2.41871100	-0.00496000
10	6	0	7.34985400	-0.03742300	0.33196900
11	6	0	4.54254400	0.04720700	-0.01997300
12	6	0	5.28770300	1.25986100	0.05618700
13	6	0	2.47818900	1.34394100	-0.28453900
14	6	0	5.21117700	-1.20861500	0.07239700
15	6	0	2.40133100	-1.12231700	-0.27574400
16	6	0	3.14683400	0.08949500	-0.20165400
17	6	0	0.33703600	0.17452300	-0.53622500
18	6	0	5.37786400	3.73709200	0.04307000
19	6	0	2.54477200	3.81191200	-0.29890800
20	6	0	3.31527100	5.03778800	-0.22091700
21	6	0	0.46643300	5.12088500	-0.55159800
22	6	0	3.22554400	2.55615800	-0.21040900
23	6	0	0.40861600	2.64028200	-0.53798300
24	6	0	1.16349500	3.85259600	-0.46323500
25	6	0	-1.67473600	3.94453000	-0.77251900
26	6	0	1.08120500	1.38620400	-0.46024400
27	6	0	-1.73083300	1.47145700	-0.77014100
28	6	0	-0.98699200	2.67997100	-0.69579400
29	6	0	-3.81489300	2.76802300	-0.95931600
30	6	0	5.14600100	-3.68728700	0.09712100
31	6	0	2.31476200	-3.59045200	-0.26273500
32	6	0	3.00635100	-4.86050300	-0.15361600
33	6	0	0.16263800	-4.77170200	-0.51917200
34	6	0	3.07280700	-2.37838800	-0.18610100
35	6	0	0.25819700	-2.29129600	-0.54111200
36	6	0	1.00690800	-1.08009900	-0.45932200
37	6	0	-1.80441700	-0.99566000	-0.80115000

38	6	0	0.93593100	-3.54791700	-0.44384800
39	6	0	-1.88836600	-3.46856500	-0.83068300
40	6	0	-1.13114100	-2.24730800	-0.72911500
41	6	0	-3.94619500	-2.17126100	-1.09410700
42	6	0	-1.05939300	0.21679100	-0.70710200
43	6	0	-3.87932100	0.30191300	-0.99546500
44	6	0	-3.13457400	1.50969000	-0.90595600
45	6	0	-5.96585500	1.59749500	-1.04380200
46	6	0	-3.20162400	-0.95104800	-0.96893800
47	6	0	-6.02300700	-0.88682100	-1.18558300
48	6	0	-5.29031200	0.34326500	-1.07740800
49	6	0	2.59695300	6.29596700	-0.32023100
50	1	0	3.17482600	7.21467700	-0.26487000
51	6	0	4.67017000	4.98344500	-0.05724100
52	1	0	5.24328600	5.90621400	0.00154100
53	6	0	6.74420500	3.67780000	0.21361000
54	1	0	7.31732100	4.60026400	0.27440900
55	6	0	8.81597400	2.37132000	0.49074700
56	1	0	9.38955600	3.29351600	0.55239600
57	6	0	10.89392800	1.06502700	0.77289600
58	1	0	11.46320000	1.98837200	0.83430300
59	6	0	11.53670300	-0.16260100	0.87081200
60	1	0	12.61266500	-0.19606700	1.00971700
61	6	0	10.81685100	-1.34975700	0.79309200
62	1	0	11.32825600	-2.30521000	0.87158600
63	6	0	8.66211200	-2.53040400	0.53107600
64	1	0	9.17769800	-3.48488500	0.61033500
65	6	0	6.51284300	-3.71005800	0.27151700
66	1	0	7.02694300	-4.66514700	0.35167900

67	6	0	4.36124400	-4.88777000	0.01750900
68	1	0	4.87446500	-5.84314700	0.10173100
69	6	0	2.21026700	-6.07278200	-0.22595400
70	1	0	2.72768500	-7.02399400	-0.13471800
71	6	0	1.25942900	6.33468200	-0.47512900
72	1	0	0.73786800	7.28540600	-0.54709500
73	6	0	-0.89158200	5.14581500	-0.70063500
74	1	0	-1.40802900	6.10117500	-0.76602400
75	6	0	-3.04970000	3.96392100	-0.90498900
76	1	0	-3.56825700	4.91933100	-0.95849300
77	6	0	-5.21192200	2.77295000	-1.03877400
78	1	0	-5.73380000	3.72484400	-1.09575500
79	6	0	-7.41836500	1.60974400	-0.94277000
80	1	0	-7.95090800	2.45754500	-1.36597400
81	6	0	-8.10215800	0.33785200	-0.93830800
82	1	0	-9.17207300	0.37642800	-1.16127800
83	6	0	-7.44431700	-0.82765800	-1.21890000
84	1	0	-7.99772300	-1.75827600	-1.31005000
85	6	0	-5.33570600	-2.10301700	-1.23010300
86	1	0	-5.90434100	-3.02668100	-1.30964400
87	6	0	-3.25160900	-3.40896600	-1.03881800
88	1	0	-3.82290200	-4.33179900	-1.10637300
89	6	0	-1.18966600	-4.71513100	-0.70359100
90	1	0	-1.76944800	-5.63426500	-0.74475600
91	6	0	0.87452400	-6.03037200	-0.39417700
92	1	0	0.29265800	-6.94692100	-0.44057200
93	7	0	-7.35514700	2.14089800	1.03621500
94	7	0	-7.22469100	3.51871500	1.53874000
95	6	0	-7.68095500	1.08087500	1.51987000

96	6	0	-8.16240300	-0.03886900	1.05789200
97	6	0	-7.97240911	-1.36972737	1.06665555
98	6	0	-6.81182950	-2.02426621	1.56081820
99	6	0	-8.92739164	-2.14212774	0.35351850
100	6	0	-6.60417469	-3.36643376	1.32860101
101	1	0	-6.07398512	-1.44592453	2.11037407
102	6	0	-8.71121662	-3.47983253	0.10897217
103	1	0	-9.81964865	-1.64069839	-0.00677294
104	6	0	-7.54299641	-4.08506087	0.58490887
105	1	0	-5.71176469	-3.87082222	1.68160049
106	1	0	-9.42212519	-4.07508557	-0.45195801
107	7	0	-7.27278983	-5.46754961	0.26116374
108	8	0	-8.05120104	-6.04780117	-0.48704616
109	8	0	-6.26537147	-5.98337095	0.72468090
110	6	0	-7.88802200	3.53209300	2.93196700
111	1	0	-7.36590100	2.85822500	3.60856500
112	1	0	-7.85430700	4.54193800	3.34257200
113	1	0	-8.92729400	3.21425200	2.85963400
114	6	0	-5.70744000	3.76942100	1.65496700
115	1	0	-5.30751600	3.44522000	0.70222800
116	1	0	-5.48234200	4.82301400	1.82827500
117	1	0	-5.27436500	3.19222600	2.47285400
118	6	0	-7.90576300	4.59948700	0.69267700
119	1	0	-7.73589300	5.56376100	1.16883700
120	1	0	-7.50843600	4.64900000	-0.31984300
121	1	0	-8.97915600	4.42068100	0.63370400

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.227402	0.853772	0.578550
2	6	0	9.751628	2.183168	0.551172
3	6	0	6.969883	1.741922	0.197173
4	6	0	7.503372	3.078735	0.168469
5	6	0	4.711883	2.632235	-0.183773
6	6	0	10.102385	-0.257577	0.784012
7	6	0	7.317102	-0.685676	0.429487
8	6	0	8.204196	-1.801349	0.636307
9	6	0	5.409130	-2.228357	0.283708
10	6	0	7.839843	0.637475	0.402848
11	6	0	5.064503	0.203487	0.051889
12	6	0	5.587535	1.529170	0.025952
13	6	0	2.810109	1.093466	-0.321902
14	6	0	5.938059	-0.903396	0.259781
15	6	0	3.157793	-1.337158	-0.088264
16	6	0	3.681026	-0.011550	-0.110491
17	6	0	0.903793	-0.445495	-0.451160
18	6	0	5.251330	3.972035	-0.215088
19	6	0	2.450936	3.524777	-0.563848
20	6	0	2.999704	4.867421	-0.599230
21	6	0	0.185668	4.427514	-0.944796
22	6	0	3.336506	2.419608	-0.350064
23	6	0	0.551506	1.984305	-0.692152
24	6	0	1.087335	3.312031	-0.727924
25	6	0	-1.716748	2.883125	-1.065832

26	6	0	1.426267	0.878971	-0.479245
27	6	0	-1.352237	0.446892	-0.807034
28	6	0	-0.825805	1.768352	-0.849980
29	6	0	-3.619415	1.341157	-1.172067
30	6	0	6.302966	-3.345141	0.490067
31	6	0	3.500731	-3.774220	0.140417
32	6	0	4.404074	-4.891444	0.344799
33	6	0	1.592149	-5.331041	-0.002105
34	6	0	4.037079	-2.444033	0.118766
35	6	0	1.249258	-2.880040	-0.224339
36	6	0	1.777502	-1.551447	-0.244961
37	6	0	-1.006234	-1.986975	-0.575758
38	6	0	2.139031	-3.986807	-0.023806
39	6	0	-0.661842	-4.434249	-0.363566
40	6	0	-0.123368	-3.092200	-0.383209
41	6	0	-2.919327	-3.540413	-0.714165
42	6	0	-0.480630	-0.659387	-0.602613
43	6	0	-3.263176	-1.090868	-0.907950
44	6	0	-2.739112	0.230105	-0.954856
45	6	0	-5.523044	-0.193788	-1.220877
46	6	0	-2.385493	-2.198263	-0.727672
47	6	0	-5.180009	-2.643400	-1.045428
48	6	0	-4.653900	-1.301279	-1.040583
49	6	0	2.078571	5.968313	-0.818729
50	1	0	2.489843	6.973816	-0.849545
51	6	0	4.340294	5.062492	-0.430604
52	1	0	4.745188	6.071875	-0.459790
53	6	0	6.603549	4.165666	-0.042812
54	1	0	7.007537	5.175311	-0.068577

55	6	0	8.867355	3.267932	0.344384
56	1	0	9.272324	4.277207	0.321956
57	6	0	11.137745	2.368923	0.731446
58	1	0	11.539001	3.378339	0.710753
59	6	0	11.979607	1.283216	0.931015
60	1	0	13.043873	1.448553	1.067976
61	6	0	11.477604	-0.013779	0.957861
62	1	0	12.145789	-0.855925	1.114955
63	6	0	9.559703	-1.566614	0.806484
64	1	0	10.231628	-2.407598	0.962900
65	6	0	7.649236	-3.117083	0.657801
66	1	0	8.320836	-3.958698	0.812666
67	6	0	5.740018	-4.667841	0.510412
68	1	0	6.412837	-5.509003	0.663581
69	6	0	3.835119	-6.227486	0.364777
70	1	0	4.512996	-7.063195	0.517038
71	6	0	0.757678	5.762071	-0.981566
72	1	0	0.081888	6.597311	-1.145072
73	6	0	-1.151821	4.203955	-1.105467
74	1	0	-1.823137	5.044524	-1.267898
75	6	0	-3.067140	2.652899	-1.223448
76	1	0	-3.739192	3.492819	-1.387167
77	6	0	-4.987469	1.101358	-1.312290
78	1	0	-5.661005	1.939650	-1.477003
79	6	0	-6.933802	-0.420643	-1.266075
80	1	0	-7.574177	0.412101	-1.545515
81	6	0	-7.454936	-1.745860	-1.338706
82	1	0	-8.390442	-1.897212	-1.871836
83	6	0	-6.536244	-2.838579	-1.272156

