

Supporting Information

Yttrium catalysts for syndioselective β -butyrolactone polymerization: on the origin of ligand-induced stereoselectivity

J. Fang, M. J.-L. Tschan, T. Roisnel, X. Trivelli, R. M. Gauvin, C. M. Thomas* and L. Maron*

General considerations

Reaction of “yttrium isopropoxide” and Salan proligand

Monitoring of the reaction between “ $\text{Y}(\text{O}i\text{Pr})_3$ ” solution in toluene with salan by ^1H NMR in C_6D_6 at 50°C

Polymer synthesis

Figure 1S. Carbonyl region and methylene region of the ^{13}C NMR spectrum (125 MHz, CDCl_3 , 40°C) of PHB prepared by polymerization of *rac*-BBL with the alkoxide complex

Figure 2S. Crystal structure for **1**

Table 1S. Summary of crystallographic data for **1**

Table 2S. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**

Table 3S. Anisotropic displacement parameters (\AA^2) for **1**

Table 4S. Bond lengths [\AA] for **1**

Table 5S. Angles [°] for **1**

Table 6S. Torsion angles [°] for **1**

Computational details

Cartesian coordinates of all optimized complexes as well as their energies

References

General considerations

All manipulations requiring oxygen free and dry atmosphere were performed under a purified argon atmosphere using standard Schlenk techniques or in a glovebox. Solvents (toluene, THF) were taken from a solvent purification system (PureSolv, Innovative technology, Inc.), dried and distilled over Na/benzophenone under argon and degassed thoroughly by freeze-vacuum-thaw cycles (4 times) prior to use. Deutarated solvents ($[D_6]$ benzene, $[D_8]$ THF from Eurisotop) were freshly distilled over Na/benzophenone under Argon and degassed prior to use. “Yttrium isopropoxide” ($Y(O^iPr)_3$) solution in toluene was purchased from Aldrich and Strem. The Yttrium isopropoxide oxide ($Y_5O(O^iPr)_{13}$) was purchased from Strem. Racemic butyrolactone (*rac*-BBL) was purchased from Aldrich and distilled two times over CaH_2 under argon and degassed thoroughly by freeze-vacuum-thaw cycles prior to use. Gel permeation chromatography (GPC) analyses were carried out using a Waters instrument GPCV 2000, equipped with a UV and a viscometry detectors. The columns used are μ Styragel columns (two HT6E and one HT2) filled with 10 μ m styrene-divinyl benzene gel balls. THF was used as eluent at a flow rate of 1.0 $mL \cdot min^{-1}$. The number average molecular masses (M_n) and polydispersity index (M_w/M_n) of the resultant polymers were calculated with reference to a polystyrene calibration. M_n values were not corrected by a Mark–Houwink factor. NMR analyses were performed on a Bruker AC 500 MHz. PHBs microstructure was determined by $^{13}C\{^1H\}$ NMR spectroscopy in $CDCl_3$ on a Bruker 500 MHz spectrometer operating at 125 MHz.

Reaction of “yttrium isopropoxide” and Salan proligand

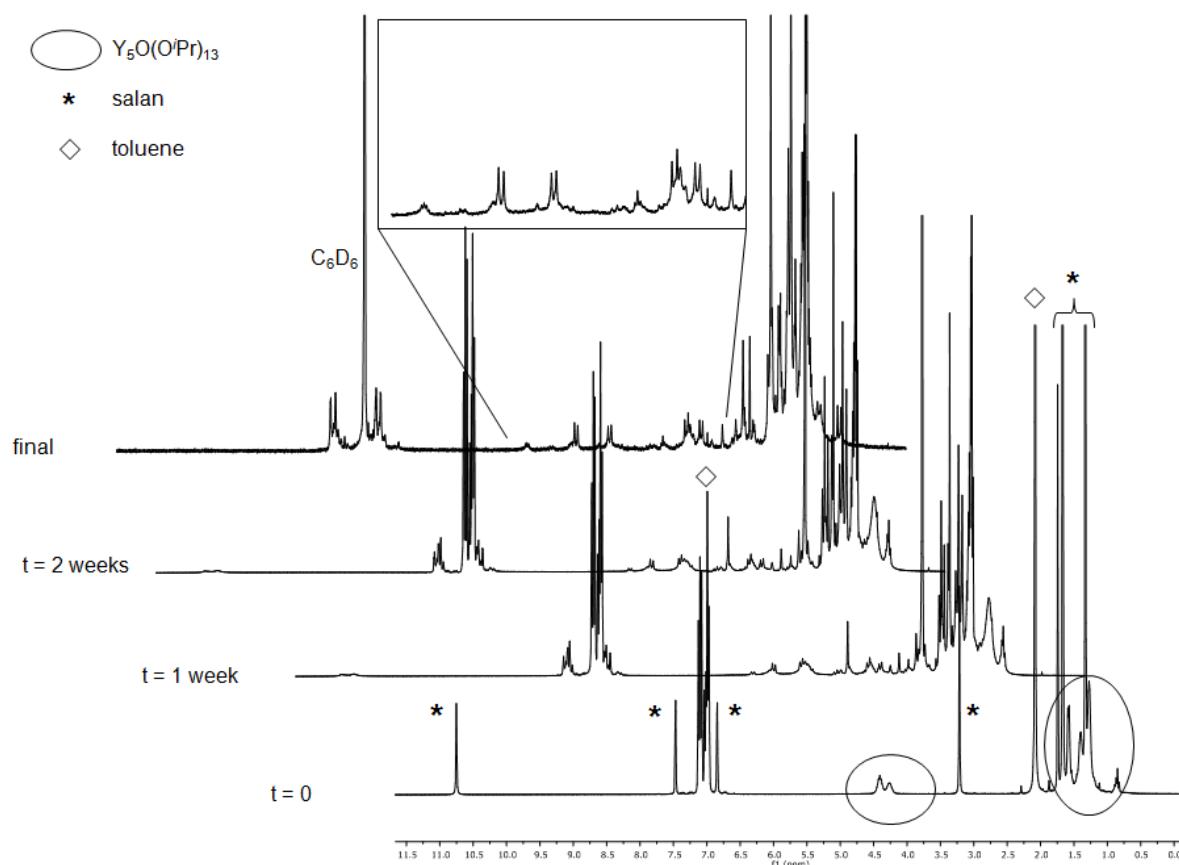
A toluene solution (1 mL) of yttrium isopropoxide oxide $Y_5O(O^iPr)_{13}$ (toluene solution, 25 w%, 187 mg of solution containing 0.19 mmol of yttrium) and salan (100 mg, 0.19 mmol) is heated up to 80°C for 6 days. After cooling down to room temperature, all volatiles are evaporated. The white solid obtained considered as mixture of **1** and **1'** in a 2:3 ratio is used without further purification for the polymerization of *rac*-BBL. Monocrystals of **1** suitable for X-ray diffraction analysis were obtained by slow evaporation of a concentrated solution of the crude mixture in hexane.

1H NMR (500 MHz, $[D_8]$ THF, 25°C): $\delta = 7.23$ (s, 2H, C_6H_2), 7.19 (s, 2H, C_6H_2), 6.86 (d, $^4J(H,H) = 2.3$ Hz, 2H, C_6H_2), 6.81 (d, $^4J(H,H) = 2.2$, 2H, C_6H_2), 4.94 (m, 1H, $OCH(CH_3)_2$), 4.33 (d, $^2J(H,H) = 12.4$ Hz, 1H, $ArCH_2N$), 4.27 (d, $^2J(H,H) = 12.9$ Hz, 1H, $ArCH_2N$), 3.16 (m, 4H, $ArCH_2N$), 3.01 (d, $^2J(H,H) = 12.4$ Hz, 1H, $ArCH_2N$), 2.65 (s, 6H, NCH_3), 2.16 (d, $^2J(H,H) = 12.4$ Hz, 1H, $ArCH_2N$), 1.88 (d, $^4J(H,H) = 13.2$ Hz, 1H, $ArCH_2N$), 1.60 (s, 18H,

$\text{C}(\text{CH}_3)_3$, 1.60 (br, 3H, $\text{OCH}(\text{CH}_3)_2$), 1.53 (br, 3H, $\text{OCH}(\text{CH}_3)_2$), 1.35 (s, 18H, $\text{C}(\text{CH}_3)_3$), 1.32 (m, 8H, $\text{N}(\text{CH}_2)_2\text{N}$), 1.27 (s, 18H, $\text{C}(\text{CH}_3)_3$), 1.26 (s, 18H, $\text{C}(\text{CH}_3)_3$).

Monitoring of the reaction between “ $\text{Y}(\text{O}i\text{Pr})_3$ ” solution in toluene with salan by ^1H NMR in C_6D_6 at 50°C

The final ^1H NMR spectrum shows the ^1H signal of the crude mixture obtained after evaporation of all volatiles (toluene, $i\text{PrOH}$ formed).



