Novel Metal-Organic Framework Linkers for Light Harvesting Applications

Supporting Information

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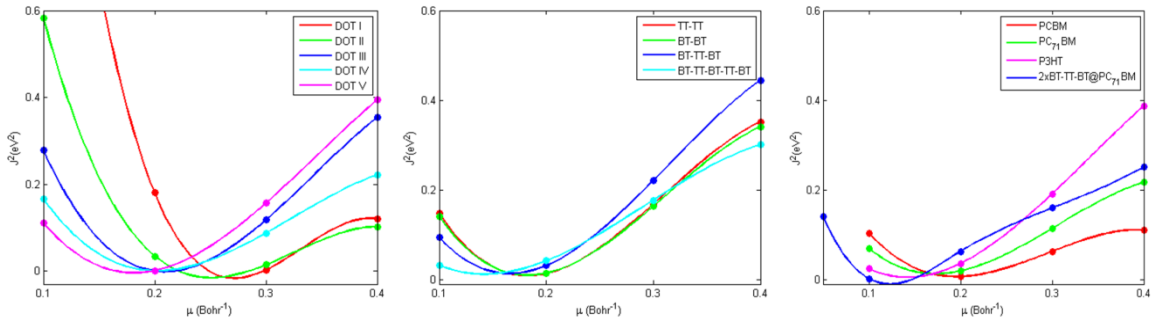

Fig. S1: Plots of J^2 as a function of μ for DOT I-V (Left), TT-TT, BT-BT, BT-TT-BT, BT-TT-BT-TT-BT (Middle), P3HT, PCBM, $PC_{71}BM$ and 2x BT-TT-BT@$PC_{71}BM$ (Right); the minimum of each curve was determined by cubic spline interpolation (optimal μ values are reported in Table 1).

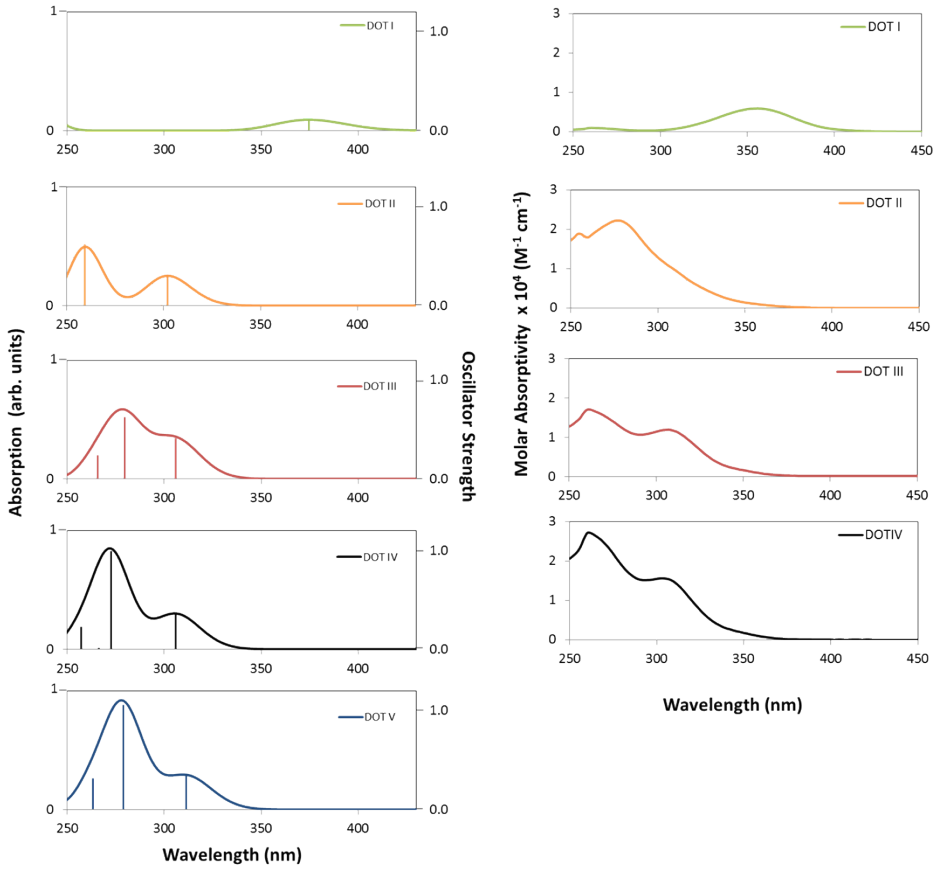

Fig. S2: The TDDFT/LC-BLYP/6-311G(d,p) predicted absorption spectra and oscillator strengths (represented by the vertical lines) of DOT I-V (left) compared to the experimental spectra (right). The TDDFT predicted absorption spectra curves were determined by Gaussian convolution using a FWHM of 3000 cm^{-1}. All experimental absorption spectra were recorded using a Shimadzu UV-3600 UV-Vis-NIR spectrophotometer in dimethylformamide (DMF) at room temperature. DOT I was purchased from Sigma-Aldrich and used without further purification and DOT II-IV were prepared according to a previously reported procedure. [1]

Synthesis of the BT-TT-BT Linker

General Remarks. All manipulations of air and/or water sensitive compounds were performed under an inert atmosphere using standard glovebox and Schlenk techniques. Xylenes was distilled from CaH_2. Reagents, unless otherwise specified, were purchased from Sigma-Aldrich and used without further purification. Tetrakis(triphenylphosphine)palladium(0) was purchased from Strem Chemicals and used as received. $CDCl_3$ was purchased from Cambridge Isotope Labs and used as received. Methyl 2-(benzyloxy)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate was prepared according to previously reported procedures.[i] Proton and carbon (^1H and ^{13}C) nuclear magnetic resonance (NMR) spectra were recorded on a Varian Inova Unity VNMR 500 MHz spectrometer at 25 ˚C. ^1H and ^{13}C NMR spectra are referenced to the residual solvent impurity peak of the given solvent. Chemical shifts are reported in ppm and coupling constants in Hz as absolute values. Flash chromatography was performed on a Teledyne Isco CombiFlash Purification System using Redi*Sep* Rf prepacked columns. Microwave assisted reactions were performed in a CEM Discover microwave reactor. Elemental analyses were performed by Galbraith Laboratories, Inc. Matrix-assisted laser desorption ionization (MALDI) mass spectra were measured on 4800 MALDI TOF/TOF analyzer from Applied Biosystems. UV-Visible spectra were recorded using a Shimadzu UV-3600 UV-Vis-NIR spectrophotometer at room temperature.

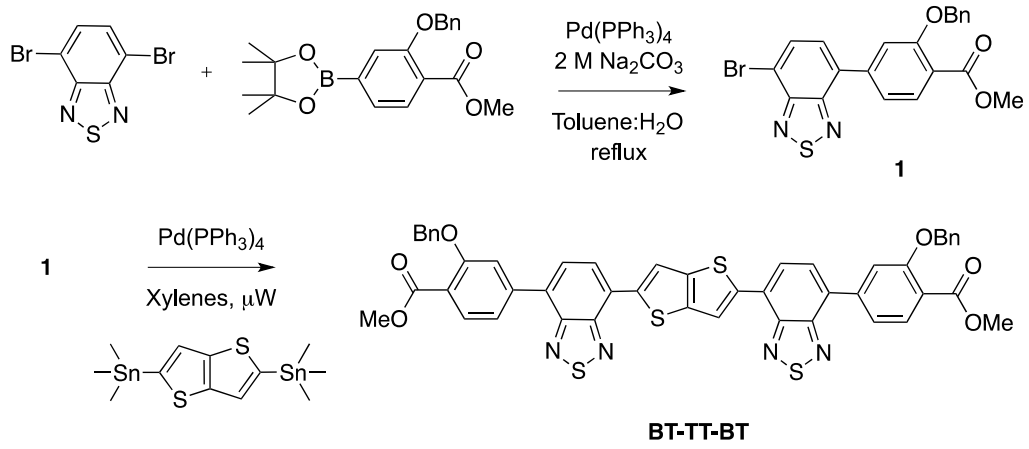

Fig. S3: Synthesis of BT-TT-BT.

Complex Synthesis:

Methyl 2-(benzyloxy)-4-(7-bromobenzo[c][1,2,5]thiadiazol-4-yl)benzoate (1)

In an argon filled glove-box, methyl 2-(benzyloxy)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (0.300 g, 0.82 mmol), 4,7-dibromo-5,6-benzo[*c*][1,2,5]thiadiazole (600 mg, 2.04 mmol) and $Pd(PPh_3)_4$ (94 mg, 0.08 mmol) were combined and 10 mL of toluene was added. The tube was sealed, removed from the glove box and an aqueous solution of degassed 2 M Na_2CO_3 (~5 mL) was added *via* cannula. The resulting mixture was heated to reflux and vigorously stirred for 12 hours. After this time, the reaction mixture was allowed to cool and volatiles were removed *in vacuo.* The residue was extracted

with $CHCl_3$ and filtered through a pad of celite. The filtrate was poured into a separatory funnel containing 50 mL DI water and the organic layer was washed with 50 mL DI water (3x), then brine. The organic layer was dried over anhydrous $MgSO_4$ and volatiles removed *in vacuo*. Purification was accomplished by flash chromatography using a (hexanes: ethyl acetate) gradient as the eluent which afforded 275 mg of a pale yellow solid (0.60 mmol, 74 %). **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K): δ 7.99 (d, J = 7.5 Hz, 1H); 7.94 (d, J = 7.5 Hz, 1H); 7.67 (s, 1H), 7.59 (d, J = 7.5 Hz, 1H), 7.54 (d, J = 7.5 Hz, 2H), 7.50 (dd, J = 7.5, 1.0 Hz, 1H), 7.41 (t, J = 7.5 Hz, 2H), 7.34 (t, J = 7.5 Hz, 1H), 5.30 (s, 2H), 3.96 (s, 3H), ppm. **^{13}C NMR** (125 MHz, $CDCl_3$, 298 K): δ 166.44, 158.28, 153.90, 152.78, 141.48, 136.66, 132.63, 132.15, 132.11, 128.59, 128.53, 127.87, 126.94, 126.72, 121.11, 120.62, 115.19, 114.25, 70.90, 52.13. **Anal. Calcd.** for $C_{21}H_{15}BrN_2O_3S$: C, 55.39; H, 3.32; N, 6.15. Found: C, 55.51; H, 3.36; N, 6.20.