84	1	0	-6.900035	-3.853845	-1.408988
85	6	0	-4.277785	-3.732227	-0.883069
86	1	0	-4.676919	-4.744519	-0.886380
87	6	0	-2.013070	-4.628769	-0.528254
88	1	0	-2.414393	-5.639731	-0.514119
89	6	0	0.251846	-5.526238	-0.167321
90	1	0	-0.151724	-6.536393	-0.148652
91	6	0	2.514660	-6.433859	0.201076
92	1	0	2.104316	-7.440045	0.219534
93	7	0	-8.212653	-0.937992	1.075057
94	7	0	-7.351898	0.012794	0.943424
95	6	0	-8.519350	-1.932844	0.453149
96	6	0	-9.241233	-3.205746	0.778863
97	6	0	-7.844715	1.307644	1.077613
98	6	0	-6.882933	2.333463	1.121503
99	6	0	-9.211983	1.638356	1.110512
100	6	0	-7.273694	3.659723	1.169382
101	1	0	-5.833943	2.056740	1.127718
102	6	0	-9.606670	2.963816	1.172204
103	1	0	-9.954335	0.846728	1.091421
104	6	0	-8.633562	3.957829	1.190985
105	1	0	-6.550264	4.465370	1.206357
106	1	0	-10.652539	3.245198	1.199430
107	7	0	-9.053681	5.356364	1.244846
108	8	0	-10.250425	5.588207	1.283425
109	8	0	-8.182858	6.209838	1.244171
110	6	0	-9.841749	-3.830786	-0.485077
111	1	0	-10.410123	-4.724590	-0.210504
112	1	0	-10.522872	-3.134153	-0.984222

113	1	0	-9.069983	-4.132731	-1.198651
114	6	0	-10.371659	-2.849988	1.760767
115	1	0	-9.965787	-2.408330	2.674418
116	1	0	-11.072318	-2.139582	1.311757
117	1	0	-10.921428	-3.759949	2.022305
118	6	0	-8.259125	-4.178636	1.451483
119	1	0	-8.783310	-5.108393	1.697535
120	1	0	-7.417852	-4.416637	0.794998
121	1	0	-7.860698	-3.746617	2.373768

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.567304	-0.565741	0.079241
2	6	0	10.377592	0.607899	-0.000442
3	6	0	7.551339	0.822410	-0.082222
4	6	0	8.370092	2.002061	-0.161529
5	6	0	5.534620	2.212868	-0.244347
6	6	0	10.178694	-1.851426	0.201435
7	6	0	7.348915	-1.624528	0.120211
8	6	0	7.971438	-2.917998	0.245037
9	6	0	5.133326	-2.687640	0.162749
10	6	0	8.158252	-0.455010	0.039826
11	6	0	5.337143	-0.235920	-0.042966
12	6	0	6.145769	0.935538	-0.119597
13	6	0	3.325685	1.153001	-0.204865

14	6	0	5.949082	-1.517507	0.084400
15	6	0	3.122212	-1.297790	-0.002533
16	6	0	3.933766	-0.125366	-0.074332
17	6	0	1.111275	0.092598	-0.164692
18	6	0	6.359256	3.395080	-0.323415
19	6	0	3.513473	3.605570	-0.407567
20	6	0	4.347830	4.788739	-0.487963
21	6	0	1.488191	5.007977	-0.573543
22	6	0	4.134792	2.323975	-0.280136
23	6	0	1.309675	2.542046	-0.365287
24	6	0	2.126006	3.712764	-0.444931
25	6	0	-0.719280	3.939337	-0.528867
26	6	0	1.919040	1.263979	-0.235553
27	6	0	-0.897295	1.482919	-0.320734
28	6	0	-0.094134	2.649408	-0.399618
29	6	0	-2.920790	2.872710	-0.475486
30	6	0	5.762087	-3.983274	0.289517
31	6	0	2.916988	-3.753535	0.203393
32	6	0	3.554369	-5.050985	0.330592
33	6	0	0.698593	-4.830420	0.237076
34	6	0	3.740432	-2.580772	0.127673
35	6	0	0.906697	-2.361952	0.034987
36	6	0	1.724517	-1.188086	-0.034128
37	6	0	-1.107640	-0.971826	-0.135844
38	6	0	1.534127	-3.646393	0.162836
39	6	0	-1.311891	-3.437137	0.059769
40	6	0	-0.483649	-2.253314	-0.008213
41	6	0	-3.328374	-2.049666	-0.134140
42	6	0	-0.290429	0.203764	-0.198701

43	6	0	-3.117521	0.421887	-0.300856
44	6	0	-2.309456	1.592309	-0.355388
45	6	0	-5.117794	1.814990	-0.375870
46	6	0	-2.498403	-0.862626	-0.189451
47	6	0	-5.349857	-0.665938	-0.398514
48	6	0	-4.517772	0.539200	-0.345239
49	6	0	3.686648	6.075254	-0.613940
50	1	0	4.311948	6.961943	-0.674571
51	6	0	5.707791	4.669599	-0.445754
52	1	0	6.328931	5.560649	-0.505581
53	6	0	7.731292	3.270386	-0.281670
54	1	0	8.352568	4.161212	-0.340684
55	6	0	9.753788	1.869608	-0.119241
56	1	0	10.376072	2.759802	-0.177699
57	6	0	11.782120	0.467226	0.043142
58	1	0	12.400694	1.358471	-0.015392
59	6	0	12.366439	-0.784676	0.160363
60	1	0	13.447878	-0.872277	0.192517
61	6	0	11.581205	-1.933142	0.239363
62	1	0	12.049126	-2.909172	0.333197
63	6	0	9.353798	-3.002893	0.281585
64	1	0	9.826040	-3.978136	0.376200
65	6	0	7.134286	-4.072418	0.326491
66	1	0	7.605832	-5.047907	0.421658
67	6	0	4.915404	-5.142041	0.370472
68	1	0	5.387779	-6.117240	0.466167
69	6	0	2.698954	-6.221697	0.409237
70	1	0	3.177148	-7.192735	0.505439
71	6	0	2.344149	6.178037	-0.655611

72	1	0	1.866384	7.149298	-0.752178
73	6	0	0.125082	5.097623	-0.612161
74	1	0	-0.347217	6.072767	-0.709547
75	6	0	-2.099486	4.024279	-0.564254
76	1	0	-2.572670	4.999238	-0.658061
77	6	0	-4.331770	2.946979	-0.481172
78	1	0	-4.800913	3.925153	-0.562597
79	6	0	-6.618195	1.911365	-0.253504
80	1	0	-6.955009	2.857979	-0.701293
81	6	0	-7.376807	0.742313	-0.899011
82	1	0	-7.591928	0.926854	-1.958117
83	6	0	-6.678766	-0.571383	-0.678724
84	1	0	-7.278887	-1.474468	-0.759101
85	6	0	-4.696013	-1.934324	-0.234874
86	1	0	-5.311027	-2.830907	-0.227584
87	6	0	-2.679569	-3.317804	-0.000872
88	1	0	-3.298349	-4.211092	0.045095
89	6	0	-0.659751	-4.711800	0.186205
90	1	0	-1.281129	-5.603107	0.239831
91	6	0	1.357240	-6.117955	0.363756
92	1	0	0.730353	-7.003741	0.420934
93	6	0	-7.246079	1.859798	1.157716
94	6	0	-6.728836	2.510249	2.421694
95	7	0	-8.381779	1.269961	1.140626
96	7	0	-8.633483	0.787077	-0.127306
97	6	0	-9.685156	-0.086813	-0.315388
98	6	0	-10.658473	-0.268884	0.687153
99	6	0	-9.817783	-0.777128	-1.536002
100	6	0	-11.726435	-1.118731	0.471053

101	1	0	-10.550420	0.260668	1.624750
102	6	0	-10.888396	-1.627990	-1.747598
103	1	0	-9.079941	-0.649562	-2.320094
104	6	0	-11.833303	-1.793435	-0.742309
105	1	0	-12.482007	-1.273530	1.231858
106	1	0	-11.001202	-2.167613	-2.680110
107	7	0	-12.955855	-2.695840	-0.962273
108	8	0	-13.017289	-3.275997	-2.034260
109	8	0	-13.769524	-2.822023	-0.062067
110	6	0	-7.761448	2.346781	3.542627
111	1	0	-7.385429	2.824377	4.453248
112	1	0	-8.715230	2.808006	3.271842
113	1	0	-7.948433	1.290442	3.753884
114	6	0	-5.410523	1.846924	2.861406
115	1	0	-5.541488	0.766267	2.980712
116	1	0	-4.600509	2.019854	2.148501
117	1	0	-5.103325	2.262771	3.827378
118	6	0	-6.498053	4.008269	2.167552
119	1	0	-7.423275	4.498452	1.845714
120	1	0	-6.160417	4.489444	3.091753
121	1	0	-5.729543	4.175053	1.408190

TsC

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.398993	-0.207380	-0.762567

2	6	0	-7.953726	-1.483961	-1.093123
3	6	0	-5.136366	-1.189532	-0.765654
4	6	0	-5.709147	-2.469989	-1.122589
5	6	0	-2.886706	-2.187626	-0.759891
6	6	0	-8.257288	0.922093	-0.595545
7	6	0	-5.451526	1.207857	-0.303103
8	6	0	-6.318443	2.345842	-0.147358
9	6	0	-3.500663	2.634037	0.117658
10	6	0	-6.000677	-0.060810	-0.605697
11	6	0	-3.197115	0.219071	-0.250706
12	6	0	-3.759146	-1.056440	-0.582696
13	6	0	-0.967794	-0.861195	0.133442
14	6	0	-4.053059	1.357962	-0.156839
15	6	0	-1.259834	1.644452	0.102013
16	6	0	-1.820998	0.355530	-0.015641
17	6	0	0.989907	0.724791	-0.246425
18	6	0	-3.466281	-3.461822	-1.144134
19	6	0	-0.663673	-3.184780	-0.783382
20	6	0	-1.241855	-4.470702	-1.123975
21	6	0	1.588350	-4.118860	-1.145307
22	6	0	-1.530613	-2.084565	-0.516564
23	6	0	1.285074	-1.698132	-0.650888
24	6	0	0.719360	-3.008779	-0.808904
25	6	0	3.502549	-2.602075	-1.258034
26	6	0	0.479964	-0.619169	-0.155963
27	6	0	3.197201	-0.173882	-0.854889
28	6	0	2.639258	-1.488930	-0.929719
29	6	0	5.432349	-1.097461	-1.331252
30	6	0	-4.373399	3.778921	0.258577