Polymer Synthesis

In a typical experiment (Table 1, entry 1), in the glovebox, a Schlenk tube was charged with a solution of the initiator (0.01 g , $1.49 \times 10^{-5} \text{ mol}$) in benzene- d_6 (1.0 mL). To this stirred solution was added rapidly β -butyrolactone (0.257 mg , 2.98 mmol , 200 equiv). The reaction solution was stirred at 25°C for the desired time. Conversion was monitored by comparing the relative magnitude of peaks corresponding to the methine hydrogen for BBL and PHB. The reaction mixture was quenched with acidic methanol (0.5 mL of a 1.2 M HCl solution in MeOH), and the polymer was precipitated with excess methanol. The polymer was then dried under vacuum to constant weight.

Solid State Structure Determination of Complex 1

A suitable single crystal of **1** was mounted onto a glass fiber using the “oil-drop” method. Diffraction data were collected at 100 K using an APEXII, Bruker-AXS diffractometer, Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$). The structure was solved by direct methods using the *SIR97* program,¹ and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*)² with the aid of the *WINGX*³ program. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm,⁴ implemented as the *SQUEEZE* option in *PLATON*.⁵ A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. Except O₄ linked hydrogen atom that was introduced in the structural model through Fourier difference maps analysis, H atoms were finally included in their calculated positions. A final refinement on F^2 with 18289 unique intensities and 739 parameters converged at $\omega R(F^2) = 0.1631$ ($R(F) = 0.0712$) for 8438 observed reflections with $I > 2\sigma(I)$. Crystal data and details of data collection and structure refinement are given in Table 1S.

Figure 1S. Carbonyl region and methylene region of the ^{13}C NMR spectrum (125 MHz, CDCl_3 , 40°C) of PHB prepared by polymerization of *rac*-BBL with the alkoxide complex

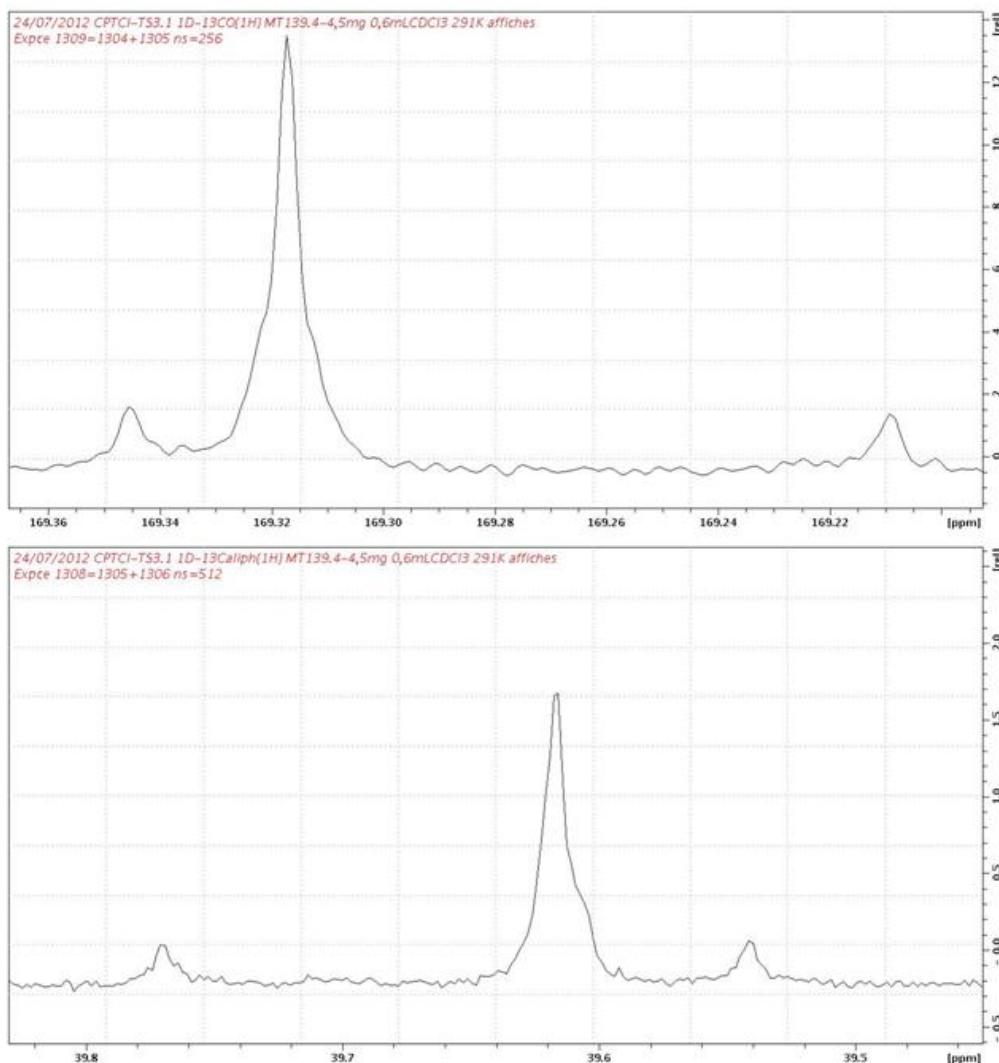


Figure 2S. Crystal structure for **1**

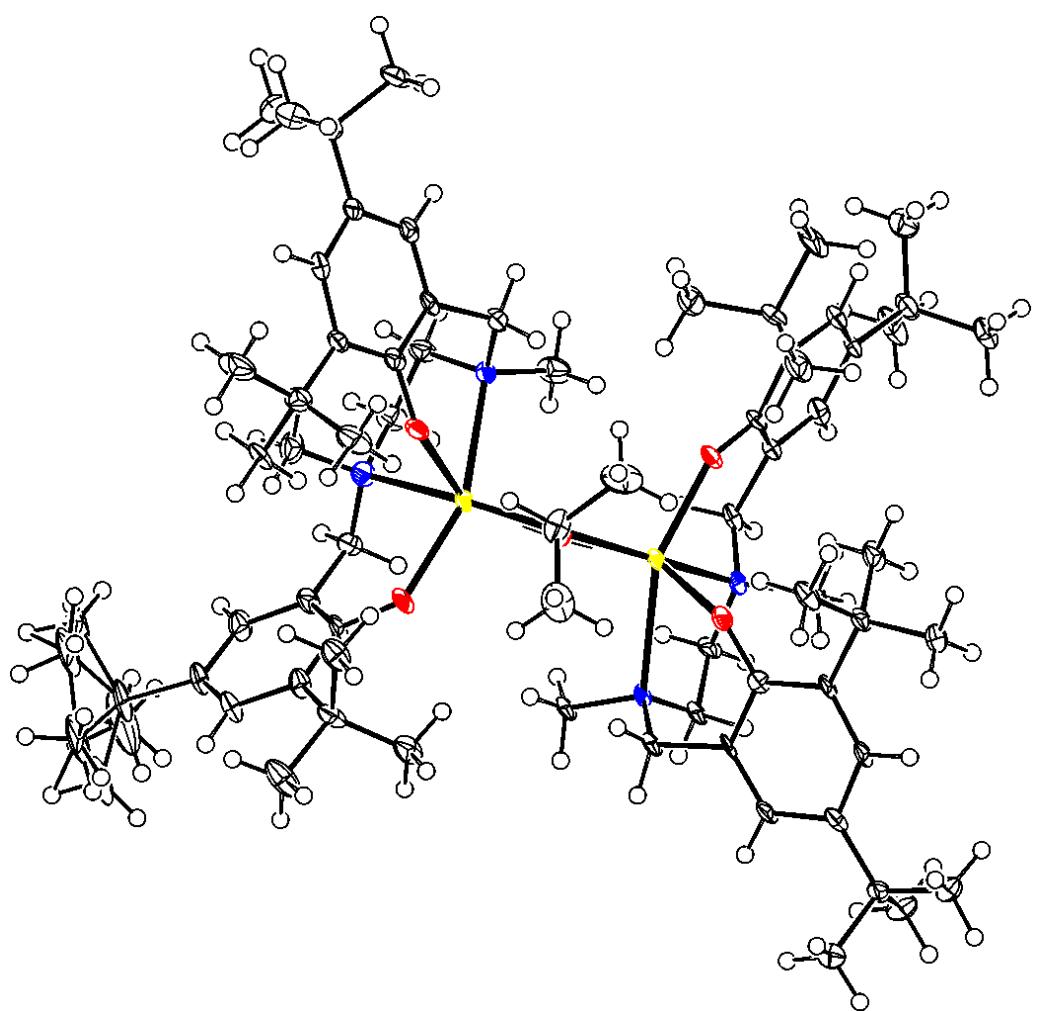


Table 1S. Summary of crystallographic data for **1**

Empirical formula	C71 H116 N4 O6 Y2
Formula weight	1299.50
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P c a b
Unit cell dimensions	a = 21.045(3) Å alpha = 90 deg. b = 24.936(3) Å beta = 90 deg. c = 30.425(4) Å gamma = 90 deg.
Volume	15966(4) Å ³
Z, Calculated density	8, 1.081 Mg/m ³
Absorption coefficient	1.491 mm ⁻¹
F(000)	5568
Crystal size	0.3 x 0.14 x 0.09 mm
Theta range for data collection	2.96 to 27.48 deg.
Limiting indices	-27<=h<=16, -31<=k<=32, -38<=l<=39
Reflections collected / unique	95920 / 18289 [R(int) = 0.1235]
Completeness to theta = 27.48	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.874 and 0.633
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	18289 / 0 / 739
Goodness-of-fit on F ²	0.894
Final R indices [I>2sigma(I)]	R1 = 0.0712, wR2 = 0.1631
R indices (all data)	R1 = 0.1566, wR2 = 0.1876
Largest diff. peak and hole	1.348 and -1.166 e.Å ⁻³