Dimethyl 4,4'-(7,7'-(thieno[3,2-b]thiophene-2,5-diyl)bis(benzo[c][1,2,5]thiadiazole-7,4-diyl))bis(2-(benzyloxy benzoate) (BT-TT-BT).

A microwave tube was loaded with **1** (100 mg, 0.22 mmol) and 2,5-bis(trimethylstannyl)thieno[3,2-*b*]thiophene (41 mg, 0.09 mmol). The tube was brought inside a glove box and $Pd(PPh_3)_4$ (5.1 mg, 4.4 mol) and 1 ml of xylenes was added. The tube was sealed, removed from the glove box and subjected to the following reaction conditions in a microwave reactor: 120 °C for 5 min, 140 °C for 5 min and 170 °C for 10 min. After this time the reaction mixture was precipitated into methanol and collected by filtration. Purification was accomplished by flash chromatography using a (hexanes: chloroform) gradient as the eluent to give 57 mg (0.004 mmol, 72.9 %) of a red solid. **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K): δ 8.55 (s, 2H), 8.00 (d, J = 7.5 Hz, 2H); 7.94 (d, J = 7.5 Hz, 2H), 7.77 (s, 2H), 7.75 (d, J = 7.5 Hz, 2H), 7.58-7.55 (m, 6H), 7.43 (t, J = 7.5 Hz, 4H), 7.36 (t, J = 7.5 Hz, 2H), 5.33 (s, 4H), 3.95 (s, 6H) ppm. **^{13}C NMR** (125 MHz, $CDCl_3$, 298 K): δ 166.47, 158.31, 153.71, 152.52, 142.18, 142.05, 140.95, 136.76, 132.09, 131.62, 128.60, 128.44, 127.86, 127.31, 126.99, 125.54, 121.08, 120.98, 120.15, 115.10, 70.81, 52.13. **MS (MALDI-TOF):** *m/z*: 888.1587, calculated 888.1205. **Anal. Calcd.** for $C_{48}H_{32}N_4O_6S_4$: C, 64.85; H, 3.63; N, 6.30. Found: C, 65.01; H, 3.71; N, 6.40.

Optimized Coordinates (DOT I-V, TT-TT, BT-BT, BT-TT-BT, BT-TT-BT-TT-BT, PCBM, $PC_{71}BM$, 2xBT-TT-BT, IRMOF-74-II(Mg), IRMOF-74-TT-TT(Mg), and IRMOF-74-BT-TT-BT(Mg))

DOT I: E(LC-BYLP) = -758.589220709 Hartree

C	-1.48526600	-0.59912800	0.00016100
C	-1.52424100	0.81215400	0.00014300
C	-0.27339200	-1.28403600	0.00017300
C	0.93217100	-0.59655400	0.00015000
C	0.89319600	0.81472800	0.00008100
C	-0.31867800	1.49963600	0.00008100
C	-2.76034200	-1.32756700	0.00013900
O	-3.85848400	-0.78688100	-0.00050600
O	-2.64370100	-2.65882300	-0.00023200
O	-2.66822500	1.51443600	0.00024900
O	2.07615500	-1.29883600	0.00021500
C	2.16827200	1.54316700	0.00000700
O	2.05163100	2.87442300	-0.00024900
O	3.26641400	1.00248100	-0.00031700
H	-0.25927700	-2.37241400	0.00020200
H	-0.33279300	2.58801400	0.00005800
H	-3.55445000	-3.01345200	-0.00061700
H	-3.41284300	0.85977500	0.00046700
H	2.82077300	-0.64417500	0.00027600
H	2.96238000	3.22905200	-0.00048200

DOT II: E(LC-BYLP) = -989.166133137 Hartree

C	4.67547300	2.62548800	-0.71782400
C	4.65793100	4.00570700	-0.99082100
C	5.87939300	1.99230200	-0.44945200
C	7.08113000	2.70733800	-0.44363100
C	7.05610800	4.09068700	-0.71737300
C	5.83467000	4.72078800	-0.99019300
C	8.31807800	4.82122200	-0.70534900
O	8.21730400	6.13000400	-0.97641600
O	9.40996200	4.30916100	-0.46910300
O	8.21015700	2.04831000	-0.17134100
H	3.71481100	4.49725500	-1.22708500
H	5.92170800	0.92945000	-0.21141000
H	5.84062200	5.78855400	-1.20838300
H	9.12770900	6.48428700	-0.93338900
H	8.95052400	2.71605500	-0.20924500
C	1.03247800	0.38084300	-0.71303100
C	1.04866500	1.69706800	-0.20657000
C	2.21251000	-0.18168700	-1.21742800
C	3.38857700	0.53446400	-1.22122600
C	3.41210900	1.84788000	-0.71693500
C	2.24901400	2.41444400	-0.21834500
C	-0.22721200	-0.35337800	-0.69129500
O	-1.28307800	0.09985000	-0.25548600
O	-0.16712300	-1.59563700	-1.19098500

O	-0.03918900	2.28904100	0.29274500
H	2.17434500	-1.19674300	-1.61235000
H	2.24116800	3.42076500	0.20046100
H	-1.07067100	-1.96115700	-1.11210800
H	-0.78503400	1.63023300	0.22108600
H	4.29696200	0.09930600	-1.63651800

DOT III: E(LC-BYLP) = -1298.29537368 Hartree

C	-0.87702300	-0.62802800	-0.64200800
C	-0.86743100	0.71464400	-1.08506300
C	0.31502100	-1.21712200	-0.19266500
C	1.49316800	-0.49981700	-0.17926200
C	1.51141300	0.84114400	-0.61606600
C	0.33565600	1.43072100	-1.06327900
C	-2.13849400	-1.35649600	-0.67310200
O	-3.20540300	-0.87967200	-1.06479100
O	-2.07261000	-2.62566100	-0.23512600
O	-1.96708200	1.33144900	-1.53254400
H	0.28400400	-2.25201400	0.14940100
H	0.31869600	2.45722700	-1.42970200
H	-2.98131500	-2.98078000	-0.31462400
H	-2.71066100	0.66497900	-1.47491400
C	2.79471400	1.59015200	-0.62245000
C	2.92797900	2.87610900	-0.06911200
C	3.91291100	0.97976600	-1.19810500
C	5.16647400	1.58546700	-1.25824800
C	5.29974000	2.87142400	-0.70491000
C	4.18154300	3.48181000	-0.12925500
C	6.30051600	0.85898000	-1.93461200
H	2.41463000	-0.95490200	0.18504900
C	1.79393800	3.60259600	0.60725200
H	3.78897700	-0.00902900	-1.64798100
H	4.30547700	4.47060500	0.32062100
C	6.58304100	3.62043200	-0.71129400
C	6.60128700	4.96139200	-1.14809900
C	7.75879800	3.03085400	-0.26408300
C	8.96188600	3.74693000	-0.24230200
C	8.97147600	5.08960400	-0.68535000
C	7.77943300	5.67869800	-1.13469400
C	10.23294400	5.81807700	-0.65424100
O	10.16705200	7.08725500	-1.09217800
O	11.29983500	5.34128100	-0.26246900
O	10.06154200	3.13011600	0.20515600
H	5.67982400	5.41647800	-1.51240900
H	7.77575900	2.00434600	0.10233400
H	7.81044900	6.71359100	-1.47675500
H	11.07574600	7.44239100	-1.01263000
H	10.80512900	3.79657400	0.14749100
H	5.90721200	0.13560100	-2.66160600
H	6.91448000	0.29794100	-1.21331700
H	6.97403800	1.54967500	-2.45901600

H	1.17997400	4.16363500	-0.11404300
H	2.18724200	4.32597500	1.33424600
H	1.12041600	2.91190100	1.13165700

DOT IV: E(LC-BYLP) = -1607.33408096 Hartree

C	5.18900600	-0.36653700	-0.48067300
C	4.97256400	0.69820500	0.41146900
C	4.16099800	-0.74895100	-1.35141500
C	2.92973000	-0.10100000	-1.39101100
C	2.71799100	0.97026800	-0.50739900
C	3.73121400	1.33895800	0.37575300
C	6.46623300	-1.12481100	-0.52850600
H	4.34244700	-1.58051700	-2.03777400
H	3.54159200	2.16001900	1.07286200
C	1.42146800	1.70647000	-0.50609300
C	1.17794500	2.72555500	-1.44170900
C	0.43968600	1.38917600	0.43084800
C	-0.80077200	2.03120200	0.47229400
C	-1.04971400	3.04258900	-0.47195500
C	-0.05265300	3.37459200	-1.39760200
C	-1.79293900	1.63788200	1.53687700
C	1.85083500	-0.54924800	-2.33949100
C	2.22367800	3.11894200	-2.44972100
H	0.65448400	0.60928200	1.16684600
H	-0.25905300	4.16544000	-2.12388900
C	-2.32999400	3.79570000	-0.51984700
C	-2.30638700	5.20532000	-0.57382300
C	-3.55029700	3.13123600	-0.54231900
C	-4.75645100	3.83909800	-0.61551900
C	-4.72319400	5.25240400	-0.66541900
C	-3.48649800	5.91668100	-0.64347200
C	-5.98828300	5.97038300	-0.74204100
O	-5.88025600	7.31041000	-0.78280700
O	-7.09478900	5.42672000	-0.76968700
O	-5.90107700	3.14617400	-0.64143300
H	-1.34802200	5.72439700	-0.54081300
H	-3.60370900	2.04248700	-0.52553000
H	-3.48397900	7.00659000	-0.67736800
H	-6.79792300	7.64769900	-0.83282600
H	-6.63925200	3.81927800	-0.69819200
C	7.68618300	-0.46675600	-0.62833900
C	6.43881300	-2.53521200	-0.50314800
C	7.61484100	-3.25330700	-0.57227800
C	8.85112100	-2.59544300	-0.67225900
C	8.88813800	-1.18168200	-0.70217100
C	10.11181600	-3.32083700	-0.75124600
O	11.21757300	-2.78332200	-0.84640600
O	10.00044000	-4.66069200	-0.71372300
C	6.00125600	1.15108600	1.41596700
O	10.03229200	-0.49510300	-0.80480800
H	7.74204700	0.62109400	-0.67363600