31	6	0	-1.536935	4.092736	0.356310
32	6	0	-2.419214	5.232051	0.535939
33	6	0	0.421161	5.590113	0.429995
34	6	0	-2.109832	2.786475	0.197763
35	6	0	0.699555	3.143289	0.074417
36	6	0	0.150906	1.832036	0.012998
37	6	0	2.913553	2.238715	-0.423459
38	6	0	-0.162730	4.267035	0.302809
39	6	0	2.650226	4.662537	0.006016
40	6	0	2.077398	3.340742	-0.105659
41	6	0	4.870648	3.745687	-0.477172
42	6	0	2.355725	0.929137	-0.518898
43	6	0	5.134608	1.325809	-0.917067
44	6	0	4.570530	0.024312	-1.054026
45	6	0	7.375760	0.393957	-1.334008
46	6	0	4.299612	2.431137	-0.611440
47	6	0	7.091492	2.818840	-0.927878
48	6	0	6.528806	1.513296	-1.064728
49	6	0	-0.344676	-5.595658	-1.315013
50	1	0	-0.786602	-6.573380	-1.486927
51	6	0	-2.592216	-4.588451	-1.279084
52	1	0	-3.027126	-5.553184	-1.531109
53	6	0	-4.825999	-3.576154	-1.304191
54	1	0	-5.253336	-4.541356	-1.567183
55	6	0	-7.076253	-2.588315	-1.272307
56	1	0	-7.501534	-3.553657	-1.537927
57	6	0	-9.342051	-1.602344	-1.238441
58	1	0	-9.765152	-2.570997	-1.489951
59	6	0	-10.175530	-0.496084	-1.065260

60	1	0	-11.248678	-0.612677	-1.182057
61	6	0	-9.651091	0.745345	-0.750999
62	1	0	-10.306133	1.602480	-0.622134
63	6	0	-7.689084	2.177643	-0.287876
64	1	0	-8.346911	3.035222	-0.165412
65	6	0	-5.732724	3.615425	0.139431
66	1	0	-6.389396	4.475862	0.247401
67	6	0	-3.772234	5.061869	0.499767
68	1	0	-4.428260	5.920382	0.627083
69	6	0	-1.810662	6.536296	0.727667
70	1	0	-2.471317	7.382112	0.898616
71	6	0	0.990751	-5.431057	-1.315224
72	1	0	1.657219	-6.271786	-1.488196
73	6	0	2.924694	-3.912752	-1.331055
74	1	0	3.576806	-4.752180	-1.563120
75	6	0	4.850101	-2.394521	-1.440421
76	1	0	5.502786	-3.241279	-1.643606
77	6	0	6.796741	-0.895618	-1.454557
78	1	0	7.446137	-1.748032	-1.639646
79	6	0	8.758525	0.604712	-1.464849
80	1	0	9.403661	-0.245792	-1.666328
81	6	0	9.299870	1.882064	-1.338348
82	1	0	10.370913	2.023308	-1.444597
83	6	0	8.486509	2.974106	-1.074933
84	1	0	8.917002	3.966455	-0.972666
85	6	0	6.239444	3.910016	-0.642002
86	1	0	6.673320	4.902018	-0.538654
87	6	0	4.003052	4.836699	-0.171885
88	1	0	4.433096	5.831335	-0.078581

89	6	0	1.768178	5.759481	0.297819
90	1	0	2.198729	6.753873	0.393686
91	6	0	-0.475804	6.704591	0.678315
92	1	0	-0.035314	7.689455	0.808379
93	6	0	-1.072830	-1.260187	1.875827
94	7	0	0.028700	-1.145027	2.445245
95	7	0	1.161491	-0.658610	2.060934
96	6	0	2.251415	-1.508087	2.155582
97	6	0	3.520289	-0.907945	2.069823
98	6	0	2.142655	-2.911741	2.172307
99	6	0	4.651095	-1.682801	1.894473
100	1	0	3.579077	0.176125	2.082092
101	6	0	3.270934	-3.693989	1.994257
102	1	0	1.163104	-3.371552	2.263360
103	6	0	4.501727	-3.065986	1.822821
104	1	0	5.631634	-1.241012	1.761159
105	1	0	3.209661	-4.773726	1.930209
106	7	0	5.656035	-3.874295	1.440775
107	8	0	5.508743	-5.083746	1.369252
108	8	0	6.696433	-3.290460	1.180532
109	6	0	-2.308188	-1.642435	2.721139
110	6	0	-1.789506	-1.909121	4.151656
111	1	0	-1.061329	-2.725056	4.164879
112	1	0	-1.315156	-1.021188	4.576249
113	1	0	-2.639234	-2.189527	4.781607
114	6	0	-3.337195	-0.499697	2.823769
115	1	0	-3.984232	-0.438735	1.949466
116	1	0	-3.977655	-0.690553	3.691232
117	1	0	-2.849590	0.470408	2.968618

118	6	0	-2.994309	-2.937710	2.242461
119	1	0	-3.539035	-3.373613	3.086360
120	1	0	-3.718010	-2.761867	1.446963
121	1	0	-2.265792	-3.678519	1.893244

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.200790	-0.867021	-0.721568
2	6	0	0.581998	-2.141119	-0.787367
3	6	0	-1.010148	0.178431	-0.404757
4	6	0	-1.617145	-1.096426	-0.427606
5	6	0	-3.204474	1.224735	-0.031148
6	6	0	2.601704	-0.752415	-0.822200
7	6	0	1.000353	1.582762	-0.590844
8	6	0	2.407494	1.706245	-0.788151
9	6	0	0.796264	4.046064	-0.502687
10	6	0	0.396810	0.308054	-0.567035
11	6	0	-1.197972	2.630801	-0.244667
12	6	0	-1.811167	1.347461	-0.224705
13	6	0	-3.397634	3.672582	0.149363
14	6	0	0.192529	2.755556	-0.447916
15	6	0	-1.406641	5.079392	-0.098565
16	6	0	-2.004135	3.800721	-0.065212
17	6	0	-3.822929	-0.058202	-0.036045
18	6	0	-4.001989	2.394411	0.166412

19	6	0	-4.200646	4.850958	0.346159
20	6	0	-3.569215	6.123177	0.309238
21	1	0	-4.179478	7.011756	0.454952
22	6	0	-2.217334	6.254677	0.090551
23	6	0	-0.012204	5.206758	-0.323810
24	6	0	2.191060	4.185037	-0.736942
25	6	0	3.009308	2.988154	-0.914004
26	6	0	3.210518	0.531037	-0.880376
27	6	0	3.408869	-1.937183	-0.942450
28	6	0	2.801669	-3.153825	-1.116268
29	1	0	3.406651	-4.040931	-1.290140
30	6	0	1.385794	-3.308653	-1.031356
31	6	0	-0.817916	-2.262026	-0.642673
32	6	0	-3.023605	-1.228712	-0.252425
33	6	0	4.866860	-1.797242	-0.871140
34	6	0	4.606933	0.641255	-1.115445
35	6	0	0.772396	-4.548723	-1.125360
36	6	0	-1.432144	-3.537890	-0.711470
37	6	0	-5.397428	2.269855	0.378094
38	6	0	0.579085	6.498983	-0.368805
39	6	0	-1.578031	7.548324	0.042348
40	6	0	-5.565529	4.715810	0.564440
41	6	0	-0.622036	-4.701029	-0.964084
42	6	0	5.441239	-0.542574	-1.107890
43	6	0	-0.250033	7.662282	-0.177689
44	6	0	-6.190897	3.453231	0.588033
45	1	0	1.377224	-5.433157	-1.312731
46	1	0	0.224723	8.639117	-0.215847
47	1	0	-2.197074	8.429679	0.186518

48	1	0	-6.172062	5.605250	0.718931
49	6	0	1.951187	6.603022	-0.592895
50	6	0	4.373650	3.051603	-1.217427
51	6	0	2.735791	5.474374	-0.771169
52	6	0	5.148943	1.907164	-1.323114
53	1	0	6.207329	1.992882	-1.553813
54	6	0	-7.564210	3.318720	0.808854
55	6	0	-6.009624	0.996293	0.382548
56	6	0	-5.211608	-0.179471	0.163621
57	6	0	-3.629054	-2.499743	-0.291213
58	6	0	-2.827664	-3.668869	-0.532872
59	6	0	-5.035836	-2.629730	-0.094856
60	6	0	-1.238550	-5.952339	-1.033086
61	6	0	-2.617360	-6.102473	-0.852078
62	6	0	-3.430182	-4.950484	-0.593151
63	6	0	-8.185274	2.066681	0.822623
64	6	0	-7.405368	0.883963	0.600745
65	6	0	-5.828965	-1.465625	0.145635
66	6	0	-3.232228	-7.381569	-0.919303
67	6	0	-4.835917	-5.105288	-0.401115
68	6	0	-5.647405	-3.913212	-0.134055
69	6	0	-7.229426	-1.588985	0.359400
70	6	0	-8.042398	-0.393114	0.604389
71	6	0	-9.582039	1.942893	1.051976
72	6	0	-10.173438	0.707543	1.059799
73	1	0	-11.240087	0.612319	1.237200
74	6	0	-9.409118	-0.453541	0.836637
75	6	0	-7.788430	-2.863890	0.324781
76	6	0	-7.020306	-3.992154	0.084567

77	6	0	-5.381665	-6.378894	-0.477514
78	6	0	-4.583672	-7.509301	-0.735771
79	1	0	-5.052713	-8.486782	-0.790399
80	1	0	-7.522460	-4.952187	0.070703
81	1	0	-10.164640	2.844095	1.221303
82	1	0	-8.164678	4.210447	0.973514
83	1	0	-0.631939	-6.833275	-1.229983
84	1	0	4.852470	4.010841	-1.374978
85	1	0	-9.922145	-1.407699	0.852502
86	1	0	-8.851632	-3.000395	0.482719
87	1	0	-2.610609	-8.249596	-1.120408
88	1	0	-6.445944	-6.530180	-0.342424
89	1	0	5.444508	-2.684943	-1.119540
90	1	0	6.440833	-0.464035	-1.523195
91	6	0	5.187058	-2.002083	1.280708
92	1	0	2.409341	7.588040	-0.623749
93	1	0	3.799295	5.611110	-0.927655
94	7	0	5.985912	-1.114909	1.483624
95	7	0	6.505384	-0.114218	0.870791
96	6	0	4.457419	-2.942714	2.202462
97	6	0	7.894999	-0.164450	0.735362
98	6	0	8.508953	0.971462	0.180019
99	6	0	8.685014	-1.274668	1.083466
100	6	0	9.873576	0.996395	-0.043775
101	1	0	7.889982	1.832821	-0.046200
102	6	0	10.053569	-1.250896	0.872414
103	1	0	8.217756	-2.147818	1.526628
104	6	0	10.629508	-0.119179	0.305854
105	1	0	10.366067	1.862244	-0.469268

106	1	0	10.683136	-2.092278	1.135705
107	7	0	12.074218	-0.096057	0.082097
108	8	0	12.713502	-1.083156	0.403702
109	8	0	12.553523	0.908676	-0.414517
110	6	0	5.158192	-2.879909	3.571665
111	1	0	6.211846	-3.163388	3.488286
112	1	0	5.103140	-1.871638	3.990443
113	1	0	4.664712	-3.574898	4.258955
114	6	0	4.527356	-4.375445	1.663316
115	1	0	4.033577	-5.049698	2.370405
116	1	0	4.021165	-4.464998	0.701274
117	1	0	5.566545	-4.700636	1.548915
118	6	0	2.997412	-2.486683	2.363637
119	1	0	2.431616	-2.590441	1.436403
120	1	0	2.520347	-3.110514	3.126944
121	1	0	2.948512	-1.443676	2.690562