Table 2S. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Y(1)	6689 (1)	1657 (1)	864 (1)	16 (1)
Y(2)	7537 (1)	2558 (1)	1597 (1)	16 (1)
O(3)	6742 (2)	1956 (1)	1555 (1)	20 (1)
O(4)	7446 (2)	2310 (1)	880 (1)	18 (1)
O(5)	7720 (2)	2401 (1)	2274 (1)	19 (1)
N(6)	8612 (2)	2076 (1)	1561 (1)	17 (1)
O(7)	7024 (2)	3291 (1)	1565 (1)	23 (1)
N(8)	6043 (2)	2336 (1)	401 (1)	16 (1)
O(9)	7308 (2)	985 (1)	856 (1)	20 (1)
O(10)	5752 (2)	1329 (1)	881 (1)	19 (1)
N(11)	8418 (2)	3244 (1)	1553 (1)	19 (1)
C(12)	7930 (2)	181 (2)	743 (2)	23 (1)
N(13)	6883 (2)	1498 (1)	57 (1)	18 (1)
C(14)	4823 (2)	873 (2)	601 (2)	16 (1)
C(15)	8656 (2)	1913 (2)	2394 (1)	16 (1)
C(16)	7122 (2)	3822 (2)	1593 (2)	19 (1)
C(17)	7698 (2)	4031 (2)	1450 (2)	21 (1)
C(18)	5373 (2)	2328 (2)	559 (2)	20 (1)
C(19)	6735 (2)	1994 (2)	-193 (2)	19 (1)
C(20)	5209 (2)	1335 (2)	658 (2)	16 (1)
C(21)	9172 (2)	1887 (2)	3109 (2)	18 (1)
C(22)	5009 (2)	1821 (2)	461 (2)	16 (1)
C(23)	8160 (2)	529 (2)	-117 (2)	22 (1)
C(24)	7663 (2)	676 (2)	595 (2)	22 (1)
C(25)	9713 (2)	1705 (2)	3409 (2)	22 (1)
C(26)	8186 (2)	2405 (2)	2997 (2)	19 (1)
C(27)	7832 (3)	-17 (2)	1217 (2)	24 (1)
C(28)	8606 (3)	3496 (2)	1979 (2)	28 (1)
C(29)	6660 (2)	4172 (2)	1762 (2)	21 (1)
C(30)	8798 (2)	-312 (2)	-302 (2)	26 (1)
C(31)	6086 (2)	2208 (2)	-72 (1)	20 (1)
C(32)	4294 (2)	918 (2)	339 (2)	18 (1)
C(33)	6504 (2)	1040 (2)	-117 (2)	24 (1)
C(34)	6286 (2)	2893 (2)	479 (2)	20 (1)
C(35)	9143 (2)	1743 (2)	2664 (2)	18 (1)
C(36)	7576 (2)	1386 (2)	-2 (2)	21 (1)
C(37)	8413 (2)	46 (2)	13 (2)	22 (1)
C(38)	8175 (2)	2245 (2)	2555 (2)	17 (1)
C(39)	3534 (2)	1415 (2)	-186 (2)	21 (1)
C(40)	4986 (2)	344 (2)	834 (2)	19 (1)
C(41)	6106 (2)	3581 (2)	2312 (2)	28 (1)
C(42)	4098 (2)	1391 (2)	121 (2)	18 (1)
C(43)	6395 (3)	1796 (2)	1938 (2)	27 (1)
C(44)	4495 (2)	-103 (2)	728 (2)	27 (1)
C(45)	5637 (2)	141 (2)	699 (2)	26 (1)
C(46)	8619 (2)	1678 (2)	1933 (1)	19 (1)
C(47)	7673 (2)	2760 (2)	3194 (2)	25 (1)
C(48)	8977 (2)	2976 (2)	1355 (2)	25 (1)
C(49)	6808 (2)	4719 (2)	1795 (2)	24 (1)

C (50)	4479 (2)	1839 (2)	203 (2)	18 (1)
C (51)	8292 (2)	-111 (2)	444 (2)	24 (1)
C (52)	8338 (2)	-711 (2)	-520 (2)	28 (1)
C (53)	8191 (2)	3670 (2)	1250 (2)	19 (1)
C (54)	8687 (3)	1762 (2)	1150 (2)	30 (1)
C (55)	7386 (2)	4932 (2)	1670 (2)	24 (1)
C (56)	7644 (3)	3301 (2)	2952 (2)	29 (1)
C (57)	7792 (2)	846 (2)	160 (2)	20 (1)
C (58)	8686 (2)	2213 (2)	3258 (2)	19 (1)
C (59)	7831 (2)	4577 (2)	1488 (2)	25 (1)
C (60)	9513 (2)	1716 (2)	3895 (2)	31 (1)
C (61)	6010 (2)	3959 (2)	1914 (2)	23 (1)
C (62)	3139 (2)	898 (2)	-180 (2)	28 (1)
C (63)	3083 (2)	1874 (2)	-55 (2)	27 (1)
C (64)	4965 (2)	439 (2)	1338 (2)	27 (1)
C (65)	8094 (3)	398 (2)	1539 (2)	32 (1)
C (66)	8174 (3)	-544 (2)	1309 (2)	39 (2)
C (67)	5665 (2)	3665 (2)	1545 (2)	28 (1)
C (68)	3768 (2)	1507 (2)	-653 (2)	31 (1)
C (70)	10279 (2)	2078 (2)	3346 (2)	31 (1)
C (71)	9916 (2)	1130 (2)	3302 (2)	30 (1)
C (72)	7126 (3)	-106 (2)	1313 (2)	33 (1)
C (73)	7795 (3)	2893 (2)	3680 (2)	40 (2)
C (74)	7022 (3)	2480 (2)	3159 (2)	34 (1)
C (75)	5561 (3)	4412 (2)	2070 (2)	39 (2)
C (76)	6411 (3)	1181 (2)	1974 (2)	42 (2)
C (77)	9112 (3)	16 (2)	-672 (2)	40 (2)
C (78)	5725 (3)	2006 (2)	1916 (2)	38 (2)
C (79)	9136 (2)	2459 (2)	1600 (2)	22 (1)
C (81)	9308 (3)	-621 (2)	-61 (2)	39 (2)
C (69A)	7565 (3)	5522 (2)	1733 (2)	35 (2)
C (80A)	7820 (4)	5767 (2)	1320 (2)	74 (3)
C (141)	7154 (8)	5818 (5)	2027 (5)	58 (2)
C (151)	8242 (7)	5515 (5)	2011 (6)	58 (2)
C (69B)	7565 (3)	5522 (2)	1733 (2)	35 (2)
C (80B)	7820 (4)	5767 (2)	1320 (2)	74 (3)
C (241)	6918 (7)	5875 (5)	1777 (5)	58 (2)
C (251)	7888 (7)	5606 (5)	2131 (5)	58 (2)