H	5.48125900	-3.04841700	-0.40966400
H	7.60956800	-4.34339900	-0.54538700
H	10.91538700	-5.00333200	-0.77575800
H	10.76713900	-1.17277000	-0.84894500
H	-1.26962900	1.20816100	2.40197500
H	-2.50284700	0.87846800	1.17410400
H	-2.38846600	2.49478100	1.87882200
H	0.94032100	-0.84134900	-1.79519800
H	2.18635300	-1.40625000	-2.93864400
H	1.55587000	0.25664500	-3.02936500
H	3.15010000	3.44453200	-1.95337800
H	1.86575200	3.93823900	-3.08741300
H	2.49955500	2.27411200	-3.09975600
H	5.50845600	1.62715600	2.27471200
H	6.69452800	1.89051100	0.98589600
H	6.61200300	0.31529000	1.78222800

DOT V: E(LC-BYLP) = -1916.50890566 Hartree

C	3.64195100	0.86811000	-0.43177300
C	3.46634400	2.04978000	0.31241600
C	2.56962000	0.36931200	-1.18432800
C	1.33371900	1.00865600	-1.24915500
C	1.16249000	2.19568400	-0.51550600
C	2.22055800	2.68223200	0.25243500
C	4.91854000	0.10752700	-0.44116700
H	2.71813000	-0.55060700	-1.75651500
H	2.06391000	3.59330400	0.83698100
C	-0.13586400	2.92906400	-0.54688700
C	-0.43573600	3.80456600	-1.60427800
C	-1.06631000	2.74366900	0.47871000
C	-2.29852600	3.40067300	0.49470300
C	-2.59839800	4.27617600	-0.56268800
C	-1.66795200	4.46157100	-1.58828500
C	-3.28594100	3.15981300	1.60561000
C	0.20849800	0.43240700	-2.06652600
C	0.55167800	4.04542300	-2.71518700
H	-0.81942400	2.05486800	1.29156900
H	-1.91483800	5.15037100	-2.40114400
C	-3.89675000	5.00955700	-0.59406800
C	-4.06798200	6.19658000	0.13958900
C	-4.95481600	4.52301700	-1.36201900
C	-6.20060100	5.15547100	-1.42200000
C	-6.37621000	6.33713600	-0.67780100
C	-5.30388200	6.83592600	0.07476300
C	-2.94276200	6.77282300	0.95696700
H	-4.79816600	3.61195000	-1.94657100
H	-5.45239200	7.75584100	0.64695500
C	6.13168500	0.74507900	-0.68032200
C	4.89808300	-1.28949600	-0.23537700
C	6.07293900	-2.01396600	-0.26740600
C	7.30203400	-1.37666200	-0.50733500

C	7.33230600	0.02349700	-0.71797000
C	8.56056200	-2.10831600	-0.55176100
O	9.66019600	-1.58852000	-0.76423400
O	8.45601000	-3.43440100	-0.34089800
C	4.54263000	2.63756200	1.19007000
O	8.46907700	0.68916300	-0.95939600
H	6.18113500	1.81797400	-0.86718600
H	3.94789700	-1.78439600	-0.03214900
H	6.07293100	-3.09177900	-0.10187300
H	9.36924200	-3.78278500	-0.40089500
H	9.20303000	0.00783400	-0.94971900
C	-7.65279700	7.09772200	-0.66840700
C	-7.63233500	8.49474700	-0.87418100
C	-8.80718900	9.21922000	-0.84214700
C	-10.03628700	8.58191700	-0.60223500
C	-10.06656600	7.18175400	-0.39162800
C	-8.86594600	6.46017000	-0.42927200
C	-11.29481100	9.31357900	-0.55778700
O	-11.19023800	10.63968200	-0.76852200
O	-12.39442700	8.79381000	-0.34515900
H	-12.10345700	10.98808500	-0.70841800
C	-7.27688200	4.56769900	-2.29966600
O	-11.20334500	6.51608300	-0.15025400
H	-6.68214600	8.98964700	-1.07739700
H	-8.80717600	10.29703700	-1.00766000
H	-8.91540200	5.38727100	-0.24243000
H	-11.93730300	7.19740500	-0.15998400
H	-2.89401700	2.43052200	2.32739500
H	-4.24133300	2.78030300	1.21285100
H	-3.52102600	4.08808100	2.14994400
H	-0.67712600	0.24028100	-1.44229100
H	0.51126600	-0.51103000	-2.54043400
H	-0.11451200	1.12560500	-2.85925400
H	1.50707000	4.42493300	-2.32242900
H	0.15975400	4.77471400	-3.43697300
H	0.78676200	3.11715400	-3.25952000
H	-2.05713600	6.96495200	0.33273700
H	-2.61975600	6.07962000	1.74969200
H	-3.24553100	7.71625800	1.43088000
H	4.09090800	3.23454300	1.99429200
H	5.21284200	3.30448900	0.62532600
H	5.17274600	1.86018900	1.64274700
H	-7.90699400	5.34507700	-2.75234100
H	-7.94709900	3.90076800	-1.73493300
H	-6.82515600	3.97072400	-3.10389000

TT-TT: E(LC-BYLP) = -3040.36831870 Hartree

C	-4.77234700	-3.73424800	0.14929700
C	-4.89289700	-2.41287400	0.62987800
C	-3.77359300	-1.61321200	0.71800000
C	-2.50517600	-2.07704200	0.32851400

C	-2.38071900	-3.39624800	-0.16452300
C	-3.52032300	-4.20561400	-0.23909500
C	-1.38924500	-1.13140300	0.46304700
O	-0.18011800	-1.66572300	0.05885800
O	-1.45000000	0.00439600	0.87511900
O	-1.22260500	-3.95273800	-0.56662200
H	-5.87236500	-2.02067900	0.90317300
H	-3.83550400	-0.58658700	1.08246300
H	-3.38388800	-5.22826100	-0.59500500
H	0.48724600	-0.96122200	0.18842900
C	-9.68601100	-7.28608700	-0.14483000
C	-8.52647100	-7.39231900	-0.87505300
S	-9.63880900	-5.94594800	0.99887100
C	-8.04367400	-5.50600300	0.45904700
C	-7.59334600	-6.38318000	-0.52259700
S	-5.99761400	-5.94838100	-1.05531800
C	-5.95586800	-4.59250200	0.06908000
C	-7.11618800	-4.48867500	0.79810500
H	-8.37856800	-8.14834400	-1.64424400
H	-7.26996800	-3.72932900	1.56218000
H	-0.50464800	-3.28811700	-0.45711300
C	-10.86713400	-8.12193300	-0.21604100
C	-12.16640200	-7.78163600	0.07566500
C	-13.04889000	-8.87546700	-0.11962000
C	-12.42875700	-10.03669400	-0.57008200
S	-10.71097900	-9.80236000	-0.72381200
S	-14.76270000	-9.11250900	0.04144200
C	-14.61458200	-10.78582100	-0.48993800
C	-13.31453800	-11.12354100	-0.78048100
C	-15.79882600	-11.64266900	-0.57437000
C	-16.92995300	-11.37570900	0.19368200
C	-18.06717800	-12.18885200	0.12469100
C	-18.05878500	-13.31159000	-0.73458400
C	-16.91133500	-13.57087800	-1.50390200
C	-15.79997600	-12.75807000	-1.43891200
C	-19.18180300	-14.24494500	-0.89357200
O	-19.10348300	-11.83845400	0.90951700
O	-19.21979800	-15.21332400	-1.61768500
O	-20.26790200	-13.91873100	-0.10321500
H	-16.95866900	-10.53547900	0.88958000
H	-16.94334000	-14.43840500	-2.16497800
H	-14.93476100	-12.95687800	-2.07118900
H	-19.82920100	-12.48975900	0.77426100
H	-20.95104900	-14.59636000	-0.28375300
H	-12.46020200	-6.78086500	0.38744100
H	-13.01881000	-12.12078900	-1.09998500

BT-BT: E(LC-BYLP) = -2462.98897824 Hartree

C	0.64367700	-1.45527400	-0.15193100
C	0.74573100	-0.07964300	0.23676300
C	1.83055000	-2.06602200	-0.48703200

C	3.08741200	-1.40783500	-0.45397600
C	3.24137900	-0.08476500	-0.09183100
C	2.02779800	0.60135700	0.26659400
N	-0.27791100	0.69714600	0.62158400
S	0.34888600	2.16252800	0.98454500
N	1.93060000	1.87654400	0.67325500
H	1.80877300	-3.10548100	-0.81887300
H	3.97221300	-1.98086300	-0.72307600
C	8.43190100	2.70514500	-0.20061000
C	-0.64408400	-2.18135400	-0.19321800
C	8.53323100	3.87366400	-0.97659800
C	9.71825300	4.58560500	-1.00216800
C	10.84316000	4.17866500	-0.27302100
C	10.75060700	3.00288600	0.49476300
C	9.55059200	2.28378200	0.51977300
C	12.04342200	5.04230200	-0.39822300
C	-0.67067400	-3.53988800	0.11602800
C	-1.85395700	-4.28391200	0.04738900
C	-3.04756200	-3.63614600	-0.34324600
C	-3.01027100	-2.26460200	-0.64507700
C	-1.83963000	-1.53736800	-0.57119500
C	-4.35479600	-4.29996900	-0.45252200
O	13.11133800	4.62895700	0.31811200
O	12.07933600	6.04632800	-1.08494900
O	11.82164400	2.57255500	1.20634700
O	-1.76340800	-5.58877000	0.37346000
O	-5.39982700	-3.78849300	-0.78288500
O	-4.30440500	-5.64318000	-0.12981700
H	7.68857100	4.20141600	-1.58265000
H	9.82645400	5.49133400	-1.60076000
H	9.49948600	1.36070100	1.10042300
H	0.22747900	-4.06224700	0.44771100
H	-3.95020600	-1.79652800	-0.94164100
H	-1.83464600	-0.47266400	-0.79276800
H	13.80328300	5.29650600	0.12838600
H	11.56731000	1.74764900	1.65745600
H	-2.65750100	-5.99151900	0.28990300
H	-5.21664400	-5.98306800	-0.23391300
C	4.55491400	0.58723600	-0.09118800
C	5.78868700	-0.13706200	0.06605600
C	4.68895300	1.95142700	-0.25012600
C	7.06976100	0.54841000	0.05215300
N	5.90751000	-1.46020900	0.25426900
C	5.94358500	2.61349300	-0.27723900
H	3.78893000	2.55604800	-0.34047100
C	7.15175900	1.96718400	-0.14273600
N	8.11297000	-0.27677000	0.22929100
S	7.50441200	-1.78586300	0.39823900
H	5.94062600	3.69842300	-0.39250100