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.381949	-1.773725	-0.881612
2	6	0	0.435215	-2.825993	-0.846207
3	6	0	-0.435535	-0.138769	-0.569687
4	6	0	-1.372269	-1.192184	-0.500412
5	6	0	-2.227940	1.495555	-0.171191
6	6	0	2.756601	-2.058655	-1.017653

7	6	0	1.869629	0.637197	-0.926269
8	6	0	3.236086	0.352192	-1.206882
9	6	0	2.369698	3.056660	-0.951693
10	6	0	0.941152	-0.415951	-0.789090
11	6	0	0.077933	2.271601	-0.528086
12	6	0	-0.868025	1.214580	-0.422992
13	6	0	-1.713868	3.901934	-0.077958
14	6	0	1.432094	1.993910	-0.807590
15	6	0	0.581319	4.679030	-0.454012
16	6	0	-0.353488	3.625145	-0.355609
17	6	0	-3.180736	0.438963	-0.096419
18	6	0	-2.653363	2.848343	0.007214
19	6	0	-2.138681	5.263875	0.113227
20	6	0	-1.171642	6.301869	0.019767
21	1	0	-1.496014	7.329275	0.169115
22	6	0	0.150623	6.039290	-0.255878
23	6	0	1.939264	4.400379	-0.754869
24	6	0	3.725228	2.789122	-1.287384
25	6	0	4.155050	1.405820	-1.468151
26	6	0	3.679964	-1.001194	-1.220098
27	6	0	3.206414	-3.426407	-1.039992
28	6	0	2.281734	-4.433446	-1.125177
29	1	0	2.605935	-5.465606	-1.230626
30	6	0	0.877570	-4.182620	-1.025299
31	6	0	-0.937109	-2.543301	-0.666720
32	6	0	-2.750998	-0.916730	-0.278584
33	6	0	4.656731	-3.672740	-0.940970
34	6	0	5.045841	-1.300386	-1.496606
35	6	0	-0.057946	-5.204737	-1.033312

36	6	0	-1.883413	-3.598346	-0.647230
37	6	0	-4.016449	3.128941	0.272433
38	6	0	2.873666	5.466813	-0.858530
39	6	0	1.132947	7.093320	-0.356242
40	6	0	-3.475906	5.526051	0.382237
41	6	0	-1.436245	-4.952739	-0.845455
42	6	0	5.529570	-2.632619	-1.309069
43	6	0	2.424633	6.818944	-0.640763
44	6	0	-4.432667	4.493711	0.466494
45	1	0	0.271399	-6.232334	-1.169817
46	1	0	3.158476	7.616949	-0.714446
47	1	0	0.802072	8.115885	-0.196576
48	1	0	-3.799401	6.553778	0.530280
49	6	0	4.200951	5.172347	-1.165637
50	6	0	5.454740	1.064362	-1.860013
51	6	0	4.612370	3.867253	-1.389032
52	6	0	5.891797	-0.250525	-1.865977
53	1	0	6.925713	-0.472642	-2.117932
54	6	0	-5.778378	4.759532	0.733850
55	6	0	-4.962152	2.081079	0.345392
56	6	0	-4.537585	0.721008	0.151295
57	6	0	-3.687539	-1.966991	-0.236242
58	6	0	-3.253263	-3.323700	-0.433949
59	6	0	-5.066109	-1.687948	0.001454
60	6	0	-2.379054	-5.981973	-0.833979
61	6	0	-3.739649	-5.730227	-0.623968
62	6	0	-4.191066	-4.385908	-0.413409
63	6	0	-6.727258	3.735607	0.810832
64	6	0	-6.322764	2.374512	0.610431

65	6	0	-5.491299	-0.338964	0.208479
66	6	0	-4.689085	-6.786768	-0.611953
67	6	0	-5.577442	-4.131057	-0.187149
68	6	0	-6.013650	-2.748115	0.038029
69	6	0	-6.860928	-0.054462	0.464917
70	6	0	-7.293869	1.330383	0.683317
71	6	0	-8.092360	4.019470	1.085236
72	6	0	-9.007875	3.003417	1.156799
73	1	0	-10.050180	3.219907	1.368937
74	6	0	-8.611655	1.667177	0.957320
75	6	0	-7.756419	-1.120395	0.498732
76	6	0	-7.345103	-2.427737	0.291038
77	6	0	-6.459449	-5.202237	-0.189271
78	6	0	-6.016517	-6.521405	-0.400956
79	1	0	-6.741013	-7.329913	-0.394720
80	1	0	-8.096308	-3.207436	0.334615
81	1	0	-8.390054	5.053156	1.237260
82	1	0	-6.096228	5.788534	0.885280
83	1	0	-2.048796	-7.006566	-0.988726
84	1	0	6.162495	1.841972	-2.124995
85	1	0	-9.371500	0.897952	1.027435
86	1	0	-8.808689	-0.945061	0.688367
87	1	0	-4.340588	-7.802961	-0.773939
88	1	0	-7.518885	-5.042159	-0.028555
89	1	0	4.984845	-4.693018	-1.137639
90	1	0	6.559370	-2.851176	-1.568376
91	6	0	4.922812	-3.843097	1.107601
92	1	0	4.926354	5.979093	-1.219599
93	1	0	5.661552	3.691275	-1.597564

94	7	0	5.734183	-3.001533	1.436400
95	7	0	6.560774	-2.160635	0.927576
96	6	0	4.294776	-4.950230	1.924454
97	6	0	6.315761	-0.826977	1.216496
98	6	0	5.077194	-0.338567	1.679099
99	6	0	7.341164	0.083364	0.903987
100	6	0	4.855963	1.023146	1.772956
101	1	0	4.281007	-1.035827	1.922026
102	6	0	7.130558	1.446717	1.009904
103	1	0	8.292221	-0.311852	0.562475
104	6	0	5.878764	1.899035	1.418222
105	1	0	3.896205	1.422217	2.080867
106	1	0	7.902050	2.164796	0.759122
107	7	0	5.613313	3.335096	1.437932
108	8	0	6.502045	4.081124	1.054726
109	8	0	4.513756	3.707653	1.805838
110	6	0	5.099550	-5.096820	3.226721
111	1	0	6.143696	-5.345580	3.016449
112	1	0	5.077204	-4.168409	3.803385
113	1	0	4.663565	-5.897599	3.833343
114	6	0	4.353763	-6.275430	1.155892
115	1	0	3.958555	-7.072843	1.793156
116	1	0	3.754219	-6.246483	0.245456
117	1	0	5.384779	-6.530924	0.890230
118	6	0	2.843988	-4.576390	2.269515
119	1	0	2.219088	-4.483136	1.379554
120	1	0	2.419608	-5.355750	2.911724
121	1	0	2.813090	-3.629350	2.817886

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.622004	0.106261	-0.877391
2	6	0	1.391228	-1.290844	-0.973946
3	6	0	-0.782964	0.462075	-0.462430
4	6	0	-0.999952	-0.932442	-0.515048
5	6	0	-3.174509	0.823287	-0.014220
6	6	0	2.926610	0.619514	-1.009838
7	6	0	0.741771	2.388095	-0.613611
8	6	0	2.054138	2.914908	-0.805759
9	6	0	-0.154752	4.686159	-0.410540
10	6	0	0.524213	0.994729	-0.643706
11	6	0	-1.657806	2.751641	-0.202629
12	6	0	-1.879118	1.346041	-0.222488
13	6	0	-4.056462	3.106761	0.249947
14	6	0	-0.363725	3.275454	-0.409315
15	6	0	-2.555155	5.031697	0.039484
16	6	0	-2.761143	3.635295	0.029139
17	6	0	-3.399118	-0.583027	-0.045692
18	6	0	-4.269197	1.709056	0.232166
19	6	0	-5.159600	3.998990	0.493983
20	6	0	-4.918674	5.399345	0.498054
21	1	0	-5.754577	6.070961	0.680540
22	6	0	-3.664724	5.918660	0.276936
23	6	0	-1.258329	5.560259	-0.183969

24	6	0	1.139681	5.227752	-0.635206
25	6	0	2.263112	4.321289	-0.864037
26	6	0	3.156850	2.022426	-0.967721
27	6	0	4.023322	-0.280501	-1.244898
28	6	0	3.790561	-1.621843	-1.417146
29	1	0	4.620451	-2.293197	-1.624084
30	6	0	2.486039	-2.175254	-1.269853
31	6	0	0.092824	-1.813596	-0.786593
32	6	0	-2.303217	-1.468870	-0.309727
33	6	0	5.364225	0.253992	-1.245246
34	6	0	4.468681	2.538613	-1.169256
35	6	0	2.259006	-3.540132	-1.352792
36	6	0	-0.127969	-3.212714	-0.857966
37	6	0	-5.566436	1.183683	0.456540
38	6	0	-1.060752	6.968502	-0.178671
39	6	0	-3.421682	7.342063	0.276489
40	6	0	-6.424641	3.472768	0.718592
41	6	0	0.975810	-4.090508	-1.146030
42	6	0	5.613159	1.626697	-1.256690
43	6	0	-2.185044	7.838760	0.058010
44	6	0	-6.662006	2.083827	0.709041
45	1	0	3.089850	-4.208530	-1.568274
46	1	0	-2.008777	8.911139	0.058442
47	1	0	-4.264373	8.003950	0.457052
48	1	0	-7.257217	4.146576	0.906923
49	6	0	0.221906	7.468554	-0.395315
50	6	0	3.545712	4.784193	-1.162355
51	6	0	1.294779	6.618368	-0.614674
52	6	0	4.617208	3.913264	-1.316406

53	1	0	5.596439	4.321225	-1.551999
54	6	0	-7.935156	1.555611	0.938633
55	6	0	-5.787048	-0.212190	0.434817
56	6	0	-4.689392	-1.103464	0.174308
57	6	0	-2.516822	-2.860415	-0.360211
58	6	0	-1.418604	-3.744881	-0.641026
59	6	0	-3.820069	-3.394903	-0.134743
60	6	0	0.751257	-5.467175	-1.205614
61	6	0	-0.517752	-6.012322	-0.986107
62	6	0	-1.623131	-5.146302	-0.698227
63	6	0	-8.170373	0.178079	0.925916
64	6	0	-7.087385	-0.725789	0.667788
65	6	0	-4.910297	-2.512477	0.139380
66	6	0	-0.731981	-7.415604	-1.041382
67	6	0	-2.916869	-5.704818	-0.471134
68	6	0	-4.034253	-4.800669	-0.179378
69	6	0	-6.211282	-3.038537	0.372716
70	6	0	-7.330768	-2.132238	0.649581
71	6	0	-9.469393	-0.346884	1.164164
72	6	0	-9.680884	-1.699806	1.147846
73	1	0	-10.672804	-2.101267	1.330443
74	6	0	-8.618693	-2.587707	0.892236
75	6	0	-6.378005	-4.420052	0.326535
76	6	0	-5.321120	-5.275526	0.058684
77	6	0	-3.067064	-7.082730	-0.536764
78	6	0	-1.980900	-7.932230	-0.819726
79	1	0	-2.144988	-9.004387	-0.861392
80	1	0	-5.524444	-6.339473	0.037903
81	1	0	-10.283705	0.345493	1.358506