Table 3S. Anisotropic displacement parameters (\AA^2) for **1**

The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Y(1)	18 (1)	6 (1)	24 (1)	0 (1)	-2 (1)	0 (1)
Y(2)	15 (1)	9 (1)	24 (1)	-1 (1)	-2 (1)	-1 (1)
O(3)	23 (2)	15 (2)	22 (2)	-2 (1)	3 (2)	-7 (1)
O(4)	19 (2)	10 (2)	26 (2)	-1 (1)	2 (2)	-2 (1)
O(5)	18 (2)	12 (2)	27 (2)	1 (1)	-1 (2)	3 (1)
N(6)	15 (2)	13 (2)	23 (2)	-3 (2)	-2 (2)	0 (2)
O(7)	21 (2)	5 (2)	42 (2)	0 (1)	-1 (2)	-2 (1)
N(8)	25 (3)	4 (2)	20 (2)	3 (2)	-4 (2)	-5 (2)
O(9)	25 (2)	10 (2)	24 (2)	-3 (1)	0 (2)	6 (1)
O(10)	21 (2)	10 (2)	27 (2)	0 (1)	-2 (2)	-2 (1)
N(11)	17 (3)	17 (2)	25 (2)	1 (2)	2 (2)	-2 (2)
C(12)	20 (3)	10 (2)	38 (3)	-6 (2)	-8 (2)	0 (2)
N(13)	22 (3)	7 (2)	25 (2)	1 (2)	-5 (2)	-3 (2)
C(14)	15 (3)	4 (2)	29 (3)	-1 (2)	5 (2)	-3 (2)
C(15)	18 (3)	6 (2)	24 (3)	0 (2)	4 (2)	-2 (2)
C(16)	22 (3)	6 (2)	30 (3)	-2 (2)	3 (2)	-2 (2)
C(17)	22 (3)	11 (2)	31 (3)	2 (2)	0 (2)	-3 (2)
C(18)	24 (2)	5 (1)	31 (2)	2 (1)	-3 (1)	0 (1)
C(19)	20 (3)	8 (2)	30 (3)	6 (2)	-2 (2)	0 (2)
C(20)	12 (3)	15 (2)	22 (3)	0 (2)	4 (2)	-1 (2)
C(21)	14 (3)	8 (2)	30 (3)	2 (2)	-2 (2)	-4 (2)
C(22)	16 (3)	3 (2)	28 (3)	-4 (2)	9 (2)	-2 (2)
C(23)	25 (3)	14 (2)	27 (3)	-3 (2)	2 (2)	-1 (2)
C(24)	23 (3)	7 (2)	35 (3)	-3 (2)	-7 (2)	5 (2)
C(25)	20 (3)	19 (3)	26 (3)	1 (2)	-1 (2)	4 (2)
C(26)	15 (3)	10 (2)	31 (3)	-2 (2)	-1 (2)	1 (2)
C(27)	30 (4)	10 (2)	33 (3)	4 (2)	-5 (2)	6 (2)
C(28)	34 (4)	21 (3)	30 (3)	0 (2)	-4 (2)	-10 (2)
C(29)	20 (3)	16 (2)	27 (3)	-4 (2)	8 (2)	-5 (2)
C(30)	25 (3)	14 (3)	40 (3)	-6 (2)	0 (3)	4 (2)
C(31)	24 (2)	5 (1)	31 (2)	2 (1)	-3 (1)	0 (1)
C(32)	16 (3)	7 (2)	31 (3)	-3 (2)	5 (2)	-3 (2)
C(33)	26 (3)	11 (2)	34 (3)	-5 (2)	-1 (2)	-5 (2)
C(34)	24 (2)	5 (1)	31 (2)	2 (1)	-3 (1)	0 (1)
C(35)	15 (3)	10 (2)	29 (3)	-2 (2)	3 (2)	-4 (2)
C(36)	27 (3)	8 (2)	26 (3)	-2 (2)	2 (2)	-1 (2)
C(37)	24 (3)	9 (2)	34 (3)	-8 (2)	-5 (2)	5 (2)
C(38)	16 (3)	9 (2)	26 (3)	3 (2)	1 (2)	-3 (2)
C(39)	11 (3)	16 (2)	35 (3)	-4 (2)	-1 (2)	2 (2)
C(40)	20 (3)	9 (2)	29 (3)	0 (2)	-1 (2)	0 (2)
C(41)	30 (4)	20 (3)	34 (3)	2 (2)	10 (3)	-1 (2)
C(42)	16 (3)	8 (2)	30 (3)	0 (2)	7 (2)	1 (2)
C(43)	29 (4)	31 (3)	20 (3)	0 (2)	2 (2)	-11 (3)
C(44)	31 (4)	13 (3)	38 (3)	-1 (2)	-7 (3)	-5 (2)
C(45)	26 (3)	13 (3)	38 (3)	-1 (2)	2 (3)	-6 (2)
C(46)	25 (3)	14 (2)	17 (3)	0 (2)	0 (2)	4 (2)
C(47)	31 (4)	25 (3)	19 (3)	-2 (2)	-4 (2)	9 (2)
C(48)	19 (3)	26 (3)	31 (3)	3 (2)	5 (2)	1 (2)
C(49)	32 (4)	11 (2)	30 (3)	-4 (2)	7 (2)	0 (2)
C(50)	21 (3)	6 (2)	28 (3)	1 (2)	1 (2)	2 (2)

C(51)	28 (3)	9 (2)	36 (3)	-4 (2)	-7 (3)	4 (2)
C(52)	31 (4)	17 (3)	35 (3)	-8 (2)	7 (3)	3 (2)
C(53)	14 (3)	16 (2)	27 (3)	3 (2)	2 (2)	-1 (2)
C(54)	28 (4)	37 (3)	25 (3)	-3 (2)	6 (2)	14 (3)
C(55)	32 (4)	10 (2)	32 (3)	-5 (2)	4 (2)	-5 (2)
C(56)	36 (4)	13 (2)	37 (3)	-8 (2)	-3 (3)	11 (2)
C(57)	22 (3)	12 (2)	25 (3)	-6 (2)	-4 (2)	5 (2)
C(58)	23 (3)	13 (2)	19 (3)	-5 (2)	4 (2)	-2 (2)
C(59)	24 (3)	18 (3)	33 (3)	-2 (2)	4 (2)	-7 (2)
C(60)	31 (4)	29 (3)	32 (3)	7 (2)	2 (3)	6 (3)
C(61)	19 (3)	16 (2)	35 (3)	3 (2)	6 (2)	6 (2)
C(62)	14 (3)	24 (3)	45 (3)	-2 (2)	-8 (2)	-4 (2)
C(63)	23 (3)	25 (3)	33 (3)	-2 (2)	-3 (2)	4 (2)
C(64)	36 (4)	9 (2)	35 (3)	5 (2)	2 (3)	-1 (2)
C(65)	43 (4)	17 (3)	36 (3)	4 (2)	-8 (3)	-1 (3)
C(66)	69 (5)	9 (3)	40 (3)	8 (2)	-8 (3)	9 (3)
C(67)	23 (3)	15 (3)	46 (3)	5 (2)	4 (3)	-4 (2)
C(68)	17 (3)	36 (3)	40 (3)	-1 (3)	-6 (3)	-1 (3)
C(70)	20 (3)	34 (3)	39 (3)	-1 (2)	-3 (2)	-3 (3)
C(71)	33 (4)	20 (3)	36 (3)	4 (2)	-4 (3)	13 (2)
C(72)	40 (4)	15 (3)	43 (3)	2 (2)	1 (3)	-2 (2)
C(73)	42 (4)	40 (3)	37 (3)	-6 (3)	4 (3)	25 (3)
C(74)	29 (4)	30 (3)	44 (4)	2 (3)	9 (3)	10 (3)
C(75)	39 (4)	23 (3)	55 (4)	-1 (3)	27 (3)	6 (3)
C(76)	35 (4)	35 (3)	56 (4)	23 (3)	2 (3)	-1 (3)
C(77)	44 (4)	14 (3)	62 (4)	-4 (3)	15 (3)	-2 (3)
C(78)	33 (4)	35 (3)	46 (4)	-2 (3)	17 (3)	-9 (3)
C(79)	15 (3)	20 (3)	31 (3)	2 (2)	2 (2)	4 (2)
C(81)	28 (4)	32 (3)	57 (4)	-13 (3)	-5 (3)	8 (3)
C(69A)	46 (4)	11 (3)	47 (4)	-11 (2)	14 (3)	-13 (3)
C(80A)	138 (8)	21 (3)	65 (5)	-3 (3)	43 (5)	-30 (4)
C(141)	65 (8)	13 (3)	96 (8)	-18 (4)	9 (5)	-16 (4)
C(151)	65 (8)	13 (3)	96 (8)	-18 (4)	9 (5)	-16 (4)
C(69B)	46 (4)	11 (3)	47 (4)	-11 (2)	14 (3)	-13 (3)
C(80B)	138 (8)	21 (3)	65 (5)	-3 (3)	43 (5)	-30 (4)
C(241)	65 (8)	13 (3)	96 (8)	-18 (4)	9 (5)	-16 (4)
C(251)	65 (8)	13 (3)	96 (8)	-18 (4)	9 (5)	-16 (4)