BT-TT-BT: E(LC-BYLP) = -3488.67070920 Hartree

C	-4.82693400	-4.11784800	-0.02868500
C	-4.78296700	-2.70941200	0.23138100
C	-3.60331400	-4.71531500	-0.26126400
C	-2.37088300	-4.01821700	-0.23927600
C	-2.27190800	-2.66476600	0.03142300
C	-3.51924500	-1.99802600	0.26585000
N	-5.83872000	-1.91514000	0.47615900
S	-5.25378900	-0.40396000	0.71798300
N	-3.64946700	-0.69059100	0.52939300
C	-0.98854500	-1.97242600	0.07324000
C	0.25559000	-2.57058200	0.02545000
S	-0.86931400	-0.20704400	0.16008200
C	0.86746200	-0.30327100	0.09922000
C	1.30540700	-1.62493700	0.03496000
S	3.04305700	-1.72380400	0.03386100
C	3.16200100	0.04241200	0.09655300
C	1.91781800	0.64093800	0.13926700
C	4.44450900	0.73700200	0.07281600
C	5.69658300	0.05647300	0.23089700
C	6.95838200	0.77123000	0.22912000
C	6.99816700	2.19343800	0.05951100
C	5.76955700	2.80584600	-0.09332800
C	4.53743200	2.10725900	-0.09636200
H	-3.58198500	-5.77896600	-0.50427400
H	-1.46563400	-4.58330700	-0.46416900
H	0.39746800	-3.64888800	-0.00511000
H	1.77661700	1.71761900	0.20789700
N	5.83384800	-1.26806100	0.38163100
N	8.02072000	-0.03745100	0.37874800
C	8.26055200	2.96037000	0.04148000
H	5.73829900	3.89181400	-0.19849100
H	3.62557900	2.68798700	-0.24033000
S	7.44251200	-1.56465200	0.50916100
C	-6.08589900	-4.89178800	-0.05703900
C	9.36208300	2.59061800	0.83185900
C	10.50705200	3.36959000	0.81637900
C	10.61778600	4.52173100	0.02612000
C	9.52122800	4.88760100	-0.77979200
C	8.36317100	4.10353500	-0.75833100
C	11.90940900	5.24800700	0.11430200
C	-6.07616500	-6.22839300	0.34297200
C	-7.23097400	-7.01796100	0.29416900
C	-8.43662500	-6.44087100	-0.16887500
C	-8.43724400	-5.09083700	-0.56065900
C	-7.29389700	-4.31832200	-0.50735400
C	-9.71670200	-7.15684600	-0.26558600
O	11.98536000	6.35630300	-0.65746300
O	12.83512800	4.89099900	0.81998600
O	9.60006800	5.98646500	-1.57337500
O	-7.10441300	-8.29504000	0.70985200
O	-10.77068600	-6.70695000	-0.65535900

O	-9.62815900	-8.47487900	0.14857400
H	9.31177800	1.69328900	1.44448300
H	11.37481300	3.11294500	1.42588000
H	7.53223400	4.38142600	-1.41414300
H	-5.17178900	-6.69575000	0.73435600
H	-9.38401900	-4.67704000	-0.91115800
H	-7.31954800	-3.27127800	-0.79998900
H	12.88329400	6.70939300	-0.48469300
H	8.75950800	6.06753800	-2.05857000
H	-7.98249100	-8.73349600	0.63155700
H	-10.52534600	-8.85340500	0.04555200

BT-TT-BT-TT-BT: E(LC-BYLP) = -5251.46384904 Hartree

C	-4.78669400	-4.15200000	0.01378700
C	-4.76478700	-2.72461300	0.14325500
C	-3.54707100	-4.75180300	-0.12706300
C	-2.32396000	-4.04055000	-0.13427900
C	-2.24594400	-2.66291700	0.00626200
C	-3.50793200	-1.99505900	0.14425400
N	-5.83668000	-1.92504400	0.28819100
S	-5.27335600	-0.38713300	0.40678000
N	-3.65788100	-0.66976300	0.28471300
C	-0.97361300	-1.95263400	0.01130500
C	0.28195500	-2.53413100	-0.02353100
S	-0.87716700	-0.17987000	0.04783400
C	0.86375300	-0.25598600	-0.00209400
C	1.31822700	-1.57576900	-0.03376500
S	3.05967700	-1.65295600	-0.05276100
C	3.15649800	0.12018100	-0.02656900
C	1.90079400	0.70220100	0.00442000
C	4.43002600	0.82561100	-0.04740100
C	5.69342100	0.15063000	-0.00543800
C	6.94625000	0.88166100	-0.02004700
C	5.73142800	2.92330000	-0.10767500
C	4.51206300	2.21152700	-0.10142000
H	-3.50646500	-5.83306400	-0.26717800
H	-1.40702900	-4.61458800	-0.27038000
H	0.43980700	-3.61041600	-0.03426500
H	1.74314000	1.77814600	0.03484400
N	5.85643400	-1.17995000	0.04989300
N	8.02548400	0.08585400	0.02691800
C	17.13699600	8.60602200	0.00793400
H	5.67598100	4.01210800	-0.13439600
H	3.59161700	2.79499100	-0.13973500
S	7.47588600	-1.46276500	0.08282600
C	-6.03426800	-4.94381900	0.02419900
C	18.13866400	8.16455600	0.89630500
C	19.36876900	8.79759000	0.92493400
C	19.66457800	9.88696000	0.09074300
C	18.66119400	10.34279000	-0.78882000
C	17.41715300	9.69942100	-0.81810300

C	21.02448500	10.46294500	0.23402400
C	-6.01593500	-6.24562700	0.53082900
C	-7.15989700	-7.05356300	0.52479900
C	-8.36591200	-6.53264000	-0.00480200
C	-8.37573500	-5.21711600	-0.50383800
C	-7.24278700	-4.42616900	-0.49262200
C	-9.63483700	-7.27177100	-0.06627600
O	21.28061000	11.51213700	-0.58353000
O	21.85700500	10.03849800	1.01714100
O	18.90442400	11.40115100	-1.60432000
O	-7.02442600	-8.29251100	1.04435800
O	-10.68885600	-6.86918700	-0.50810000
O	-9.53615400	-8.55413800	0.45303700
H	17.93511700	7.34574800	1.58597400
H	20.15745700	8.47906900	1.60782900
H	16.64313500	10.07738500	-1.48875700
H	-5.11404500	-6.66753600	0.97547500
H	-9.32050500	-4.84589500	-0.90336700
H	-7.27669000	-3.40682400	-0.86935500
H	22.20181600	11.76735800	-0.36616900
H	18.09522500	11.56854600	-2.12083600
H	-7.89574300	-8.74781100	0.98488200
H	-10.42674000	-8.95187500	0.36557400
C	6.97893900	2.31292400	-0.07563700
C	8.21979700	3.07430600	-0.10171300
C	8.33490500	4.44286300	-0.27478800
S	9.80331700	2.30303300	0.12259000
C	9.67595200	4.88101600	-0.21266400
H	7.48143400	5.09541100	-0.44572700
C	10.59463100	3.85142200	0.00082000
S	10.47151000	6.42275900	-0.38089500
C	11.93706900	4.28620100	0.04007900
C	12.05311400	5.65402600	-0.13670500
H	12.79296600	3.62995300	0.18276800
C	13.29333400	6.41755800	-0.10602800
C	13.36048400	7.80521700	-0.46273700
C	14.50290200	5.84954100	0.26404300
C	14.61301000	8.54315500	-0.44409800
N	12.30662000	8.54635400	-0.83439500
C	15.72224500	6.56681300	0.28074200
H	14.52924400	4.80084800	0.56154100
C	15.83727100	7.90611200	-0.05224600
N	14.46718500	9.83033800	-0.80857500
S	12.87288800	10.05914700	-1.13612200
H	16.62460700	6.02115600	0.55974400

PCBM: E(LC-BYLP) = -2896.99144319 Hartree

C	-0.89030000	0.67479800	-0.02068200
C	0.55906200	0.74294800	-0.06069600
C	1.19409400	1.97955500	0.03311300
C	0.40899700	3.19555700	0.15369300

C	-0.97817900	3.12607300	0.18904700
C	-1.64206000	1.83578700	0.10510900
C	-1.31604300	-0.37667200	-0.92613000
C	-0.13913100	-0.97030300	-1.52232100
C	1.03915700	-0.26717100	-0.97884600
C	2.13570600	-0.00585900	-1.77554500
C	2.32201600	2.26100500	-0.81949100
C	1.06279200	4.23177700	-0.62759400
C	0.30083300	5.15066600	-1.34063800
C	-1.14822500	5.07723700	-1.30075300
C	-1.77321600	4.08686600	-0.55125800
C	-2.93366700	3.39362200	-1.08671700
C	-2.85556600	2.00462100	-0.67705600
C	-3.26792800	0.99926300	-1.54283900
C	-2.48672500	-0.21890400	-1.66515500
C	-0.17015100	-1.37923800	-2.84013500
C	-1.36229300	-1.16888800	-3.61999700
C	-2.50878200	-0.62390500	-3.04869900
C	-3.30704200	0.33433900	-3.79426100
C	-3.77665200	1.34114100	-2.86031300
C	-3.84789100	2.67257700	-3.25472100
C	-3.41820100	3.72138900	-2.34810200
C	-2.76064400	4.75215800	-3.13255600
C	-1.65165100	5.41417200	-2.62096100
C	2.24921100	3.65293000	-1.23061600
C	0.65682900	4.71114500	-5.40694700
C	1.81328600	4.55714200	-4.65230100
C	2.59480100	3.33799400	-4.76258800
C	2.17933200	2.31646500	-5.61266100
C	0.97338400	2.48272000	-6.40239000
C	-1.22084100	3.58989500	-6.27339700
C	-1.68998900	4.59977300	-5.34417900
C	-0.52929200	5.29278700	-4.80867800
C	-0.51200800	5.69333800	-3.47737900
C	0.69423200	5.53164000	-2.68658400
C	1.83245100	4.97703800	-3.26159800
C	3.09076800	3.00430700	-3.45090000
C	3.15337500	1.66915900	-3.06105000
C	2.78091600	0.60533700	-3.96320700
C	2.26950900	0.93329900	-5.20307600
C	1.09362400	0.22908000	-5.74804100
C	0.30545000	1.19684600	-6.47917600
C	-1.08571300	1.13964700	-6.46155500
C	-1.86427800	2.36073200	-6.34935600
C	-2.78213100	4.33761700	-4.52469000
C	-3.45467600	3.05357600	-4.60079500
C	-3.00643600	2.08690400	-5.49441900
C	-2.92980700	0.69794700	-5.07952200
C	-1.73895900	0.11930100	-5.67983300
C	-0.96870900	-0.79319300	-4.96391900
C	0.47368200	-0.77481400	-5.02992000