82	1	0	-8.763241	2.233414	1.132493
83	1	0	1.583729	-6.132243	-1.423236
84	1	0	3.729370	5.845314	-1.283888
85	1	0	-8.835639	-3.649112	0.889511
86	1	0	-7.353235	-4.859820	0.497991
87	1	0	0.111624	-8.063849	-1.260953
88	1	0	-4.036172	-7.538126	-0.371661
89	1	0	6.174413	-0.433728	-1.480911
90	1	0	6.502712	1.994974	-1.761502
91	1	0	0.379663	8.543768	-0.385035
92	1	0	2.273890	7.059138	-0.760774
93	7	0	6.442333	0.805112	1.183475
94	6	0	6.771811	1.809368	0.592931
95	7	0	5.592630	-0.145227	1.039289
96	6	0	7.555259	3.033332	0.967364
97	6	0	6.073775	-1.444821	1.152949
98	6	0	5.097672	-2.456092	1.205131
99	6	0	7.437033	-1.794558	1.155489
100	6	0	5.469094	-3.789774	1.222827
101	1	0	4.053772	-2.165133	1.239291
102	6	0	7.812601	-3.126261	1.187976
103	1	0	8.190281	-1.012870	1.136569
104	6	0	6.823872	-4.106386	1.208942
105	1	0	4.732283	-4.583470	1.260902
106	1	0	8.854183	-3.424138	1.191767
107	7	0	7.224226	-5.512447	1.228297
108	8	0	8.417696	-5.762350	1.245849
109	8	0	6.340951	-6.352873	1.220621
110	6	0	8.270057	3.615585	-0.256629

111	1	0	8.895423	4.457064	0.057222
112	1	0	8.915409	2.867305	-0.727998
113	1	0	7.565289	3.984284	-1.005253
114	6	0	8.607929	2.596649	2.003015
115	1	0	8.127540	2.176287	2.890153
116	1	0	9.283729	1.845132	1.583286
117	1	0	9.201455	3.467316	2.300669
118	6	0	6.611263	4.069108	1.598518
119	1	0	7.189054	4.955858	1.880761
120	1	0	5.822374	4.371796	0.905843
121	1	0	6.141268	3.659858	2.497363

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.013281	-0.929868	-1.087711
2	6	0	1.235991	-2.106235	-1.221819
3	6	0	-0.039213	0.365852	-0.660259
4	6	0	-0.797969	-0.823499	-0.699267
5	6	0	-2.073740	1.659693	-0.184500
6	6	0	3.418393	-0.998853	-1.145919
7	6	0	2.128825	1.512614	-0.827745
8	6	0	3.543830	1.459343	-0.987947
9	6	0	2.238789	3.977723	-0.681959
10	6	0	1.369408	0.324895	-0.849483
11	6	0	0.083898	2.816400	-0.429975

12	6	0	-0.682349	1.617199	-0.417747
13	6	0	-1.963161	4.110694	0.028561
14	6	0	1.476983	2.772712	-0.647208
15	6	0	0.181488	5.268038	-0.244771
16	6	0	-0.568628	4.072192	-0.214545
17	6	0	-2.841036	0.459228	-0.180481
18	6	0	-2.717068	2.913891	0.052229
19	6	0	-2.613365	5.374890	0.253699
20	6	0	-1.831333	6.561706	0.211605
21	1	0	-2.325743	7.516512	0.375923
22	6	0	-0.477378	6.530468	-0.030655
23	6	0	1.579371	5.226281	-0.484092
24	6	0	3.642196	3.945525	-0.909857
25	6	0	4.309645	2.655145	-1.078238
26	6	0	4.190512	0.192285	-1.067557
27	6	0	4.068533	-2.268742	-1.349834
28	6	0	3.303187	-3.386315	-1.594227
29	1	0	3.791170	-4.344934	-1.757465
30	6	0	1.882074	-3.350429	-1.537462
31	6	0	-0.159680	-2.064060	-1.009562
32	6	0	-2.198529	-0.792931	-0.452281
33	6	0	5.495082	-2.348688	-1.171154
34	6	0	5.605719	0.118924	-1.138782
35	6	0	1.115603	-4.501311	-1.651880
36	6	0	-0.925280	-3.254179	-1.078178
37	6	0	-4.110962	2.954480	0.304120
38	6	0	2.325797	6.436431	-0.520466
39	6	0	0.316099	7.736562	-0.076627
40	6	0	-3.979162	5.402211	0.504074

41	6	0	-0.274491	-4.494387	-1.410638
42	6	0	6.258142	-1.186587	-0.959706
43	6	0	1.645681	7.690139	-0.311092
44	6	0	-4.751298	4.222824	0.540376
45	1	0	1.603651	-5.447551	-1.876202
46	1	0	2.235434	8.602406	-0.343540
47	1	0	-0.188077	8.685826	0.082977
48	1	0	-4.470999	6.356573	0.677012
49	6	0	3.699238	6.373030	-0.749859
50	6	0	5.676057	2.536154	-1.340734
51	6	0	4.340867	5.157295	-0.934896
52	6	0	6.310480	1.296335	-1.362446
53	1	0	7.379134	1.254906	-1.551315
54	6	0	-6.124500	4.250344	0.798240
55	6	0	-4.869758	1.761157	0.324020
56	6	0	-4.225440	0.500955	0.071179
57	6	0	-2.950273	-1.983423	-0.477684
58	6	0	-2.308092	-3.230239	-0.791757
59	6	0	-4.349799	-1.951030	-0.207518
60	6	0	-1.031875	-5.667658	-1.443260
61	6	0	-2.398376	-5.665067	-1.148826
62	6	0	-3.054246	-4.433048	-0.821418
63	6	0	-6.888615	3.079899	0.829996
64	6	0	-6.261339	1.813356	0.586414
65	6	0	-4.990040	-0.703727	0.071598
66	6	0	-3.154223	-6.867730	-1.167998
67	6	0	-4.451472	-4.430718	-0.530279
68	6	0	-5.107409	-3.155129	-0.221487
69	6	0	-6.386196	-0.663332	0.339181

70	6	0	-7.044892	0.619414	0.610242
71	6	0	-8.283567	3.120609	1.098775
72	6	0	-9.015980	1.963693	1.125049
73	1	0	-10.081002	1.995089	1.332979
74	6	0	-8.401833	0.720403	0.881573
75	6	0	-7.090253	-1.864800	0.326060
76	6	0	-6.470063	-3.074086	0.052939
77	6	0	-5.137542	-5.636206	-0.561088
78	6	0	-4.492276	-6.846941	-0.876823
79	1	0	-5.069308	-7.766262	-0.887460
80	1	0	-7.081885	-3.968289	0.054405
81	1	0	-8.751515	4.083818	1.281729
82	1	0	-6.611190	5.205912	0.978876
83	1	0	-0.543834	-6.608475	-1.687383
84	1	0	6.277915	3.421486	-1.512354
85	1	0	-9.023257	-0.166610	0.909955
86	1	0	-8.154869	-1.876995	0.527054
87	1	0	-2.648948	-7.797550	-1.413598
88	1	0	-6.197736	-5.670113	-0.340182
89	1	0	5.987583	-3.291845	-1.378068
90	1	0	7.320371	-1.233200	-1.197079
91	1	0	4.274296	7.294881	-0.774263
92	1	0	5.413566	5.162184	-1.090411
93	7	0	5.999921	-2.158692	1.530887
94	6	0	6.594371	-1.190966	1.101287
95	7	0	5.389263	-3.203629	1.100734
96	6	0	7.516748	-0.220516	1.799168
97	6	0	4.049307	-3.313482	1.462501
98	6	0	3.446798	-4.568915	1.274410

99	6	0	3.259032	-2.223498	1.873379
100	6	0	2.083252	-4.732042	1.454014
101	1	0	4.075117	-5.400470	0.972535
102	6	0	1.892139	-2.373661	2.031329
103	1	0	3.718997	-1.250046	2.015835
104	6	0	1.319601	-3.621744	1.800657
105	1	0	1.593796	-5.685186	1.292948
106	1	0	1.256227	-1.534998	2.291294
107	7	0	-0.135995	-3.755752	1.876712
108	8	0	-0.788532	-2.746115	2.082599
109	8	0	-0.614066	-4.864443	1.705011
110	6	0	8.740665	0.080353	0.927463
111	1	0	9.423807	0.727339	1.486796
112	1	0	9.277216	-0.837929	0.667761
113	1	0	8.464765	0.598423	0.008851
114	6	0	7.988199	-0.864125	3.113496
115	1	0	7.137612	-1.095838	3.759811
116	1	0	8.535679	-1.791293	2.920280
117	1	0	8.651621	-0.169747	3.640069
118	6	0	6.736370	1.066684	2.112763
119	1	0	7.394625	1.765049	2.641127
120	1	0	6.368274	1.552904	1.206801
121	1	0	5.882235	0.845840	2.760891

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.162702	-3.281285	-0.014974
2	6	0	1.836842	-3.707106	-0.269833
3	6	0	2.437726	-0.930785	-0.183689
4	6	0	1.109654	-1.359362	-0.407155
5	6	0	1.720200	1.415343	-0.371702
6	6	0	4.183439	-4.233304	0.193641
7	6	0	4.801105	-1.456745	0.234454
8	6	0	5.835162	-2.415885	0.446798
9	6	0	6.456100	0.369936	0.437299
10	6	0	3.473715	-1.882768	0.014717
11	6	0	4.087703	0.888507	0.024103
12	6	0	2.746242	0.464056	-0.174886
13	6	0	3.371037	3.236729	-0.222457
14	6	0	5.111604	-0.060220	0.233511
15	6	0	5.728560	2.716597	0.189032
16	6	0	4.396930	2.288063	-0.000405
17	6	0	0.375826	0.992395	-0.554275
18	6	0	2.033205	2.809785	-0.398117
19	6	0	3.686927	4.639478	-0.275600
20	6	0	5.035972	5.038118	-0.079819
21	1	0	5.276131	6.098386	-0.114386
22	6	0	6.038286	4.121596	0.150707
23	6	0	6.756728	1.764627	0.412509
24	6	0	7.494861	-0.574648	0.657028
25	6	0	7.175990	-2.000321	0.668810
26	6	0	5.515247	-3.806183	0.433372
27	6	0	3.869964	-5.638211	0.156502
28	6	0	2.581466	-6.045309	-0.107216