Table 4S. Bond lengths [Å] for **1**

Y(1)-O(9)	2.123 (3)
Y(1)-O(10)	2.134 (3)
Y(1)-O(3)	2.234 (3)
Y(1)-O(4)	2.278 (3)
Y(1)-N(13)	2.520 (4)
Y(1)-N(8)	2.587 (3)
Y(1)-Y(2)	3.6338 (7)
Y(2)-O(7)	2.125 (3)
Y(2)-O(5)	2.131 (3)
Y(2)-O(3)	2.250 (3)
Y(2)-O(4)	2.274 (3)
Y(2)-N(11)	2.527 (4)
Y(2)-N(6)	2.564 (4)
O(3)-C(43)	1.433 (5)
O(4)-H(4)	0.84 (5)
O(5)-C(38)	1.342 (5)
N(6)-C(79)	1.464 (6)
N(6)-C(54)	1.486 (5)
N(6)-C(46)	1.503 (5)
O(7)-C(16)	1.342 (5)
N(8)-C(31)	1.478 (5)
N(8)-C(18)	1.489 (6)
N(8)-C(34)	1.501 (5)
O(9)-C(24)	1.336 (5)
O(10)-C(20)	1.331 (5)
N(11)-C(48)	1.481 (6)
N(11)-C(53)	1.485 (5)
N(11)-C(28)	1.494 (6)
C(12)-C(51)	1.391 (6)
C(12)-C(24)	1.428 (6)
C(12)-C(27)	1.540 (7)
N(13)-C(19)	1.486 (5)
N(13)-C(33)	1.490 (5)
N(13)-C(36)	1.495 (6)
C(14)-C(32)	1.375 (6)
C(14)-C(20)	1.419 (6)
C(14)-C(40)	1.536 (6)
C(15)-C(35)	1.381 (6)
C(15)-C(38)	1.397 (6)
C(15)-C(46)	1.523 (6)
C(16)-C(17)	1.391 (6)
C(16)-C(29)	1.403 (6)
C(17)-C(59)	1.394 (6)
C(17)-C(53)	1.504 (6)
C(18)-C(22)	1.509 (6)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(31)	1.510 (6)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(22)	1.415 (6)
C(21)-C(58)	1.384 (6)
C(21)-C(35)	1.402 (6)
C(21)-C(25)	1.529 (6)
C(22)-C(50)	1.363 (6)
C(23)-C(37)	1.376 (6)

C(23)-C(57)	1.389 (6)
C(23)-H(23)	0.9500
C(24)-C(57)	1.416 (6)
C(25)-C(70)	1.524 (7)
C(25)-C(71)	1.530 (6)
C(25)-C(60)	1.538 (6)
C(26)-C(58)	1.402 (6)
C(26)-C(38)	1.402 (6)
C(26)-C(47)	1.520 (6)
C(27)-C(66)	1.523 (6)
C(27)-C(65)	1.528 (6)
C(27)-C(72)	1.530 (7)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(49)	1.402 (6)
C(29)-C(61)	1.539 (6)
C(30)-C(81)	1.513 (7)
C(30)-C(37)	1.538 (6)
C(30)-C(52)	1.538 (6)
C(30)-C(77)	1.541 (7)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(42)	1.415 (6)
C(32)-H(32)	0.9500
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35)	0.9500
C(36)-C(57)	1.506 (6)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(51)	1.392 (6)
C(39)-C(42)	1.513 (6)
C(39)-C(68)	1.521 (7)
C(39)-C(62)	1.534 (6)
C(39)-C(63)	1.538 (6)
C(40)-C(45)	1.517 (6)
C(40)-C(64)	1.552 (6)
C(40)-C(44)	1.554 (6)
C(41)-C(61)	1.548 (6)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-C(50)	1.397 (6)
C(43)-C(78)	1.505 (7)
C(43)-C(76)	1.536 (7)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(73)	1.536 (6)
C(47)-C(56)	1.538 (6)

C (47) -C (74)	1.541 (7)
C (48) -C (79)	1.525 (6)
C (48) -H (48A)	0.9900
C (48) -H (48B)	0.9900
C (49) -C (55)	1.381 (6)
C (49) -H (49)	0.9500
C (50) -H (50)	0.9500
C (51) -H (51)	0.9500
C (52) -H (52A)	0.9800
C (52) -H (52B)	0.9800
C (52) -H (52C)	0.9800
C (53) -H (53A)	0.9900
C (53) -H (53B)	0.9900
C (54) -H (54A)	0.9800
C (54) -H (54B)	0.9800
C (54) -H (54C)	0.9800
C (55) -C (59)	1.403 (7)
C (55) -C (69A)	1.532 (6)
C (56) -H (56A)	0.9800
C (56) -H (56B)	0.9800
C (56) -H (56C)	0.9800
C (58) -H (58)	0.9500
C (59) -H (59)	0.9500
C (60) -H (60A)	0.9800
C (60) -H (60B)	0.9800
C (60) -H (60C)	0.9800
C (61) -C (67)	1.527 (6)
C (61) -C (75)	1.547 (6)
C (62) -H (62A)	0.9800
C (62) -H (62B)	0.9800
C (62) -H (62C)	0.9800
C (63) -H (63A)	0.9800
C (63) -H (63B)	0.9800
C (63) -H (63C)	0.9800
C (64) -H (64A)	0.9800
C (64) -H (64B)	0.9800
C (64) -H (64C)	0.9800
C (65) -H (65A)	0.9800
C (65) -H (65B)	0.9800
C (65) -H (65C)	0.9800
C (66) -H (66A)	0.9800
C (66) -H (66B)	0.9800
C (66) -H (66C)	0.9800
C (67) -H (67A)	0.9800
C (67) -H (67B)	0.9800
C (67) -H (67C)	0.9800
C (68) -H (68A)	0.9800
C (68) -H (68B)	0.9800
C (68) -H (68C)	0.9800
C (70) -H (70A)	0.9800
C (70) -H (70B)	0.9800
C (70) -H (70C)	0.9800
C (71) -H (71A)	0.9800
C (71) -H (71B)	0.9800
C (71) -H (71C)	0.9800
C (72) -H (72A)	0.9800
C (72) -H (72B)	0.9800
C (72) -H (72C)	0.9800
C (73) -H (73A)	0.9800
C (73) -H (73B)	0.9800
C (73) -H (73C)	0.9800

C (74)-H (74A)	0.9800
C (74)-H (74B)	0.9800
C (74)-H (74C)	0.9800
C (75)-H (75A)	0.9800
C (75)-H (75B)	0.9800
C (75)-H (75C)	0.9800
C (76)-H (76A)	0.9800
C (76)-H (76B)	0.9800
C (76)-H (76C)	0.9800
C (77)-H (77A)	0.9800
C (77)-H (77B)	0.9800
C (77)-H (77C)	0.9800
C (78)-H (78A)	0.9800
C (78)-H (78B)	0.9800
C (78)-H (78C)	0.9800
C (79)-H (79A)	0.9900
C (79)-H (79B)	0.9900
C (81)-H (81A)	0.9800
C (81)-H (81B)	0.9800
C (81)-H (81C)	0.9800
C (69A)-C (141)	1.446(16)
C (69A)-C (80A)	1.498(7)
C (69A)-C (151)	1.657(17)
C (80A)-H (80A)	0.9800
C (80A)-H (80B)	0.9800
C (80A)-H (80C)	0.9800
C (141)-H (14A)	0.9800
C (141)-H (14B)	0.9800
C (141)-H (14C)	0.9800
C (151)-H (15A)	0.9800
C (151)-H (15B)	0.9800
C (151)-H (15C)	0.9800
C (241)-H (24A)	0.9800
C (241)-H (24B)	0.9800
C (241)-H (24C)	0.9800
C (251)-H (25A)	0.9800
C (251)-H (25B)	0.9800
C (251)-H (25C)	0.9800