C	1.01321400	-1.32474900	-3.74811400
C	2.30419900	-0.55848500	-3.15288500
C	2.62468600	4.01572200	-2.51652600
C	2.75895900	1.29148500	-1.71785800
C	0.23099200	3.65221200	-6.30702400
C	2.32237000	-2.03546300	-3.48623800
C	2.32027000	-2.97568900	-2.30303000
C	3.31117000	-2.87827500	-1.32464700
C	1.39333000	-4.01650500	-2.23222900
C	3.37013200	-3.80279900	-0.28547800
H	4.03637100	-2.06249300	-1.37406300
C	1.45108100	-4.94367000	-1.19463900
H	0.61216400	-4.09243400	-2.99245900
C	2.43872800	-4.83690100	-0.21818000
H	4.14465100	-3.71296800	0.47775900
H	0.71809400	-5.75043200	-1.14650800
H	2.48143900	-5.55959900	0.59808600
C	3.17620900	-2.66555800	-4.59444200
H	4.08458800	-3.03739800	-4.08920600
H	2.63207600	-3.57366600	-4.91158300
C	3.61014100	-1.88182100	-5.82808900
H	4.17667400	-0.98394600	-5.54562600
H	2.75287500	-1.53015800	-6.41588500
C	4.48403700	-2.75356500	-6.72033700
H	3.95242600	-3.66865700	-7.03237000
H	5.38835000	-3.10100600	-6.19427000
C	4.91415300	-2.02229300	-7.96617900
O	4.55317800	-0.91286600	-8.29147800
O	5.76860600	-2.76866900	-8.70005300
C	6.21266300	-2.13565700	-9.91320100
H	6.88913700	-2.85203700	-10.38898800
H	5.35649100	-1.91236100	-10.56411700
H	6.73316000	-1.19555100	-9.68560300

$PC_{71}BM$: E(LC-BYLP) = -3277.80647065 Hartree

C	10.43174000	2.43573600	0.04657000
C	10.08911400	2.25804900	1.44274000
C	11.36100900	3.40834100	-0.33268900
C	10.69453000	3.03870300	2.40963200
C	9.90828200	3.56367100	3.51067900
C	8.54039000	3.22197900	3.67431200
C	7.74542500	4.15066100	4.39111300
C	9.96875300	4.07892200	-2.20913400
C	8.99225700	3.09592800	-1.80415000
C	11.15715200	4.21715300	-1.51001100
C	9.22145700	2.27851700	-0.70888000
C	8.13484600	1.98209100	0.21010900
C	6.81057900	2.41889000	-0.04299900
C	5.97252100	2.56664000	1.09116600
C	7.89635400	2.39075800	2.64704700
C	8.67020400	1.96589900	1.53545500

C	6.50739900	2.55304400	2.41688900
C	10.99732900	6.82677900	-1.83047000
C	9.67206400	6.52339000	-2.43561100
C	11.84523200	5.52825100	-1.31089300
C	9.21854300	5.24785000	-2.67706500
C	7.80383600	4.94685000	-2.56382300
C	6.84052200	5.94881500	-2.28439400
C	5.62484200	5.51407400	-1.69666100
C	6.56352800	3.27037900	-1.21546900
C	7.66410800	3.62742600	-2.03670800
C	5.48773200	4.19294200	-1.17024200
C	11.95998900	6.64450600	0.95870400
C	11.20475200	7.80799500	0.48305600
C	12.17992400	5.54739100	0.14227500
C	10.68908100	7.84140500	-0.79047400
C	9.34615300	8.32689600	-0.99429500
C	8.58935700	8.92931600	0.04407200
C	7.18222800	8.92571200	-0.11888100
C	7.32224900	7.29353200	-1.98088800
C	8.72350100	7.52200000	-1.99505700
C	6.55684000	8.11697100	-1.11779800
C	11.67182900	4.03624500	2.02701000
C	11.46805800	5.17734600	2.87354100
C	11.99196000	4.22560200	0.67992800
C	11.59451900	6.45229800	2.34297300
C	10.65477600	7.48552300	2.73098100
C	9.64941300	7.25219800	3.70520300
C	8.50172900	8.08196300	3.63614900
C	9.14716200	8.92416900	1.39372600
C	10.41023200	8.30883700	1.59002800
C	8.25360400	8.90524400	2.49504900
C	9.50501800	5.89627800	4.25415100
C	10.38206200	4.88259600	3.79395000
C	8.22086000	5.46817000	4.67701500
C	6.16830100	8.21980300	3.34525100
C	7.21885200	7.64772200	4.16125600
C	7.08065600	6.36894200	4.66947800
C	5.01961700	7.48336700	3.06232400
C	5.09490800	8.23998800	0.72205100
C	6.29065000	9.00054600	1.02292800
C	6.81632900	8.98774700	2.30316200
C	4.47046900	7.49347400	1.71798900
C	4.15911200	5.62815000	0.14225500
C	4.81601200	6.40732600	-0.88620400
C	5.27102300	7.68350500	-0.60397500
C	3.99076700	6.15537100	1.42115500
C	4.64712000	3.99949800	2.40854700
C	4.82833800	3.46243900	1.07734500
C	4.59024000	4.25649400	-0.02977300
C	4.23905200	5.32180400	2.58274700
C	5.88772300	5.60059400	4.38714400

C	6.30654500	4.22828300	4.19839700
C	5.70061500	3.44657900	3.23218700
C	4.87441200	6.14164500	3.59618500
C	12.39044800	6.50016100	-2.32945100
C	13.48598100	7.41764600	-1.83279000
C	12.70881900	6.13105200	-3.78483500
C	13.39812600	8.79641400	-2.03846800
C	14.64323300	6.88553800	-1.25957900
H	12.78847900	7.09281100	-4.32293500
H	13.73718800	5.72753900	-3.76514300
C	11.82862300	5.18495200	-4.59512500
C	14.44915800	9.63351600	-1.66920700
H	12.49191700	9.21659700	-2.48147400
C	15.69550700	7.72068100	-0.88906000
H	14.71338100	5.80804200	-1.09256600
H	10.80262300	5.56511200	-4.68570700
H	11.74947000	4.20065600	-4.11452200
C	12.40516400	5.00301900	-5.99430200
C	15.59928500	9.09672000	-1.09198600
H	14.36762600	10.70971800	-1.82882100
H	16.59223000	7.29525200	-0.43607000
H	13.42423100	4.58258400	-5.96402600
H	12.49906200	5.96820000	-6.52060200
C	11.54607000	4.09491200	-6.83830800
H	16.42057300	9.75188600	-0.79783700
O	10.50000600	3.59056900	-6.49061800
O	12.09232700	3.90549300	-8.06153000
C	11.31992600	3.05027400	-8.92621700
H	11.20377500	2.05538500	-8.47538100
H	10.32185100	3.47723900	-9.09409700
H	11.88354700	2.99275900	-9.86224400

$PC_{71}BM$@2xBT-TT-BT: E(LC-BYLP) = -10255.9422723 Hartree

C	11.67592100	-5.45380400	-2.03566300
C	10.29829600	-5.45984000	-2.16053200
C	12.33687900	-4.65711700	-1.07880100
H	12.29068100	-6.07917400	-2.68477000
C	9.51734900	-4.62925700	-1.32450600
H	9.81626600	-6.08652600	-2.90813000
C	13.81050500	-4.72893800	-1.01985600
C	11.55506100	-3.84342500	-0.19468300
C	10.15643000	-3.83589400	-0.36637600
C	8.04976600	-4.56808700	-1.45726800
O	14.43380800	-3.98283500	-0.16263300
O	14.45518200	-5.48457900	-1.79249700
O	12.11415800	-3.05475700	0.85904200
H	9.57050700	-3.21797900	0.31533100
C	7.23933600	-5.73471800	-1.62814700
C	7.35631000	-3.36348900	-1.40237700
H	15.39560300	-5.38459200	-1.62753200
H	13.06913200	-3.15282800	0.86062200