29	1	0	2.351148	-7.107574	-0.146468
30	6	0	1.535047	-5.112679	-0.338018
31	6	0	0.809697	-2.755807	-0.465848
32	6	0	0.068101	-0.409080	-0.580330
33	6	0	4.932896	-6.586682	0.389696
34	6	0	6.534493	-4.772484	0.650421
35	6	0	0.239706	-5.518699	-0.641367
36	6	0	-0.510177	-3.182716	-0.748895
37	6	0	1.008562	3.758847	-0.621027
38	6	0	8.093023	2.206435	0.607908
39	6	0	7.408245	4.528454	0.354334
40	6	0	2.672601	5.559695	-0.526451
41	6	0	-0.794903	-4.588688	-0.868469
42	6	0	6.197222	-6.173212	0.626240
43	6	0	8.382009	3.617508	0.573082
44	6	0	1.334790	5.158225	-0.712441
45	1	0	0.017733	-6.580801	-0.714782
46	1	0	9.411083	3.931699	0.726202
47	1	0	7.635113	5.590747	0.327235
48	1	0	2.916926	6.617692	-0.585772
49	6	0	9.090983	1.255757	0.824806
50	6	0	8.150264	-2.984099	0.885162
51	6	0	8.798564	-0.098025	0.848201
52	6	0	7.838933	-4.334046	0.877932
53	1	0	8.621595	-5.068665	1.047270
54	6	0	0.313382	6.070911	-1.006336
55	6	0	-0.333253	3.334647	-0.768415
56	6	0	-0.648295	1.940606	-0.718078
57	6	0	-1.254544	-0.835795	-0.803924

58	6	0	-1.542365	-2.234963	-0.927676
59	6	0	-2.312371	0.114241	-0.898186
60	6	0	-2.088296	-4.988902	-1.223676
61	6	0	-3.109816	-4.059553	-1.449162
62	6	0	-2.848204	-2.661685	-1.270241
63	6	0	-1.013397	5.662349	-1.185281
64	6	0	-1.355519	4.278530	-1.029279
65	6	0	-2.011327	1.520290	-0.815971
66	6	0	-4.409000	-4.468869	-1.857713
67	6	0	-3.898630	-1.712222	-1.452092
68	6	0	-3.633196	-0.307018	-1.150385
69	6	0	-3.040482	2.465774	-0.881892
70	6	0	-2.717943	3.858357	-1.146349
71	6	0	-2.038412	6.583570	-1.532210
72	6	0	-3.326562	6.149951	-1.726741
73	1	0	-4.097340	6.853375	-2.026560
74	6	0	-3.669814	4.799519	-1.534695
75	6	0	-4.400059	2.000768	-0.669130
76	6	0	-4.677111	0.620553	-0.996990
77	6	0	-5.139152	-2.166630	-1.878699
78	6	0	-5.389000	-3.537713	-2.086369
79	1	0	-5.685927	0.363395	-1.296334
80	1	0	-1.778852	7.630486	-1.661200
81	1	0	0.559619	7.125018	-1.110452
82	1	0	-2.301806	-6.049013	-1.339514
83	1	0	9.180467	-2.700186	1.064182
84	1	0	-4.699121	4.498225	-1.698829
85	1	0	-5.194827	2.698095	-0.924339
86	1	0	-4.602719	-5.528621	-1.998299

87	1	0	10.114608	1.588771	0.974452
88	1	0	9.612421	-0.793188	1.015545
89	1	0	4.687477	-7.644936	0.367717
90	1	0	6.992648	-6.893126	0.799324
91	1	0	-6.375098	-3.851309	-2.415092
92	1	0	-5.950015	-1.466926	-2.048484
93	7	0	-5.151907	0.987154	1.614701
94	6	0	-4.688804	2.066661	1.261292
95	7	0	-5.317421	-0.176054	1.097574
96	6	0	-4.316174	3.225769	2.164232
97	6	0	-6.625922	-0.661817	1.118044
98	6	0	-7.760425	0.134776	1.356795
99	6	0	-6.787074	-2.030954	0.840472
100	6	0	-9.027387	-0.423043	1.303523
101	1	0	-7.635886	1.187860	1.588522
102	6	0	-8.049519	-2.590791	0.776578
103	1	0	-5.898627	-2.632672	0.683038
104	6	0	-9.155574	-1.775834	1.006444
105	1	0	-9.917642	0.167290	1.484670
106	1	0	-8.195685	-3.643375	0.566439
107	7	0	-10.493274	-2.362423	0.944264
108	8	0	-10.579262	-3.547615	0.671271
109	8	0	-11.444051	-1.631889	1.166473
110	6	0	-4.930428	4.530793	1.646069
111	1	0	-6.014928	4.430997	1.526258
112	1	0	-4.741869	5.328321	2.372273
113	1	0	-4.495644	4.836205	0.693613
114	6	0	-4.895289	2.926632	3.558886
115	1	0	-5.981983	2.805484	3.515887

116	1	0	-4.464964	2.012380	3.975341
117	1	0	-4.663463	3.761728	4.227815
118	6	0	-2.788571	3.345590	2.287221
119	1	0	-2.558602	4.100329	3.047073
120	1	0	-2.347372	2.394732	2.602234
121	1	0	-2.318163	3.656687	1.353573

TsE1-r1c2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.838144	-2.742571	-0.321069
2	6	0	1.572794	-3.323629	-0.578252
3	6	0	1.827574	-0.496409	-0.414539
4	6	0	0.562247	-1.081763	-0.647083
5	6	0	0.815097	1.744778	-0.486503
6	6	0	3.969697	-3.565353	-0.139628
7	6	0	4.239277	-0.734626	-0.022603
8	6	0	5.385740	-1.562985	0.157454
9	6	0	5.652437	1.278831	0.243397
10	6	0	2.974682	-1.317454	-0.252131
11	6	0	3.234447	1.508496	-0.138249
12	6	0	1.956254	0.924418	-0.346774
13	6	0	2.218043	3.754986	-0.262792
14	6	0	4.371283	0.689049	0.028227
15	6	0	4.629098	3.522552	0.099102
16	6	0	3.360552	2.935929	-0.099144

17	6	0	-0.466226	1.160008	-0.668895
18	6	0	0.942706	3.167067	-0.440419
19	6	0	2.347005	5.187734	-0.245672
20	6	0	3.638545	5.746062	-0.049204
21	1	0	3.741581	6.828731	-0.033928
22	6	0	4.754175	4.955659	0.124296
23	6	0	5.772672	2.700397	0.273963
24	6	0	6.803576	0.465153	0.424039
25	6	0	6.665222	-0.989135	0.388993
26	6	0	5.240703	-2.981519	0.104816
27	6	0	3.831014	-4.997169	-0.205607
28	6	0	2.598434	-5.554442	-0.464174
29	1	0	2.498099	-6.636063	-0.517242
30	6	0	1.442976	-4.753648	-0.668117
31	6	0	0.436983	-2.501823	-0.749467
32	6	0	-0.591814	-0.264935	-0.767802
33	6	0	5.005789	-5.811333	-0.002166
34	6	0	6.373001	-3.818993	0.294077
35	6	0	0.202399	-5.310254	-0.961104
36	6	0	-0.822266	-3.079445	-1.037261
37	6	0	-0.201983	3.984678	-0.587199
38	6	0	7.044387	3.300422	0.478947
39	6	0	6.064687	5.524579	0.331650
40	6	0	1.214979	5.979636	-0.427437
41	6	0	-0.937247	-4.506825	-1.173084
42	6	0	6.211501	-5.250005	0.236184
43	6	0	7.150210	4.736927	0.501003
44	6	0	-0.065613	5.417386	-0.604576
45	1	0	0.101540	-6.390942	-1.024775

46	1	0	8.132877	5.174199	0.657006
47	1	0	6.155029	6.607304	0.348926
48	1	0	1.319517	7.061999	-0.432881
49	6	0	8.156673	2.475979	0.652017
50	6	0	7.755049	-1.849778	0.574664
51	6	0	8.038721	1.096029	0.626129
52	6	0	7.614407	-3.227362	0.530427
53	1	0	8.483267	-3.862903	0.679867
54	6	0	-1.210596	6.199419	-0.814670
55	6	0	-1.481776	3.394931	-0.720139
56	6	0	-1.608273	1.973167	-0.747936
57	6	0	-1.854920	-0.847000	-0.988642
58	6	0	-1.966333	-2.263625	-1.174660
59	6	0	-3.027466	-0.044754	-0.964784
60	6	0	-2.184632	-5.056314	-1.489545
61	6	0	-3.319477	-4.255285	-1.668495
62	6	0	-3.222970	-2.838809	-1.478313
63	6	0	-2.479887	5.627334	-0.970547
64	6	0	-2.629560	4.204559	-0.885714
65	6	0	-2.907943	1.380858	-0.811869
66	6	0	-4.582405	-4.820359	-1.993075
67	6	0	-4.398626	-2.032464	-1.552422
68	6	0	-4.305907	-0.620994	-1.174647
69	6	0	-4.052311	2.181123	-0.755727
70	6	0	-3.929510	3.610357	-0.966257
71	6	0	-3.635421	6.417374	-1.220574
72	6	0	-4.863051	5.823832	-1.390160
73	1	0	-5.732083	6.432036	-1.621705
74	6	0	-5.015970	4.431605	-1.264575

75	6	0	-5.311652	1.516541	-0.429940
76	6	0	-5.435230	0.137534	-0.877293
77	6	0	-5.599607	-2.631423	-1.905720
78	6	0	-5.687165	-4.018107	-2.132238
79	1	0	-6.427835	-0.260398	-1.035978
80	1	0	-3.524792	7.495391	-1.297524
81	1	0	-1.109713	7.281083	-0.864539
82	1	0	-2.278131	-6.135653	-1.583414
83	1	0	8.742367	-1.443372	0.759509
84	1	0	-5.998024	3.996486	-1.420918
85	1	0	-6.213196	2.110966	-0.587945
86	1	0	-4.651401	-5.895003	-2.138194
87	1	0	9.131662	2.930059	0.808288
88	1	0	8.936315	0.504872	0.763997
89	1	0	4.892578	-6.891061	-0.046345
90	1	0	7.091594	-5.869066	0.389031
91	1	0	-6.645422	-4.452017	-2.401000
92	1	0	-6.499740	-2.033047	-1.997046
93	7	0	-5.595347	0.278103	1.826385
94	6	0	-5.423566	1.427308	1.421408
95	7	0	-5.821026	-0.892919	1.341148
96	6	0	-5.453507	2.658886	2.314332
97	6	0	-4.826441	-1.830772	1.563934
98	6	0	-3.502264	-1.495177	1.909400
99	6	0	-5.159713	-3.181127	1.334892
100	6	0	-2.530498	-2.480226	1.981700
101	1	0	-3.239840	-0.457635	2.092576
102	6	0	-4.198361	-4.168198	1.420881
103	1	0	-6.184093	-3.418739	1.068374

104	6	0	-2.886353	-3.799951	1.725823
105	1	0	-1.496134	-2.241702	2.202455
106	1	0	-4.429659	-5.208934	1.229483
107	7	0	-1.847554	-4.823883	1.746492
108	8	0	-2.178186	-5.979916	1.529763
109	8	0	-0.700327	-4.466887	1.958345
110	6	0	-6.459930	3.683230	1.776241
111	1	0	-7.451586	3.234041	1.653512
112	1	0	-6.547671	4.505022	2.494354
113	1	0	-6.139085	4.109349	0.824652
114	6	0	-5.901772	2.222590	3.718750
115	1	0	-6.893696	1.762549	3.690300
116	1	0	-5.202355	1.499785	4.147025
117	1	0	-5.940299	3.100830	4.371455
118	6	0	-4.049435	3.275188	2.421784
119	1	0	-4.076376	4.083085	3.161045
120	1	0	-3.324175	2.528096	2.761298
121	1	0	-3.698551	3.696683	1.479408