Table 5S. Angles [°] for **1**

O(9)-Y(1)-O(10)	105.33(11)
O(9)-Y(1)-O(3)	104.11(11)
O(10)-Y(1)-O(3)	98.70(11)
O(9)-Y(1)-O(4)	97.79(12)
O(10)-Y(1)-O(4)	156.75(11)
O(3)-Y(1)-O(4)	72.86(11)
O(9)-Y(1)-N(13)	76.37(11)
O(10)-Y(1)-N(13)	96.54(12)
O(3)-Y(1)-N(13)	163.99(11)
O(4)-Y(1)-N(13)	91.17(11)
O(9)-Y(1)-N(8)	146.34(11)
O(10)-Y(1)-N(8)	77.23(11)
O(3)-Y(1)-N(8)	108.69(11)
O(4)-Y(1)-N(8)	84.94(11)
N(13)-Y(1)-N(8)	70.02(12)
O(9)-Y(1)-Y(2)	101.17(8)
O(10)-Y(1)-Y(2)	132.48(8)
O(3)-Y(1)-Y(2)	36.02(8)
O(4)-Y(1)-Y(2)	36.99(8)
N(13)-Y(1)-Y(2)	127.97(8)
N(8)-Y(1)-Y(2)	100.83(8)
O(7)-Y(2)-O(5)	107.10(11)
O(7)-Y(2)-O(3)	101.11(12)
O(5)-Y(2)-O(3)	93.80(11)
O(7)-Y(2)-O(4)	98.47(11)
O(5)-Y(2)-O(4)	153.06(11)
O(3)-Y(2)-O(4)	72.65(11)
O(7)-Y(2)-N(11)	77.77(12)
O(5)-Y(2)-N(11)	92.46(12)
O(3)-Y(2)-N(11)	173.69(11)
O(4)-Y(2)-N(11)	101.29(11)
O(7)-Y(2)-N(6)	148.19(12)
O(5)-Y(2)-N(6)	78.14(11)
O(3)-Y(2)-N(6)	109.93(11)
O(4)-Y(2)-N(6)	84.68(11)
N(11)-Y(2)-N(6)	70.61(12)
O(7)-Y(2)-Y(1)	104.71(9)
O(5)-Y(2)-Y(1)	124.60(8)
O(3)-Y(2)-Y(1)	35.72(7)
O(4)-Y(2)-Y(1)	37.08(8)
N(11)-Y(2)-Y(1)	138.32(9)
N(6)-Y(2)-Y(1)	96.78(8)
C(43)-O(3)-Y(1)	130.3(3)
C(43)-O(3)-Y(2)	121.3(3)
Y(1)-O(3)-Y(2)	108.26(12)
Y(2)-O(4)-Y(1)	105.93(12)
Y(2)-O(4)-H(4)	125(4)
Y(1)-O(4)-H(4)	126(4)
C(38)-O(5)-Y(2)	143.0(3)
C(79)-N(6)-C(54)	109.3(4)
C(79)-N(6)-C(46)	111.3(3)
C(54)-N(6)-C(46)	106.5(3)
C(79)-N(6)-Y(2)	110.8(3)
C(54)-N(6)-Y(2)	112.1(3)
C(46)-N(6)-Y(2)	106.7(3)
C(16)-O(7)-Y(2)	140.1(3)
C(31)-N(8)-C(18)	111.7(3)
C(31)-N(8)-C(34)	109.5(3)

C(18)-N(8)-C(34)	106.5 (3)
C(31)-N(8)-Y(1)	110.9 (2)
C(18)-N(8)-Y(1)	108.3 (2)
C(34)-N(8)-Y(1)	109.9 (2)
C(24)-O(9)-Y(1)	143.7 (3)
C(20)-O(10)-Y(1)	140.9 (3)
C(48)-N(11)-C(53)	109.0 (3)
C(48)-N(11)-C(28)	109.3 (4)
C(53)-N(11)-C(28)	108.9 (3)
C(48)-N(11)-Y(2)	107.4 (3)
C(53)-N(11)-Y(2)	106.3 (3)
C(28)-N(11)-Y(2)	115.7 (3)
C(51)-C(12)-C(24)	117.5 (4)
C(51)-C(12)-C(27)	121.1 (4)
C(24)-C(12)-C(27)	121.4 (4)
C(19)-N(13)-C(33)	110.1 (3)
C(19)-N(13)-C(36)	107.3 (3)
C(33)-N(13)-C(36)	109.7 (3)
C(19)-N(13)-Y(1)	109.5 (3)
C(33)-N(13)-Y(1)	112.3 (3)
C(36)-N(13)-Y(1)	107.8 (3)
C(32)-C(14)-C(20)	117.9 (4)
C(32)-C(14)-C(40)	121.1 (4)
C(20)-C(14)-C(40)	121.0 (4)
C(35)-C(15)-C(38)	120.8 (4)
C(35)-C(15)-C(46)	117.9 (4)
C(38)-C(15)-C(46)	121.0 (4)
O(7)-C(16)-C(17)	119.0 (4)
O(7)-C(16)-C(29)	122.0 (4)
C(17)-C(16)-C(29)	119.0 (4)
C(16)-C(17)-C(59)	121.1 (4)
C(16)-C(17)-C(53)	120.2 (4)
C(59)-C(17)-C(53)	118.7 (4)
N(8)-C(18)-C(22)	115.4 (4)
N(8)-C(18)-H(18A)	108.4
C(22)-C(18)-H(18A)	108.4
N(8)-C(18)-H(18B)	108.4
C(22)-C(18)-H(18B)	108.4
H(18A)-C(18)-H(18B)	107.5
N(13)-C(19)-C(31)	111.0 (4)
N(13)-C(19)-H(19A)	109.4
C(31)-C(19)-H(19A)	109.4
N(13)-C(19)-H(19B)	109.4
C(31)-C(19)-H(19B)	109.4
H(19A)-C(19)-H(19B)	108.0
O(10)-C(20)-C(22)	118.8 (4)
O(10)-C(20)-C(14)	123.0 (4)
C(22)-C(20)-C(14)	118.2 (4)
C(58)-C(21)-C(35)	115.8 (4)
C(58)-C(21)-C(25)	122.1 (4)
C(35)-C(21)-C(25)	122.1 (4)
C(50)-C(22)-C(20)	121.0 (4)
C(50)-C(22)-C(18)	120.1 (4)
C(20)-C(22)-C(18)	118.8 (4)
C(37)-C(23)-C(57)	122.7 (4)
C(37)-C(23)-H(23)	118.7
C(57)-C(23)-H(23)	118.7
O(9)-C(24)-C(57)	119.4 (4)
O(9)-C(24)-C(12)	122.1 (4)
C(57)-C(24)-C(12)	118.5 (4)
C(70)-C(25)-C(21)	108.9 (4)

C(70)-C(25)-C(71)	109.1 (4)
C(21)-C(25)-C(71)	111.1 (4)
C(70)-C(25)-C(60)	108.9 (4)
C(21)-C(25)-C(60)	111.4 (4)
C(71)-C(25)-C(60)	107.4 (4)
C(58)-C(26)-C(38)	117.2 (4)
C(58)-C(26)-C(47)	120.6 (4)
C(38)-C(26)-C(47)	122.2 (4)
C(66)-C(27)-C(65)	107.3 (4)
C(66)-C(27)-C(72)	107.4 (4)
C(65)-C(27)-C(72)	109.0 (4)
C(66)-C(27)-C(12)	112.6 (4)
C(65)-C(27)-C(12)	109.6 (4)
C(72)-C(27)-C(12)	110.8 (4)
N(11)-C(28)-H(28A)	109.5
N(11)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(11)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(49)-C(29)-C(16)	118.6 (4)
C(49)-C(29)-C(61)	120.7 (4)
C(16)-C(29)-C(61)	120.7 (4)
C(81)-C(30)-C(37)	111.6 (4)
C(81)-C(30)-C(52)	109.0 (4)
C(37)-C(30)-C(52)	108.2 (4)
C(81)-C(30)-C(77)	108.6 (4)
C(37)-C(30)-C(77)	112.0 (4)
C(52)-C(30)-C(77)	107.3 (4)
N(8)-C(31)-C(19)	111.7 (4)
N(8)-C(31)-H(31A)	109.3
C(19)-C(31)-H(31A)	109.3
N(8)-C(31)-H(31B)	109.3
C(19)-C(31)-H(31B)	109.3
H(31A)-C(31)-H(31B)	107.9
C(14)-C(32)-C(42)	125.1 (4)
C(14)-C(32)-H(32)	117.5
C(42)-C(32)-H(32)	117.5
N(13)-C(33)-H(33A)	109.5
N(13)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
N(13)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
N(8)-C(34)-H(34A)	109.5
N(8)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
N(8)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(15)-C(35)-C(21)	121.8 (4)
C(15)-C(35)-H(35)	119.1
C(21)-C(35)-H(35)	119.1
N(13)-C(36)-C(57)	114.9 (4)
N(13)-C(36)-H(36A)	108.5
C(57)-C(36)-H(36A)	108.5
N(13)-C(36)-H(36B)	108.5
C(57)-C(36)-H(36B)	108.5
H(36A)-C(36)-H(36B)	107.5
C(23)-C(37)-C(51)	116.4 (4)
C(23)-C(37)-C(30)	122.2 (4)