N	7.69384300	-7.00962400	-1.66474900
C	5.79101500	-5.64727400	-1.73017800
H	7.92537400	-2.43989500	-1.28434300
C	5.95520000	-3.26984500	-1.53238200
S	6.39413500	-7.95182500	-1.81990600
C	5.11818900	-4.37472000	-1.70067700
N	5.20387800	-6.86008300	-1.84372100
H	5.51048100	-2.27335500	-1.49597500
C	3.67927200	-4.24603300	-1.83337200
C	2.72372300	-5.25510500	-1.90488300
S	2.93677400	-2.65177100	-1.92529000
C	1.42218700	-4.73506700	-2.02552600
H	2.98943300	-6.30718900	-1.86783900
C	1.35515100	-3.33005700	-2.05030800
S	-0.14909500	-5.42415900	-2.15072000
C	0.04653400	-2.81797400	-2.17212200
C	-0.90085000	-3.83618400	-2.24531100
H	-0.22992000	-1.76817800	-2.21151700
C	-2.34240800	-3.75148200	-2.38153800
C	-3.12826200	-4.89641500	-2.52439600
C	-3.07357700	-2.51239400	-2.37732500
C	-4.52947900	-4.87182000	-2.64624400
H	-2.64045800	-5.87263800	-2.54216100
C	-4.52728800	-2.49398000	-2.47728400
N	-2.54041400	-1.27273300	-2.29181400
C	-5.28259200	-3.70187500	-2.61850600
H	-5.05270500	-5.82497600	-2.73398300
N	-5.03765500	-1.23991900	-2.46318400
S	-3.78044500	-0.23709500	-2.33083900
C	-6.75130600	-3.75124000	-2.73345700
C	-7.33246200	-4.69493000	-3.58813200
C	-7.59300700	-2.91519000	-1.96390500
C	-8.72571900	-4.85704600	-3.69849600
H	-6.70619300	-5.31962900	-4.22595200
C	-8.96593700	-3.07686700	-2.03594200
H	-7.16039100	-2.16713300	-1.30259000
C	-9.04825100	-2.95393100	2.15172200
C	-9.56499100	-4.04281300	-2.87016300
O	-9.22543400	-5.81850100	-4.63164700
H	-9.62580000	-2.45251300	-1.43191200
C	-7.64703400	-2.97852600	2.27356900
C	-9.80136300	-1.78398700	2.17945900
H	-9.57147700	-3.90708800	2.06398200
C	-11.03690700	-4.15689900	-2.85836500
H	-10.18498900	-5.82427800	-4.60292600
C	-6.86118000	-1.83359300	2.41642700
H	-7.15923000	-3.95474900	2.25580400
C	-9.04606000	-0.57609200	2.32068100
C	-11.27007800	-1.83335200	2.06450800
O	-11.59244900	-5.06843400	-3.59454200
O	-11.74075200	-3.40350800	-2.13684400

C	-7.59234200	-0.59450800	2.42063400
C	-5.41962200	-1.91829500	2.55265500
N	-9.55642100	0.67796700	2.33477400
C	-11.85122700	-2.77704400	1.20982700
C	-12.11177900	-0.99730200	2.83406100
H	-12.66957000	-3.60122700	-2.27755300
N	-7.05918500	0.64515500	2.50615100
C	-4.47223100	-0.90008800	2.62583600
S	-4.66786700	-3.50627100	2.64724600
S	-8.29921600	1.68079300	2.46712600
C	-13.24448500	-2.93916000	1.09946300
H	-11.22495800	-3.40174300	0.57200600
C	-13.48470900	-1.15897900	2.76202300
H	-11.67916300	-0.24924500	3.49537600
C	-3.16362100	-1.41216900	2.74765700
H	-4.74869200	0.14971000	2.58644800
C	-3.09658500	-2.81717800	2.77243900
C	-14.08375600	-2.12492800	1.92779500
O	-13.74420600	-3.90061200	0.16631800
H	-14.14457200	-0.53462500	3.36605300
S	-1.58199100	-0.73388600	2.87266800
C	-1.79504900	-3.33721600	2.89308200
C	-15.55567900	-2.23901000	1.93960000
H	-14.70376000	-3.90639000	0.19503900
C	-0.83949400	-2.32814700	2.96458700
H	-1.52933200	-4.38930300	2.93011900
O	-16.11122100	-3.15054600	1.20342400
O	-16.25952400	-1.48561900	2.66112100
C	0.59941700	-2.45683200	3.09728900
H	-17.18834200	-1.68333800	2.52041200
C	1.43642900	-1.35195600	3.26558100
C	1.27224300	-3.72938500	3.06778700
C	2.83754500	-1.44560300	3.39558200
H	0.99171600	-0.35547000	3.30198400
C	2.72056400	-3.81683000	3.16981900
N	0.68510600	-4.94219400	2.95424400
C	3.53099400	-2.65019900	3.34069700
H	3.40660200	-0.52200700	3.51362300
N	3.17507200	-5.09173600	3.13321600
S	1.87536300	-6.03393600	2.97806000
C	4.99858400	-2.71137200	3.47345200
C	5.77952400	-3.54195200	2.63743400
C	5.63766400	-1.91800900	4.43158300
C	7.15715000	-3.53591500	2.76230200
H	5.29749400	-4.16863800	1.88983500
C	7.03628900	-1.92553600	4.60328200
H	5.05173500	-1.30009100	5.11329600
C	7.81811400	-2.73923100	3.71915700
H	7.77191600	-4.16128800	2.11318800
O	7.59539200	-1.13687200	5.65700000
C	9.29173300	-2.81105000	3.77810900

H	8.55036000	-1.23494000	5.65858800
O	9.91504300	-2.06494900	4.63532600
O	9.93641000	-3.56669000	3.00546800
H	10.87683100	-3.46670400	3.17043400
C	4.47457800	6.43095800	-2.74476400
C	4.84577900	5.08303100	-3.13206600
C	4.82618300	6.92470900	-1.47860100
C	5.57164400	4.28046300	-2.25741400
C	5.23572200	2.87541700	-2.11957400
C	4.23483900	2.26613200	-2.93015200
C	3.60804100	1.10873300	-2.38900100
C	2.61758100	7.92164600	-1.19500600
C	2.23973500	7.39042600	-2.48688700
C	3.90829700	7.73025200	-0.70481600
C	3.15181700	6.67034400	-3.25664400
C	2.71178600	5.48784300	-3.97853000
C	1.34260200	5.10298100	-4.01092900
C	1.08263800	3.72395700	-4.24936000
C	3.46617000	3.11507700	-3.85648200
C	3.75902500	4.50883300	-3.90365300
C	2.12897100	2.74434000	-4.17346600
C	2.87541900	7.38900600	1.71532700
C	1.56959200	7.48439200	1.01282900
C	4.21787800	7.53562300	0.74113700
C	1.44172700	7.79732500	-0.33003400
C	0.36792900	7.21077100	-1.11029500
C	-0.61909800	6.36624900	-0.52784200
C	-1.27888600	5.45575900	-1.40170200
C	0.37529400	5.87438300	-3.21433300
C	0.85496300	6.96657200	-2.43583700
C	-0.78852900	5.21372600	-2.72779400
C	4.98905800	5.30717800	1.67289300
C	3.80773300	5.18896500	2.53352900
C	5.13058200	6.35979100	0.77189300
C	2.78615100	6.12061700	2.47751200
C	1.41642300	5.67396800	2.47839100
C	1.05583600	4.31611000	2.70465200
C	-0.22133200	3.91374400	2.22326300
C	-0.45749700	5.99258400	0.87637800
C	0.67101700	6.50403500	1.58008900
C	-0.96886500	4.74085300	1.31993500
C	5.95514600	4.79107300	-0.95617200
C	5.82964000	3.70849300	-0.01713500
C	5.57895400	6.08683500	-0.56942700
C	5.34191500	3.96243500	1.26531600
C	4.42016600	3.02531700	1.87598000
C	4.05826100	1.80351500	1.23706100
C	2.80753700	1.24021500	1.61868300
C	2.13151800	3.32911100	2.79634500
C	3.47426000	3.77966400	2.64741300
C	1.85761500	1.99398900	2.38552200

C	4.56062500	1.54540100	-0.12380400
C	5.39373200	2.52225200	-0.73569700
C	3.76958000	0.75357800	-1.00609300
C	0.64939300	0.57704500	0.94441700
C	2.06424100	0.36827200	0.72742300
C	2.53241900	0.14165200	-0.55873400
C	-0.25909100	0.52937900	-0.11822900
C	-1.44603000	2.49079800	0.79569600
C	-0.50262000	2.52954700	1.89778400
C	0.52720500	1.59687400	1.96393800
C	-1.32762900	1.50984800	-0.19872100
C	-1.75529500	3.21164700	-1.94158800
C	-1.86756200	4.22292900	-0.90764700
C	-1.71847000	3.87048400	0.43181500
C	-1.48775500	1.87922300	-1.59887800
C	0.12582900	1.71748200	-3.46623300
C	-0.15201200	3.09763600	-3.80788300
C	-1.07253400	3.82947900	-3.06330300
C	-0.52391300	1.11861500	-2.37833200
C	1.60625700	0.10261800	-1.66994600
C	2.27162400	0.71147500	-2.79991500
C	1.54499000	1.50914000	-3.67858800
C	0.23640800	0.29697800	-1.45966600
C	3.95402500	8.42706700	1.92632100
C	4.84225800	8.16886400	3.11700100
C	3.69894500	9.93107100	1.81165600
C	4.27752500	7.98632600	4.38470500
C	6.23387100	8.17663100	2.96696900
H	3.25649300	10.23934300	2.77846800
H	4.69798700	10.40632400	1.77430000
C	2.84383200	10.46511700	0.67108700
C	5.10121000	7.80734900	5.50088700
H	3.18769600	7.96158100	4.47949600
C	7.06066600	7.99785900	4.08109900
H	6.65742800	8.29839900	1.96553300
H	1.83368700	10.03271700	0.69210300
H	3.27156000	10.20028900	-0.30651200
C	2.72201000	11.98201200	0.75615000
C	6.49412300	7.81147000	5.34887500
H	4.65730300	7.65623200	6.48790200
H	8.14659400	7.99506200	3.95949500
H	3.70992200	12.47493900	0.70080200
H	2.28063100	12.29865400	1.71930100
C	1.85449700	12.50525200	-0.36671400
H	7.13883000	7.66313200	6.21863100
O	1.30485200	11.81515600	-1.21194000
O	1.75510700	13.85837600	-0.32232800
C	0.93173100	14.40609600	-1.37515700
H	1.34845200	14.14167900	-2.36041300
H	-0.08942400	13.99679800	-1.31158600
H	0.93544900	15.49273500	-1.22019100