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.267328	-2.497396	-0.094086
2	6	0	3.160172	-3.348899	-0.317576
3	6	0	2.778201	-0.534029	-0.205521
4	6	0	1.670168	-1.388767	-0.399924

5	6	0	1.296860	1.427371	-0.349414
6	6	0	5.558435	-3.044374	0.072015
7	6	0	5.187960	-0.225292	0.163468
8	6	0	6.492606	-0.775296	0.341480
9	6	0	6.119625	2.053777	0.389180
10	6	0	4.081765	-1.077088	-0.042675
11	6	0	3.710781	1.736096	0.005609
12	6	0	2.590761	0.881582	-0.180559
13	6	0	2.231544	3.700170	-0.196215
14	6	0	5.000921	1.192403	0.187661
15	6	0	4.629984	4.012647	0.190686
16	6	0	3.523317	3.156652	0.003071
17	6	0	0.171120	0.574122	-0.506379
18	6	0	1.117464	2.845333	-0.365743
19	6	0	2.052260	5.127361	-0.229806
20	6	0	3.185303	5.961550	-0.035700
21	1	0	3.047348	7.040246	-0.054746
22	6	0	4.441862	5.439887	0.175313
23	6	0	5.924625	3.466867	0.391769
24	6	0	7.422091	1.518790	0.583219
25	6	0	7.613325	0.070725	0.559097
26	6	0	6.668508	-2.190279	0.297295
27	6	0	5.742928	-4.470052	0.010019
28	6	0	4.662142	-5.291392	-0.223346
29	1	0	4.807983	-6.367879	-0.277199
30	6	0	3.351716	-4.772635	-0.397152
31	6	0	1.861904	-2.803810	-0.463728
32	6	0	0.362673	-0.848147	-0.536042
33	6	0	7.073083	-4.999498	0.193775

34	6	0	7.962289	-2.751543	0.474150
35	6	0	2.258278	-5.597170	-0.646251
36	6	0	0.756147	-3.656846	-0.685140
37	6	0	-0.172192	3.390409	-0.572744
38	6	0	7.030474	4.336805	0.591553
39	6	0	5.591624	6.288344	0.380824
40	6	0	0.783481	5.649887	-0.457424
41	6	0	0.957971	-5.077995	-0.802203
42	6	0	8.125466	-4.181581	0.416589
43	6	0	6.819522	5.762116	0.581729
44	6	0	-0.339277	4.818340	-0.640841
45	1	0	2.408686	-6.671317	-0.724455
46	1	0	7.680534	6.406642	0.738041
47	1	0	5.440693	7.364295	0.370910
48	1	0	0.650577	6.728506	-0.498237
49	6	0	8.295354	3.782290	0.788850
50	6	0	8.871035	-0.522118	0.736396
51	6	0	8.484327	2.410034	0.783864
52	6	0	9.041724	-1.896011	0.695457
53	1	0	10.032567	-2.320413	0.833893
54	6	0	-1.612714	5.339145	-0.895900
55	6	0	-1.291532	2.539780	-0.720370
56	6	0	-1.120709	1.118090	-0.654440
57	6	0	-0.740883	-1.701256	-0.705452
58	6	0	-0.546659	-3.115850	-0.796248
59	6	0	-2.064781	-1.164630	-0.753220
60	6	0	-0.144206	-5.896694	-1.079799
61	6	0	-1.435798	-5.374094	-1.212825
62	6	0	-1.651612	-3.967532	-1.036558

63	6	0	-2.725151	4.509768	-1.074423
64	6	0	-2.573633	3.087794	-0.967179
65	6	0	-2.260482	0.262911	-0.741288
66	6	0	-2.548162	-6.201946	-1.523026
67	6	0	-2.975240	-3.433237	-1.102209
68	6	0	-3.167896	-2.021389	-0.822065
69	6	0	-3.551954	0.800328	-0.926232
70	6	0	-3.711363	2.238716	-1.114819
71	6	0	-4.009161	5.046948	-1.360628
72	6	0	-5.084209	4.213216	-1.533940
73	1	0	-6.062640	4.624183	-1.765285
74	6	0	-4.939164	2.819071	-1.405076
75	6	0	-4.668543	-0.061758	-0.878106
76	6	0	-4.476817	-1.456223	-0.574196
77	6	0	-4.021821	-4.288180	-1.446208
78	6	0	-3.803566	-5.660616	-1.656462
79	1	0	-5.330665	-2.094078	-0.787391
80	1	0	-4.118460	6.124512	-1.445127
81	1	0	-1.740740	6.417134	-0.962530
82	1	0	0.008461	-6.966729	-1.199574
83	1	0	9.744622	0.094975	0.909668
84	1	0	-5.817176	2.197973	-1.537375
85	1	0	-5.621091	0.250855	-1.286167
86	1	0	-2.383017	-7.265934	-1.667469
87	1	0	9.143786	4.443162	0.945319
88	1	0	9.488323	2.032825	0.936758
89	1	0	7.205176	-6.077035	0.147651
90	1	0	9.123992	-4.587749	0.554226
91	1	0	-4.643755	-6.294748	-1.921673

92	1	0	-5.028645	-3.901244	-1.559473
93	6	0	-4.660004	-1.499185	1.396099
94	7	0	-5.267172	-0.478973	1.695055
95	7	0	-5.637034	0.601851	1.099617
96	6	0	-4.136241	-2.567486	2.334076
97	6	0	-7.025329	0.741956	0.994282
98	6	0	-7.935376	-0.310399	1.209945
99	6	0	-7.512170	2.004600	0.611637
100	6	0	-9.293035	-0.110805	1.024994
101	1	0	-7.568840	-1.280606	1.529083
102	6	0	-8.867029	2.207869	0.419635
103	1	0	-6.800666	2.814527	0.490962
104	6	0	-9.740628	1.143070	0.623602
105	1	0	-10.012312	-0.905441	1.182181
106	1	0	-9.263662	3.173066	0.128905
107	7	0	-11.173539	1.351161	0.421669
108	8	0	-11.539247	2.455933	0.058433
109	8	0	-11.917799	0.407111	0.626201
110	6	0	-4.594950	-2.197829	3.755835
111	1	0	-4.177384	-1.235962	4.065049
112	1	0	-5.685431	-2.132738	3.813145
113	1	0	-4.253076	-2.970007	4.452660
114	6	0	-4.728167	-3.932630	1.961413
115	1	0	-4.412736	-4.259413	0.969357
116	1	0	-4.387295	-4.678175	2.687495
117	1	0	-5.823016	-3.904685	1.992361
118	6	0	-2.600024	-2.616465	2.313090
119	1	0	-2.263109	-3.252693	3.138397
120	1	0	-2.210180	-3.039767	1.386805

121	1	0	-2.170108	-1.619293	2.451142

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.360694	2.935793	-0.099124
2	6	0	-2.218225	3.754901	-0.262807
3	6	0	-1.956308	0.924344	-0.346744
4	6	0	-0.815189	1.744754	-0.486492
5	6	0	-0.562214	-1.081777	-0.647038
6	6	0	-4.629264	3.522360	0.099131
7	6	0	-4.371325	0.688869	0.028266
8	6	0	-5.652504	1.278595	0.243441
9	6	0	-5.385688	-1.563209	0.157474
10	6	0	-3.234526	1.508366	-0.138215
11	6	0	-2.974642	-1.317573	-0.252113
12	6	0	-1.827566	-0.496478	-0.414498
13	6	0	-1.572673	-3.323684	-0.578282
14	6	0	-4.239260	-0.734800	-0.022575
15	6	0	-3.969566	-3.565513	-0.139660
16	6	0	-2.838046	-2.742682	-0.321077
17	6	0	0.591811	-0.264897	-0.767744
18	6	0	-0.436893	-2.501831	-0.749456
19	6	0	-1.442805	-4.753695	-0.668220
20	6	0	-2.598231	-5.554540	-0.464289
21	1	0	-2.497858	-6.636156	-0.517403

22	6	0	-3.830828	-4.997323	-0.205684
23	6	0	-5.240592	-2.981736	0.104814
24	6	0	-6.665189	-0.989416	0.389042
25	6	0	-6.803609	0.464866	0.424069
26	6	0	-5.772801	2.700155	0.274002
27	6	0	-4.754406	4.955462	0.124312
28	6	0	-3.638816	5.745914	-0.049223
29	1	0	-3.741902	6.828579	-0.033962
30	6	0	-2.347254	5.187643	-0.245712
31	6	0	-0.942864	3.167038	-0.440447
32	6	0	0.466161	1.160038	-0.668871
33	6	0	-6.064941	5.524324	0.331679
34	6	0	-7.044543	3.300125	0.478976
35	6	0	-1.215269	5.979596	-0.427518
36	6	0	0.201785	3.984700	-0.587271
37	6	0	0.822374	-3.079391	-1.037301
38	6	0	-6.372853	-3.819260	0.294081
39	6	0	-5.005568	-5.811538	-0.002252
40	6	0	-0.202220	-5.310238	-0.961288
41	6	0	0.065347	5.417402	-0.604668
42	6	0	-7.150429	4.736625	0.501038
43	6	0	-6.211297	-5.250264	0.236142
44	6	0	0.937390	-4.506755	-1.173275
45	1	0	-1.319857	7.061954	-0.432980
46	1	0	-7.091364	-5.869364	0.388985
47	1	0	-4.892318	-6.891260	-0.046473
48	1	0	-0.101330	-6.390919	-1.025031
49	6	0	-7.614272	-3.227685	0.530496
50	6	0	-8.038788	1.095687	0.626112

51	6	0	-7.754970	-1.850107	0.574761
52	6	0	-8.156799	2.475633	0.652011
53	1	0	-9.131813	2.929670	0.808252
54	6	0	2.184768	-5.056168	-1.489892
55	6	0	1.966408	-2.263523	-1.174673
56	6	0	1.854946	-0.846907	-0.988584
57	6	0	1.608174	1.973248	-0.747952
58	6	0	1.481604	3.395012	-0.720212
59	6	0	2.907866	1.380991	-0.811875
60	6	0	1.210295	6.199490	-0.814754
61	6	0	2.479618	5.627464	-0.970592
62	6	0	2.629349	4.204695	-0.885781
63	6	0	3.319584	-4.255087	-1.668799
64	6	0	3.223052	-2.838635	-1.478438
65	6	0	3.027444	-0.044604	-0.964767
66	6	0	3.635139	6.417565	-1.220506
67	6	0	3.929338	3.610557	-0.966244
68	6	0	4.052213	2.181323	-0.755774
69	6	0	4.305924	-0.620775	-1.174726
70	6	0	4.398668	-2.032232	-1.552584
71	6	0	4.582505	-4.820081	-1.993542
72	6	0	5.687227	-4.017775	-2.132687
73	1	0	6.645476	-4.451622	-2.401580
74	6	0	5.599636	-2.631115	-1.906034
75	6	0	5.435196	0.137837	-0.877544
76	6	0	5.311553	1.516779	-0.430062
77	6	0	5.015798	4.431870	-1.264365
78	6	0	4.862823	5.824094	-1.389942
79	1	0	6.213072	2.111260	-0.587987