C (51) -C (37) -C (30)	121.4 (4)
O (5) -C (38) -C (15)	117.7 (4)
O (5) -C (38) -C (26)	122.8 (4)
C (15) -C (38) -C (26)	119.6 (4)
C (42) -C (39) -C (68)	109.2 (4)
C (42) -C (39) -C (62)	112.6 (4)
C (68) -C (39) -C (62)	108.2 (4)
C (42) -C (39) -C (63)	110.7 (4)
C (68) -C (39) -C (63)	109.2 (4)
C (62) -C (39) -C (63)	106.8 (4)
C (45) -C (40) -C (14)	111.2 (4)
C (45) -C (40) -C (64)	110.1 (4)
C (14) -C (40) -C (64)	108.6 (3)
C (45) -C (40) -C (44)	107.7 (4)
C (14) -C (40) -C (44)	111.9 (4)
C (64) -C (40) -C (44)	107.2 (4)
C (61) -C (41) -H (41A)	109.5
C (61) -C (41) -H (41B)	109.5
H (41A) -C (41) -H (41B)	109.5
C (61) -C (41) -H (41C)	109.5
H (41A) -C (41) -H (41C)	109.5
H (41B) -C (41) -H (41C)	109.5
C (50) -C (42) -C (32)	114.6 (4)
C (50) -C (42) -C (39)	122.0 (4)
C (32) -C (42) -C (39)	123.4 (4)
O (3) -C (43) -C (78)	110.2 (4)
O (3) -C (43) -C (76)	108.9 (4)
C (78) -C (43) -C (76)	111.8 (4)
O (3) -C (43) -H (43)	108.6
C (78) -C (43) -H (43)	108.6
C (76) -C (43) -H (43)	108.6
C (40) -C (44) -H (44A)	109.5
C (40) -C (44) -H (44B)	109.5
H (44A) -C (44) -H (44B)	109.5
C (40) -C (44) -H (44C)	109.5
H (44A) -C (44) -H (44C)	109.5
H (44B) -C (44) -H (44C)	109.5
C (40) -C (45) -H (45A)	109.5
C (40) -C (45) -H (45B)	109.5
H (45A) -C (45) -H (45B)	109.5
C (40) -C (45) -H (45C)	109.5
H (45A) -C (45) -H (45C)	109.5
H (45B) -C (45) -H (45C)	109.5
N (6) -C (46) -C (15)	116.1 (3)
N (6) -C (46) -H (46A)	108.3
C (15) -C (46) -H (46A)	108.3
N (6) -C (46) -H (46B)	108.3
C (15) -C (46) -H (46B)	108.3
H (46A) -C (46) -H (46B)	107.4
C (26) -C (47) -C (73)	112.7 (4)
C (26) -C (47) -C (56)	110.4 (4)
C (73) -C (47) -C (56)	106.2 (4)
C (26) -C (47) -C (74)	109.9 (4)
C (73) -C (47) -C (74)	108.2 (4)
C (56) -C (47) -C (74)	109.3 (4)
N (11) -C (48) -C (79)	111.0 (4)
N (11) -C (48) -H (48A)	109.4
C (79) -C (48) -H (48A)	109.4
N (11) -C (48) -H (48B)	109.4
C (79) -C (48) -H (48B)	109.4
H (48A) -C (48) -H (48B)	108.0

C (55) -C (49) -C (29)	123.3 (5)
C (55) -C (49) -H (49)	118.4
C (29) -C (49) -H (49)	118.4
C (22) -C (50) -C (42)	123.0 (4)
C (22) -C (50) -H (50)	118.5
C (42) -C (50) -H (50)	118.5
C (12) -C (51) -C (37)	124.6 (4)
C (12) -C (51) -H (51)	117.7
C (37) -C (51) -H (51)	117.7
C (30) -C (52) -H (52A)	109.5
C (30) -C (52) -H (52B)	109.5
H (52A) -C (52) -H (52B)	109.5
C (30) -C (52) -H (52C)	109.5
H (52A) -C (52) -H (52C)	109.5
H (52B) -C (52) -H (52C)	109.5
N (11) -C (53) -C (17)	113.4 (4)
N (11) -C (53) -H (53A)	108.9
C (17) -C (53) -H (53A)	108.9
N (11) -C (53) -H (53B)	108.9
C (17) -C (53) -H (53B)	108.9
H (53A) -C (53) -H (53B)	107.7
N (6) -C (54) -H (54A)	109.5
N (6) -C (54) -H (54B)	109.5
H (54A) -C (54) -H (54B)	109.5
N (6) -C (54) -H (54C)	109.5
H (54A) -C (54) -H (54C)	109.5
H (54B) -C (54) -H (54C)	109.5
C (49) -C (55) -C (59)	117.1 (4)
C (49) -C (55) -C (69A)	123.5 (4)
C (59) -C (55) -C (69A)	119.4 (5)
C (47) -C (56) -H (56A)	109.5
C (47) -C (56) -H (56B)	109.5
H (56A) -C (56) -H (56B)	109.5
C (47) -C (56) -H (56C)	109.5
H (56A) -C (56) -H (56C)	109.5
H (56B) -C (56) -H (56C)	109.5
C (23) -C (57) -C (24)	120.2 (4)
C (23) -C (57) -C (36)	118.6 (4)
C (24) -C (57) -C (36)	121.0 (4)
C (21) -C (58) -C (26)	124.8 (4)
C (21) -C (58) -H (58)	117.6
C (26) -C (58) -H (58)	117.6
C (17) -C (59) -C (55)	120.9 (5)
C (17) -C (59) -H (59)	119.5
C (55) -C (59) -H (59)	119.5
C (25) -C (60) -H (60A)	109.5
C (25) -C (60) -H (60B)	109.5
H (60A) -C (60) -H (60B)	109.5
C (25) -C (60) -H (60C)	109.5
H (60A) -C (60) -H (60C)	109.5
H (60B) -C (60) -H (60C)	109.5
C (67) -C (61) -C (29)	111.6 (4)
C (67) -C (61) -C (75)	106.6 (4)
C (29) -C (61) -C (75)	112.6 (4)
C (67) -C (61) -C (41)	110.2 (4)
C (29) -C (61) -C (41)	109.2 (4)
C (75) -C (61) -C (41)	106.5 (4)
C (39) -C (62) -H (62A)	109.5
C (39) -C (62) -H (62B)	109.5
H (62A) -C (62) -H (62B)	109.5
C (39) -C (62) -H (62C)	109.5

H (62A) -C (62) -H (62C)	109.5
H (62B) -C (62) -H (62C)	109.5
C (39) -C (63) -H (63A)	109.5
C (39) -C (63) -H (63B)	109.5
H (63A) -C (63) -H (63B)	109.5
C (39) -C (63) -H (63C)	109.5
H (63A) -C (63) -H (63C)	109.5
H (63B) -C (63) -H (63C)	109.5
C (40) -C (64) -H (64A)	109.5
C (40) -C (64) -H (64B)	109.5
H (64A) -C (64) -H (64B)	109.5
C (40) -C (64) -H (64C)	109.5
H (64A) -C (64) -H (64C)	109.5
H (64B) -C (64) -H (64C)	109.5
C (27) -C (65) -H (65A)	109.5
C (27) -C (65) -H (65B)	109.5
H (65A) -C (65) -H (65B)	109.5
C (27) -C (65) -H (65C)	109.5
H (65A) -C (65) -H (65C)	109.5
H (65B) -C (65) -H (65C)	109.5
C (27) -C (66) -H (66A)	109.5
C (27) -C (66) -H (66B)	109.5
H (66A) -C (66) -H (66B)	109.5
C (27) -C (66) -H (66C)	109.5
H (66A) -C (66) -H (66C)	109.5
H (66B) -C (66) -H (66C)	109.5
C (61) -C (67) -H (67A)	109.5
C (61) -C (67) -H (67B)	109.5
H (67A) -C (67) -H (67B)	109.5
C (61) -C (67) -H (67C)	109.5
H (67A) -C (67) -H (67C)	109.5
H (67B) -C (67) -H (67C)	109.5
C (39) -C (68) -H (68A)	109.5
C (39) -C (68) -H (68B)	109.5
H (68A) -C (68) -H (68B)	109.5
C (39) -C (68) -H (68C)	109.5
H (68A) -C (68) -H (68C)	109.5
H (68B) -C (68) -H (68C)	109.5
C (25) -C (70) -H (70A)	109.5
C (25) -C (70) -H (70B)	109.5
H (70A) -C (70) -H (70B)	109.5
C (25) -C (70) -H (70C)	109.5
H (70A) -C (70) -H (70C)	109.5
H (70B) -C (70) -H (70C)	109.5
C (25) -C (71) -H (71A)	109.5
C (25) -C (71) -H (71B)	109.5
H (71A) -C (71) -H (71B)	109.5
C (25) -C (71) -H (71C)	109.5
H (71A) -C (71) -H (71C)	109.5
H (71B) -C (71) -H (71C)	109.5
C (27) -C (72) -H (72A)	109.5
C (27) -C (72) -H (72B)	109.5
H (72A) -C (72) -H (72B)	109.5
C (27) -C (72) -H (72C)	109.5
H (72A) -C (72) -H (72C)	109.5
H (72B) -C (72) -H (72C)	109.5
C (47) -C (73) -H (73A)	109.5
C (47) -C (73) -H (73B)	109.5
H (73A) -C (73) -H (73B)	109.5
C (47) -C (73) -H (73C)	109.5
H (73A) -C (73) -H (73C)	109.5