IRMOF-74-II (Mg) : E(HSE06) = -763.618915 eV

C	11.55744634	3.33206904	5.93855981
C	8.01560695	7.64879898	0.00872745
C	6.88717674	8.32948778	6.33147703
C	5.77896696	8.63529636	0.28514329
C	11.79020382	0.91276407	6.20149953
C	11.81405128	2.19204105	6.73432571
C	9.13279983	7.41090987	5.90903004
C	13.19777483	8.34470331	3.66318923
C	8.04126387	7.25303120	1.38651096
C	-2.88174282	11.68068151	0.89061652
C	2.27062948	10.58956137	5.44266538
C	0.64411045	15.60312190	3.16598711
C	11.22824383	3.11103159	4.56106303
C	13.55281227	8.17039409	2.28536342
C	2.62642411	10.76477721	6.82044888
C	0.31591360	15.82385276	4.54381291
C	-2.90906448	11.28509917	2.26811331
C	11.20175389	1.79713882	4.05598232
C	14.70101277	8.80765297	1.77798369
C	3.77932897	10.12641808	0.49769931
C	0.29535140	17.13687998	5.05119264
C	-4.03454043	10.60663049	2.77319402
C	11.49061250	0.68147643	4.83987762
C	15.52099716	9.61923596	2.55976449
C	4.59725382	9.31855255	6.54403305
C	0.58961759	18.25242859	4.26941185
C	-5.14554875	10.30035891	1.98929872
C	15.17190862	9.76302854	3.92160048
C	5.82905298	8.26095370	1.64697723
C	-5.09457052	10.67539243	0.62767680
C	4.24783951	9.17519745	5.18219911
C	0.88839910	18.02162842	2.90757587
C	14.05496200	9.14084551	4.45673974
C	6.92448905	7.60041376	2.18048319
C	-3.99777610	11.33430093	0.09485063
C	3.12885778	9.79501445	4.64869314
C	0.90643407	16.74320904	2.37243660
C	10.87908687	4.20049693	3.62992540
C	12.78603690	7.31853385	1.35720443
C	1.86288030	11.61431354	0.92014629
C	-0.03980548	14.73432338	5.47197190
C	-1.79067659	11.52604299	3.19925093
H	6.92365074	8.63644942	5.28547983
H	12.03676308	0.06262420	0.01522761
H	10.91713050	1.67419984	3.01029973
H	14.94943318	8.62192484	0.73246428
H	4.02716173	10.31117395	1.54369651
H	0.01045033	17.25951364	6.09671205
H	-3.99908536	10.29862497	3.81887660

H	15.78356807	10.40041684	4.56322652
H	4.97270739	8.47480190	2.28977366
H	-5.95435895	10.46493308	6.81394872
H	4.86040946	8.53973157	4.53940267
H	1.13563345	18.86972408	2.26594982
H	13.79264164	9.26321657	5.50871322
H	6.94952685	7.31093412	3.23186372
H	2.86548720	9.67229000	3.59731260
H	1.14336119	16.57691952	1.32046312
H	12.05514028	2.35761681	0.95650663
H	-3.97456018	11.62584895	5.87266971
O	11.64045803	4.54441232	6.50838721
O	10.13192504	6.70279833	6.32677346
O	10.48689177	3.95676618	2.44325828
O	12.10986572	7.80557880	4.23543273
O	9.04999690	6.57749440	1.95890688
O	-1.87247438	12.35747125	0.32078912
O	1.18190747	11.12675467	4.87026946
O	0.71964148	14.39130649	2.59374360
O	10.99238829	5.42031793	4.04634407
O	11.67214005	6.80979852	1.77437145
O	0.75072061	12.12692840	0.50240288
O	0.07502796	13.51514695	5.05480488
O	-0.79003933	12.23281417	2.78283227
O	13.19493821	7.09275686	0.17307463
O	9.12153457	7.87450226	4.72326260
O	-1.80623801	11.06454596	4.38591805
O	2.27027538	11.83584020	2.10591374
O	-0.43948024	14.97605798	6.65610171
Mg	10.42697106	5.40063777	1.04430708
Mg	11.97428616	6.32356938	5.59705676
Mg	10.39913734	7.20554485	3.32172868
Mg	-0.52500430	11.73297382	5.78486926
Mg	1.05311427	12.60933338	3.50744766
Mg	-0.49710802	13.53442006	1.23211957
Tv	21.84435129	0.00000000	0.00000000
Tv	-10.89831216	18.93152069	0.00000000
Tv	-0.00340034	0.00196605	6.82917633

IRMOF-74-TT-TT (Mg) : E(HSE06) = -1647.325520 eV

C	3.68945004	0.52727283	24.93803551
C	-0.87880466	-2.00890801	17.59717256
C	1.37217728	5.74223835	18.84462218
C	-2.26953952	0.52489661	26.04387681
C	-0.06423101	-3.01806883	17.11431272
C	2.17425966	6.64178582	18.16422648
C	-0.95489996	1.03864582	25.93390191
C	1.25523251	-3.15176914	17.61008947
C	-0.51906886	1.52489315	24.69554235
C	1.71275340	-2.23986446	18.56852089
C	3.95781897	5.00112975	18.15753334

C	3.20023070	20.20491904	6.27098717
C	-1.30737838	17.04782929	10.56833503
C	0.94182590	22.26787703	11.09310143
C	-2.24906404	20.70412035	6.18943226
C	0.03733274	16.71305152	10.20233422
C	2.28325651	22.10543398	11.56809797
C	-1.27646667	20.58670557	7.29258889
C	0.99463327	17.70364307	9.66906651
C	3.25098331	21.18263138	10.94145803
C	-1.39543289	-0.08038152	19.06103177
C	0.86634729	3.53588161	19.84885347
C	3.14145395	0.99677944	22.57438308
C	-0.43902669	-1.09401208	18.57594356
C	1.81830296	4.44948340	19.18795395
C	4.11078504	1.01877991	23.68520416
C	0.90974336	-1.19015427	19.05095115
C	3.16620689	4.08039786	18.86673613
C	-1.33575477	1.49949898	23.54836428
C	-2.10535094	16.05215421	11.15730675
C	0.12842343	23.23340055	11.71211081
C	2.38181788	20.30991529	5.13085894
C	-1.64916199	14.74429887	11.35845071
C	0.56388899	23.99263413	12.80337552
C	2.81193482	20.93505518	3.95464251
C	-0.34108942	14.40711888	10.93518364
C	-2.66984078	21.47290035	3.90494355
C	0.46995834	15.38113830	10.37497930
C	2.70000645	22.86148976	12.68485542
C	-1.83601917	21.34569912	5.00264085
C	1.87046808	23.78233964	13.30457661
C	0.36978372	8.61753707	14.73470517
C	-0.65813787	8.10287534	15.55677571
C	-1.40135293	9.08657849	16.23223952
C	-2.41466423	8.56880405	17.06967214
C	1.91166896	21.01991236	2.80681419
C	1.75691319	22.04967285	1.89122172
C	-0.33909659	24.98632189	13.38260640
C	-0.55485874	25.32118409	14.71022504
C	-0.71593922	-8.31903849	15.06699698
C	-0.46448089	-8.63756808	13.74001662
C	-2.12793858	26.70986473	13.61790687
C	-1.58158494	26.28766493	14.84230025
C	-2.94925525	0.88906481	31.71494905
C	-0.89031232	20.21848598	0.20380910
C	0.12494397	20.51233879	1.13993780
C	0.73441751	21.76535922	0.95552332
C	-2.43922540	7.18228012	17.04840673
C	0.42409259	10.00361953	14.78525596
C	1.34308371	10.89319036	14.12071541
C	1.51435848	12.25326143	14.33709838
C	2.50954531	12.79709703	13.49702355

C	3.11972162	11.86232914	12.64233141
C	4.12593014	12.41433597	11.81361477
C	-2.52308800	13.77834876	12.02062809
C	5.11200976	-7.37576981	15.57984099
C	5.00207907	-6.86063231	16.86389427
C	3.94862910	-5.92291199	16.96331180
C	3.24165829	-5.72341762	15.76503253
C	2.20946438	-4.76263339	15.85768443
C	2.13692513	-4.21030107	17.12710343
C	2.89786379	0.95230274	30.62623968
C	2.78185720	1.91424036	29.63172723
C	1.74291425	1.60692290	28.72298848
C	1.05391771	0.41873357	29.02064351
C	0.02738485	0.10169454	28.10319345
C	-0.05972779	1.04107294	27.08759837
C	3.49000359	6.27013539	17.79485969
H	-2.63560109	0.16713990	27.00575860
H	-0.44818133	-3.73298378	16.38752989
H	1.78064389	7.61556021	17.87461870
H	2.66786209	0.15277935	25.01671812
H	4.88626056	-1.91006591	17.23639784
H	0.34990144	6.01216283	19.11296634
H	0.50315707	1.88575754	24.57662366
H	2.73932901	-2.29409559	18.93323422
H	-1.80773953	4.70502247	17.92709079
H	3.66453065	16.32646277	11.42912095
H	-0.89030361	23.34361737	11.33979765
H	1.36282187	19.92939475	5.20758939
H	1.48995096	15.13860069	10.07337950
H	-3.07059112	22.71250424	13.04398493
H	-0.81691935	21.73294489	4.96660485
H	0.04324896	13.40039700	11.09817263
H	-2.30756526	21.94204126	2.99043405
H	2.23683513	24.37782120	14.14050171
H	1.06240674	8.01589333	14.14887663
H	3.71305515	9.16396749	17.69511247
H	2.33299890	22.97154232	1.93509619
H	-0.02204613	24.84994064	15.53387189
H	-0.98990427	-8.17443249	12.90680901
H	-1.46659405	19.29558607	0.17680049
H	0.94671897	12.81422955	15.07727044
H	-2.09021144	11.86548842	11.06953168
H	-1.11352692	-7.13225148	17.67420166
H	1.57096058	-4.44437262	15.03614904
H	3.43547894	2.78195229	29.56396817
H	-0.59898927	-0.78684029	28.14235924
Mg	1.30562030	20.57795450	8.56821125
Mg	3.56815119	18.80564945	8.98242994
Mg	-0.96056186	20.06440820	10.31048170
Mg	2.81919550	1.12154189	19.51781522
Mg	-1.70730701	2.54138253	20.67543039