80	1	0	4.651528	-5.894707	-2.138784
81	1	0	2.278291	-6.135492	-1.583897
82	1	0	1.109364	7.281150	-0.864619
83	1	0	-8.936366	0.504491	0.763918
84	1	0	6.499737	-2.032696	-1.997393
85	1	0	6.427816	-0.260027	-1.036323
86	1	0	3.524461	7.495578	-1.297453
87	1	0	-8.483099	-3.863263	0.679966
88	1	0	-8.742293	-1.443744	0.759674
89	1	0	-6.155331	6.607046	0.348955
90	1	0	-8.133114	5.173854	0.657044
91	1	0	5.731855	6.432349	-1.621351
92	1	0	5.997907	3.996815	-1.420534
93	6	0	5.423515	1.427409	1.421381
94	7	0	5.595717	0.278255	1.826251
95	7	0	5.821515	-0.892814	1.341275
96	6	0	5.453026	2.658924	2.314413
97	6	0	4.826918	-1.830649	1.563986
98	6	0	5.160206	-3.181027	1.335084
99	6	0	3.502722	-1.495010	1.909357
100	6	0	4.198863	-4.168090	1.421225
101	1	0	6.184591	-3.418658	1.068598
102	6	0	2.530955	-2.480046	1.981709
103	1	0	3.240282	-0.457456	2.092433
104	6	0	2.886838	-3.799805	1.726063
105	1	0	4.430173	-5.208854	1.229993
106	1	0	1.496581	-2.241506	2.202400
107	7	0	1.848040	-4.823726	1.746879
108	8	0	0.700805	-4.466683	1.958623

109	8	0	2.178673	-5.979799	1.530366
110	6	0	5.900839	2.222497	3.718941
111	1	0	5.201416	1.499466	4.146824
112	1	0	6.892881	1.762687	3.690814
113	1	0	5.938914	3.100640	4.371804
114	6	0	6.459589	3.683361	1.776743
115	1	0	6.138829	4.109855	0.825285
116	1	0	6.547368	4.504904	2.495135
117	1	0	7.451213	3.234126	1.653929
118	6	0	4.048914	3.275175	2.421487
119	1	0	4.075722	4.083316	3.160486
120	1	0	3.698072	3.696348	1.478967
121	1	0	3.323651	2.528148	2.761174

TsF

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.422833	1.569011	-0.931095
2	6	0	-1.606010	2.726786	-0.967935
3	6	0	-0.494127	0.253173	-0.098668
4	6	0	0.383388	1.370978	-0.418940
5	6	0	1.594145	-1.193661	-0.089165
6	6	0	-3.818938	1.687214	-1.094024
7	6	0	-2.636847	-0.852483	-0.691933
8	6	0	-4.045785	-0.752467	-0.922885
9	6	0	-2.819280	-3.325819	-0.868382

10	6	0	-1.848733	0.293718	-0.630157
11	6	0	-0.657698	-2.276284	-0.381551
12	6	0	0.120515	-1.122285	0.192877
13	6	0	1.407173	-3.630013	-0.462119
14	6	0	-2.018865	-2.161572	-0.610231
15	6	0	-0.775234	-4.686070	-0.830537
16	6	0	-0.006497	-3.529966	-0.568749
17	6	0	2.384850	-0.038153	-0.114797
18	6	0	2.202163	-2.463772	-0.273061
19	6	0	2.035551	-4.912945	-0.569021
20	6	0	1.228587	-6.062167	-0.781097
21	1	0	1.713773	-7.033285	-0.847093
22	6	0	-0.135921	-5.970786	-0.923775
23	6	0	-2.186248	-4.592953	-0.950078
24	6	0	-4.224911	-3.229107	-1.019599
25	6	0	-4.861891	-1.910760	-0.972889
26	6	0	-4.640460	0.531791	-1.039117
27	6	0	-4.421282	2.984842	-1.246369
28	6	0	-3.619729	4.100631	-1.306810
29	1	0	-4.072189	5.082677	-1.423965
30	6	0	-2.207260	4.009951	-1.185112
31	6	0	-0.206514	2.624960	-0.745926
32	6	0	1.771317	1.268343	-0.262104
33	6	0	-5.862323	3.081805	-1.271245
34	6	0	-6.054703	0.663172	-1.088713
35	6	0	-1.404648	5.147549	-1.215619
36	6	0	0.598538	3.789496	-0.794373
37	6	0	3.615786	-2.578341	-0.243872
38	6	0	-2.960162	-5.764651	-1.178171

39	6	0	-0.954281	-7.138894	-1.152828
40	6	0	3.421466	-5.015776	-0.458413
41	6	0	-0.013254	5.073522	-1.028883
42	6	0	-6.637286	1.978786	-1.178171
43	6	0	-2.295695	-7.039547	-1.272953
44	6	0	4.232661	-3.880976	-0.299346
45	1	0	-1.864159	6.120164	-1.374930
46	1	0	-2.904793	-7.922469	-1.448020
47	1	0	-0.457531	-8.102455	-1.226400
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49	6	0	-4.340720	-5.640429	-1.318464
50	6	0	-6.250551	-1.747123	-0.998331
51	6	0	-4.956648	-4.400095	-1.246014
52	6	0	-6.836412	-0.489293	-1.035139
53	1	0	-7.918770	-0.396174	-1.039173
54	6	0	5.622765	-3.982860	-0.179821
55	6	0	4.420727	-1.426224	-0.113410
56	6	0	3.803285	-0.138410	-0.110391
57	6	0	2.591173	2.423655	-0.354154
58	6	0	1.991886	3.702326	-0.579974
59	6	0	4.004895	2.321214	-0.222731
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61	6	0	2.167158	6.153294	-0.818780
62	6	0	2.788233	4.880202	-0.602110
63	6	0	6.432902	-2.852920	-0.029232
64	6	0	5.835100	-1.551056	-0.021320
65	6	0	4.613981	1.031842	-0.103020
66	6	0	2.966797	7.325873	-0.807390
67	6	0	4.195110	4.807587	-0.402999

68	6	0	4.814053	3.491099	-0.242384
69	6	0	6.029089	0.921807	-0.001529
70	6	0	6.658371	-0.396926	0.083004
71	6	0	7.840327	-2.966979	0.111795
72	6	0	8.615147	-1.843010	0.253583
73	1	0	9.690447	-1.932821	0.372905
74	6	0	8.031833	-0.565993	0.235857
75	6	0	6.784127	2.093109	-0.014207
76	6	0	6.194629	3.340034	-0.130861
77	6	0	4.929387	5.989633	-0.388393
78	6	0	4.318245	7.238468	-0.588142
79	1	0	8.286797	-3.957360	0.109885
80	1	0	6.083969	-4.967293	-0.203751
81	1	0	0.321565	7.189901	-1.195975
82	1	0	-6.898823	-2.615529	-0.979034
83	1	0	8.682967	0.293170	0.343709
84	1	0	2.487448	8.287054	-0.969968
85	1	0	-4.936940	-6.530131	-1.502895
86	1	0	-6.029333	-4.349752	-1.391746
87	1	0	-6.306878	4.070589	-1.336172
88	1	0	-7.720332	2.061190	-1.165817
89	1	0	4.928311	8.136038	-0.571404
90	1	0	5.999259	5.968753	-0.219461
91	1	0	6.842996	4.207623	-0.153897
92	1	0	7.864816	2.046410	0.046658
93	6	0	-0.014467	-1.312512	1.871936
94	6	0	0.425647	-2.462186	2.805956
95	7	0	-0.548035	-0.307083	2.403839
96	7	0	-0.822295	0.817743	1.792671

97	6	0	-2.136585	1.282220	2.023742
98	6	0	-3.222626	0.410955	2.186580
99	6	0	-2.350128	2.666093	1.972782
100	6	0	-4.517079	0.910674	2.203141
101	1	0	-3.044261	-0.658434	2.251909
102	6	0	-3.637486	3.176905	2.001783
103	1	0	-1.489657	3.320431	1.873168
104	6	0	-4.702118	2.282805	2.081275
105	1	0	-5.380260	0.257512	2.258044
106	1	0	-3.832397	4.239733	1.930144
107	7	0	-6.068778	2.802119	1.976470
108	8	0	-6.205932	4.001176	1.803828
109	8	0	-6.987285	2.003690	2.043546
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111	1	0	0.505652	-1.121266	4.540943
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113	1	0	0.306055	-2.845376	4.923882
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115	1	0	-1.340808	-3.631067	2.221718
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117	1	0	-0.281875	-4.409624	3.408285
118	6	0	1.952333	-2.675279	2.830977
119	1	0	2.304412	-3.290176	2.003684
120	1	0	2.492875	-1.722504	2.814766
121	1	0	2.214887	-3.196510	3.757466

References

([1]) Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, X. H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, A, J. C. Burant, S. S. Iyengar, S. J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, O. A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. G. Fox, Gaussian, Inc., Wallingford CT, **2009**.

([2]) J.L. Delgado, S. Filippone, A. Martín-Domenech, M. Altable, E. Maroto, F. Langa, N. Martín, R. Martínez-Alvarez, J. Am. Soc. Mass Spectrom. **2011**, *22*, 557-567.

([3]) Y. Hernández, V. Nicolosi, M. Lotya, F. M. Blighe, Z. Sun, S. De, I. T. McGovern, B. Holland, M. Byrne, Y. K. Gunko, J. J. Boland, P. Niraj, G. Duesberg, S. Krishnamurthy, R. Goodhue, J. Hutchison, V. Scardaci, A. C. Ferrari, J. N. Coleman, *Nat. Nanotechnol.* **2008**, ***3***, 563-568.

([4]) Boehm, H. P. *Carbon,* **2002**, *40*, 145 –149.

([5]) Stankovich, S.; Dikin, D. A.; Piner, R. D.; Kohlhaas, K. A.; Kleinhammes, A.; Jia, Y.; Wu, Y.; Nguyen, S. T.; Ruoff, R. S. *Carbon,* **2007**, *45*, 1558-1565.

([6]) (a) Del Canto, E.; Flavin, K.; Movia, D.; Navio, C.; Bittencourt, C.; Giordani, S. *Chem. Mater*., **2011**, *23*, 67–74.

([7]) Quintana, M.; Tapia, J. I.; Prato, M. *Beilstein J. Nanotechnol*., **2014**, *5*, 2328-2338

([8]) Matsumoto, M.; Saito, Y.; Park, C.; Fukushima, T.; Aida, T. *Nat. Chem*, **2015**, *7*, 730-736.

([9]) (a) Allongue, P.; Delamar, M.; Desbat, B.; Fagebaume, O.; Hitmi, R.; Pinson, J.; Saveant, J. M. *J. Am. Chem. Soc.,***1997**, *119,* 201-207; (b) Sinitskii, A.; Dimiev, A.; Corley, D. A.; Fursina, A. A.; Kosynkin, D. V.; Tour, J. M. *ACS Nano*, **2010**, *4*, 1949-1954.

([10]) T. Nomoto, S. Yagi, G. Kutluk, K. Soda, E. Hashimoto and M. Taniguchi, *J. Surface Anal.,* **2005**, *12*, 238-243.

([11]) Touhara, H.; Okino, F. *Carbon,* **2000**, *38*, 241- 267.

([12]) Yang, G.; Hu, H.; Zhou, Y.; Hu, Y.; Huang, H.; Nie, F.; Shi, W. *Sci. Rep*. **2012**, *2*, 698.