Mg	0.55520172	0.83309944	21.31629740
O	2.67028613	19.66241958	7.38286960
O	-1.85532240	18.25954540	10.37183867
O	0.40684888	21.53708674	10.09984623
O	-1.63696714	19.98707225	8.38559037
O	0.62474991	18.94532737	9.58904972
O	2.88748346	20.50840113	9.89299158
O	-0.09373014	21.04502894	7.17623721
O	2.17253744	17.36407475	9.32161849
O	-2.35679813	21.06170378	11.39936040
O	4.21494600	-0.01433340	18.58528207
O	-0.31024677	3.91852072	20.15305987
O	1.95956429	0.55533638	22.74785405
O	-1.02668815	0.73245123	20.00379295
O	1.23628578	2.31551992	20.08958348
O	3.50131606	1.45202296	21.41391463
O	1.45472197	-0.31850817	19.91708781
O	3.71947877	2.90691092	19.21852475
O	-0.80414377	1.90058813	22.37900659
S	-0.81679956	10.66422647	15.84003542
S	-1.22098819	6.52937681	15.96836028
S	0.81376344	19.69323737	2.48617230
S	-1.37833970	25.89420594	12.30408187
S	0.30982921	-9.23587358	16.15888572
S	-1.85868314	2.22856294	32.03510580
S	2.42135120	10.29632839	12.86776920
S	3.17699848	14.36304663	13.26244119
S	3.89084901	-6.71156409	14.50558736
S	3.32890689	-4.90768047	18.20791347
S	1.70507940	-0.32388975	30.43698326
S	1.11386498	2.32696696	27.28983143
Tv	6.78984792	0.00000000	0.00000000
Tv	-2.67888302	36.32079435	0.00000000
Tv	-1.87373764	-20.36667214	32.41494020

IRMOF-74-BT-TT-BT (Mg) : E(HSE06) = -1288.505197 eV

C	-0.12711093	16.06570616	11.63587617
C	5.01440771	15.46257613	13.37731471
C	5.11198105	16.79878746	13.76956706
C	5.95611513	17.73601898	13.14674989
C	-0.06609002	17.42412980	12.08354611
C	4.74123375	2.25699312	26.10954696
C	0.02183247	-0.58585938	19.04912450
C	2.41646435	7.37168447	20.05078195
C	5.57757789	2.23819954	27.21188909
C	0.80633898	-1.64064742	18.61735228
C	3.23438979	8.31533566	19.45581635
C	0.04114128	2.70564118	27.08494758
C	2.16762195	-1.69087000	18.97856495
C	4.56491606	7.97482873	19.12051516
C	0.48709699	3.15643626	25.83920708

C	2.70849444	-0.68763221	19.78044477
C	5.03558757	6.69330951	19.42389945
C	5.68592346	24.17011733	6.80302464
C	1.12288258	20.81791504	10.89004673
C	3.42339857	26.09159169	11.69292877
C	0.17800054	24.62484094	6.72325871
C	2.48186167	20.52908835	10.53899563
C	4.79043188	25.94214514	12.09772516
C	1.13109516	24.51324670	7.84679764
C	3.42721035	21.56055617	10.06772564
C	5.71464890	24.96874236	11.47859442
C	-0.37818394	1.51031881	20.28332814
C	1.92381488	5.14326318	21.00219455
C	4.21599937	2.65172874	23.72463113
C	0.54257655	0.43067258	19.86979566
C	2.87276595	6.07409936	20.35936612
C	5.17666204	2.70257259	24.84388919
C	1.92386627	0.38779914	20.25182070
C	4.23276920	5.72913732	20.06542620
C	-0.33140964	3.13967246	24.69313076
C	0.32813128	19.76330083	11.37562356
C	2.65551087	27.10049485	12.31509608
C	4.87795106	24.29474009	5.65887566
C	0.80662594	18.45304728	11.48987106
C	3.19266429	27.92483048	13.30227177
C	5.33575941	24.87716590	4.47283958
C	2.13221434	18.17113857	11.08614598
C	-0.20386103	25.36894204	4.42151403
C	2.94049878	19.19910579	10.63203359
C	5.30092940	26.76191684	13.12155412
C	0.61951411	25.22778943	5.52650489
C	5.45533396	8.93421902	18.44087833
C	-0.57749042	8.55071604	17.39369986
C	0.28016645	9.44388612	16.71882329
C	0.40483259	10.79497241	17.04852488
C	5.54344367	10.31071504	18.82101641
C	4.52645452	27.74316215	13.71693308
C	5.84487980	15.09761273	12.26058633
C	-0.41426414	11.22925321	18.15008058
C	4.13697259	14.53489123	14.06530138
C	3.84895033	13.20323089	13.77656465
C	2.92955500	12.65658336	14.69602589
C	2.51018528	13.55639409	15.69284124
C	1.59240363	13.02013786	16.61430918
C	1.29527952	11.68992959	16.33381958
C	2.39890538	29.04365692	13.87547990
C	2.53394777	30.33736312	13.39944547
C	1.49512735	28.87007962	14.96216369
C	1.81680826	31.42918766	13.93552455
C	0.75146763	29.98932519	15.52127519
C	0.90835907	31.31796031	14.98893825

C	2.99211422	-2.83382138	18.50715239
C	2.86892044	-4.10426155	19.04616670
C	3.90837452	-2.70417091	17.42302703
C	3.61160566	-5.21186955	18.57773603
C	4.66586770	-3.84080550	16.92408640
C	4.52389353	-5.14305929	17.52387425
C	4.41735110	24.91560439	3.31951389
C	4.27753839	26.03290190	2.43709872
C	3.57249586	23.84137044	3.05655181
C	3.27677122	26.04211412	1.37761398
C	2.62444948	23.83418392	2.01717146
C	2.41702466	24.91083695	1.15448548
C	0.98035529	2.73582483	28.22152205
C	1.82070810	3.82244725	28.43894599
C	1.14374459	1.64093346	29.12629102
C	2.78585301	3.86148655	29.46496271
C	2.16274125	1.66097238	30.16555817
C	3.01655571	2.80508503	30.34716768
C	1.39229802	24.87326105	0.12932517
C	0.08157618	4.08246436	33.69794923
C	0.19196618	32.47328173	15.49913351
C	-0.29230244	-9.96217443	16.56276231
C	5.25386148	-6.30812154	17.05716386
C	6.15666717	-6.39968888	16.00198746
C	-0.23516779	-7.71531122	15.83124973
C	6.10242664	-8.64424037	16.74551135
C	4.05758161	2.86055607	31.35554182
C	4.54000976	1.83639321	32.16396937
C	5.58162284	2.27991827	33.00157784
C	-0.95850124	3.64141070	32.85411899
H	5.21488639	1.88249989	28.17433770
H	0.38870250	-2.43103321	17.99328257
H	2.85406364	9.30962902	19.23059019
H	3.70947863	1.91278821	26.19597920
H	5.83665809	-0.51680043	18.75961421
H	1.38331752	7.61735942	20.30102065
H	1.52033787	3.48194517	25.71344265
H	3.75717352	-0.71932940	20.07949297
H	6.07045365	6.42275307	19.21009661
H	6.15974983	19.99717351	11.63684340
H	1.62549888	27.23294560	11.98067986
H	3.84607856	23.95198842	5.73870338
H	3.97153940	18.99890751	10.33713230
H	-0.52701732	26.60883528	13.42646467
H	1.64964955	25.58529227	5.49208651
H	2.51868062	17.15631771	11.15594838
H	0.16978191	25.83387449	3.51128878
H	4.93971827	28.38781520	14.49306393
H	4.50568177	17.14873231	14.60696432
H	5.97291693	18.75245728	13.54239502
H	4.29672372	12.68542127	12.93310082

H	1.14942053	13.54729691	17.45378929
H	0.87678870	9.04578678	15.89563320
H	6.25271166	7.51410178	17.05451493
H	3.22450275	30.52389537	12.57536788
H	1.99321998	32.41155307	13.49314530
H	2.17081189	-4.25932540	19.87042777
H	3.45044112	-6.17176296	19.07247533
H	3.65345972	22.95169515	3.68267649
H	2.00679878	22.94132063	1.90476604
H	1.72406600	4.69307868	27.78826173
H	3.40009698	4.76028165	29.54724320
H	0.48656436	5.08958650	33.74242510
H	6.29528442	-10.82815197	17.15772850
H	-0.43224988	-5.53966515	15.39869572
H	4.13629407	0.82891000	32.12509730
Mg	3.73509519	24.46590486	9.12266790
Mg	6.03433500	22.68488561	9.45873413
Mg	1.45944581	23.86355870	10.83843802
Mg	3.88724767	2.74109534	20.67103019
Mg	-0.68761448	4.15839087	21.81381074
Mg	1.60868763	2.46937080	22.46912709
N	0.56910138	15.54346762	10.59863044
N	4.86244103	10.89114988	19.83721494
N	-0.44597213	12.47205491	18.68202688
N	5.90003410	13.88135358	11.67236861
N	1.24000506	27.69571357	15.58989189
N	-0.04326298	29.62109996	16.55213261
N	4.98668474	27.18451008	2.49854261
N	3.26866467	27.19800770	0.67737682
N	4.14841375	-1.56262289	16.73210597
N	5.45360283	-3.51742008	15.87267131
N	0.44256164	0.48301968	29.09840408
N	2.19246069	0.51862329	30.88752144
O	5.13476817	23.64057346	7.91083687
O	0.56559383	22.03822705	10.77645254
O	2.84457878	25.33438711	10.74330761
O	0.73680181	23.93469815	8.93884246
O	3.02367018	22.79178751	10.01569420
O	5.30006229	24.28960607	10.45732925
O	2.32172664	24.95670541	7.74764686
O	4.61967856	21.25771623	9.73823759
O	0.03538789	24.81902566	11.91736301
O	5.30158768	1.57050144	19.82291437
O	0.73402020	5.50432281	21.27809817
O	3.02358812	2.23912227	23.90051074
O	0.03976103	2.38691239	21.14008397
O	2.32112753	3.93857168	21.26839515
O	4.60384420	3.04554840	22.55198042
O	2.49899652	1.31561613	21.03676406
O	4.78729796	4.54348667	20.38220249
O	0.21267749	3.51248939	23.51905185

S	0.11417681	14.00028622	10.47459657
S	5.34634200	12.42873220	19.88960810
S	3.26452405	15.08901690	15.48921171
S	2.16525927	11.12459794	14.91081130
S	-0.28497497	1.54337300	34.19517878
S	0.84330909	-8.48370419	14.73067109
S	5.01514726	-7.86778183	17.83726121
S	4.89908755	4.37462510	31.66193167
S	0.16940235	28.02893769	16.74918379
S	4.41932251	28.13226711	1.32155899
S	5.22356853	-1.94102050	15.59298198
S	1.03810146	-0.43707235	30.28264035
Tv	6.86425701	0.00000000	0.00000000
Tv	-0.41042125	42.52042939	0.00000000
Tv	-0.83730293	-21.81725726	34.38057108

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