H(73B)-C(73)-H(73C)	109.5
C(47)-C(74)-H(74A)	109.5
C(47)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(47)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
C(61)-C(75)-H(75A)	109.5
C(61)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
C(61)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
C(43)-C(76)-H(76A)	109.5
C(43)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5
C(43)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
C(30)-C(77)-H(77A)	109.5
C(30)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
C(30)-C(77)-H(77C)	109.5
H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
C(43)-C(78)-H(78A)	109.5
C(43)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(43)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
N(6)-C(79)-C(48)	110.3(4)
N(6)-C(79)-H(79A)	109.6
C(48)-C(79)-H(79A)	109.6
N(6)-C(79)-H(79B)	109.6
C(48)-C(79)-H(79B)	109.6
H(79A)-C(79)-H(79B)	108.1
C(30)-C(81)-H(81A)	109.5
C(30)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(30)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(141)-C(69A)-C(80A)	121.6(7)
C(141)-C(69A)-C(55)	115.0(6)
C(80A)-C(69A)-C(55)	111.9(4)
C(141)-C(69A)-C(151)	101.8(8)
C(80A)-C(69A)-C(151)	97.2(7)
C(55)-C(69A)-C(151)	105.5(6)
C(69A)-C(80A)-H(80A)	109.5
C(69A)-C(80A)-H(80B)	109.5
H(80A)-C(80A)-H(80B)	109.5
C(69A)-C(80A)-H(80C)	109.5
H(80A)-C(80A)-H(80C)	109.5
H(80B)-C(80A)-H(80C)	109.5
C(69A)-C(141)-H(14A)	109.5
C(69A)-C(141)-H(14B)	109.5
H(14A)-C(141)-H(14B)	109.5
C(69A)-C(141)-H(14C)	109.5
H(14A)-C(141)-H(14C)	109.5
H(14B)-C(141)-H(14C)	109.5

C (69A) -C (151) -H (15A)	109.5
C (69A) -C (151) -H (15B)	109.5
H (15A) -C (151) -H (15B)	109.5
C (69A) -C (151) -H (15C)	109.5
H (15A) -C (151) -H (15C)	109.5
H (15B) -C (151) -H (15C)	109.5
H (24A) -C (241) -H (24B)	109.5
H (24A) -C (241) -H (24C)	109.5
H (24B) -C (241) -H (24C)	109.5
H (25A) -C (251) -H (25B)	109.5
H (25A) -C (251) -H (25C)	109.5
H (25B) -C (251) -H (25C)	109.5

Table 6S. Torsion angles [°] for **1**

O(9)-Y(1)-Y(2)-O(7)	172.68 (12)
O(10)-Y(1)-Y(2)-O(7)	-64.20 (14)
O(3)-Y(1)-Y(2)-O(7)	-88.64 (16)
O(4)-Y(1)-Y(2)-O(7)	84.55 (16)
N(13)-Y(1)-Y(2)-O(7)	91.34 (14)
N(8)-Y(1)-Y(2)-O(7)	18.32 (12)
O(9)-Y(1)-Y(2)-O(5)	-63.92 (13)
O(10)-Y(1)-Y(2)-O(5)	59.19 (15)
O(3)-Y(1)-Y(2)-O(5)	34.76 (17)
O(4)-Y(1)-Y(2)-O(5)	-152.05 (17)
N(13)-Y(1)-Y(2)-O(5)	-145.26 (15)
N(8)-Y(1)-Y(2)-O(5)	141.71 (13)
O(9)-Y(1)-Y(2)-O(3)	-98.68 (16)
O(10)-Y(1)-Y(2)-O(3)	24.43 (17)
O(4)-Y(1)-Y(2)-O(3)	173.19 (19)
N(13)-Y(1)-Y(2)-O(3)	179.98 (17)
N(8)-Y(1)-Y(2)-O(3)	106.96 (16)
O(9)-Y(1)-Y(2)-O(4)	88.13 (16)
O(10)-Y(1)-Y(2)-O(4)	-148.76 (17)
O(3)-Y(1)-Y(2)-O(4)	-173.19 (19)
N(13)-Y(1)-Y(2)-O(4)	6.79 (17)
N(8)-Y(1)-Y(2)-O(4)	-66.23 (16)
O(9)-Y(1)-Y(2)-N(11)	84.66 (16)
O(10)-Y(1)-Y(2)-N(11)	-152.23 (17)
O(3)-Y(1)-Y(2)-N(11)	-176.67 (19)
O(4)-Y(1)-Y(2)-N(11)	-3.47 (19)
N(13)-Y(1)-Y(2)-N(11)	3.31 (17)
N(8)-Y(1)-Y(2)-N(11)	-69.71 (16)
O(9)-Y(1)-Y(2)-N(6)	16.33 (12)
O(10)-Y(1)-Y(2)-N(6)	139.44 (13)
O(3)-Y(1)-Y(2)-N(6)	115.00 (16)
O(4)-Y(1)-Y(2)-N(6)	-71.80 (15)
N(13)-Y(1)-Y(2)-N(6)	-65.01 (13)
N(8)-Y(1)-Y(2)-N(6)	-138.04 (12)
O(9)-Y(1)-O(3)-C(43)	-85.7 (4)
O(10)-Y(1)-O(3)-C(43)	22.6 (4)
O(4)-Y(1)-O(3)-C(43)	-179.7 (4)
N(13)-Y(1)-O(3)-C(43)	-175.4 (4)
N(8)-Y(1)-O(3)-C(43)	102.0 (4)
Y(2)-Y(1)-O(3)-C(43)	-175.4 (4)
O(9)-Y(1)-O(3)-Y(2)	89.66 (14)
O(10)-Y(1)-O(3)-Y(2)	-162.02 (13)
O(4)-Y(1)-O(3)-Y(2)	-4.28 (12)
N(13)-Y(1)-O(3)-Y(2)	-0.1 (5)
N(8)-Y(1)-O(3)-Y(2)	-82.65 (15)
O(7)-Y(2)-O(3)-C(43)	-84.3 (3)
O(5)-Y(2)-O(3)-C(43)	23.9 (3)
O(4)-Y(2)-O(3)-C(43)	-179.8 (3)
N(11)-Y(2)-O(3)-C(43)	-163.6 (10)
N(6)-Y(2)-O(3)-C(43)	102.7 (3)
Y(1)-Y(2)-O(3)-C(43)	175.9 (4)
O(7)-Y(2)-O(3)-Y(1)	99.79 (14)
O(5)-Y(2)-O(3)-Y(1)	-151.95 (13)
O(4)-Y(2)-O(3)-Y(1)	4.29 (12)
N(11)-Y(2)-O(3)-Y(1)	20.6 (11)
N(6)-Y(2)-O(3)-Y(1)	-73.19 (15)
O(7)-Y(2)-O(4)-Y(1)	-103.23 (13)

O(5)-Y(2)-O(4)-Y(1)	58.4 (3)
O(3)-Y(2)-O(4)-Y(1)	-4.16 (11)
N(11)-Y(2)-O(4)-Y(1)	177.65 (13)
N(6)-Y(2)-O(4)-Y(1)	108.66 (13)
O(9)-Y(1)-O(4)-Y(2)	-98.25 (13)
O(10)-Y(1)-O(4)-Y(2)	75.7 (3)
O(3)-Y(1)-O(4)-Y(2)	4.18 (12)
N(13)-Y(1)-O(4)-Y(2)	-174.65 (13)
N(8)-Y(1)-O(4)-Y(2)	115.52 (14)
O(7)-Y(2)-O(5)-C(38)	-134.8 (4)
O(3)-Y(2)-O(5)-C(38)	122.3 (4)
O(4)-Y(2)-O(5)-C(38)	64.3 (5)
N(11)-Y(2)-O(5)-C(38)	-56.9 (4)
N(6)-Y(2)-O(5)-C(38)	12.7 (4)
Y(1)-Y(2)-O(5)-C(38)	102.8 (4)
O(7)-Y(2)-N(6)-C(79)	14.6 (4)
O(5)-Y(2)-N(6)-C(79)	-88.8 (3)
O(3)-Y(2)-N(6)-C(79)	-178.5 (3)
O(4)-Y(2)-N(6)-C(79)	112.1 (3)
N(11)-Y(2)-N(6)-C(79)	8.2 (3)
Y(1)-Y(2)-N(6)-C(79)	147.2 (3)
O(7)-Y(2)-N(6)-C(54)	-107.8 (3)
O(5)-Y(2)-N(6)-C(54)	148.8 (3)
O(3)-Y(2)-N(6)-C(54)	59.0 (3)
O(4)-Y(2)-N(6)-C(54)	-10.3 (3)
N(11)-Y(2)-N(6)-C(54)	-114.3 (3)
Y(1)-Y(2)-N(6)-C(54)	24.8 (3)
O(7)-Y(2)-N(6)-C(46)	136.0 (3)
O(5)-Y(2)-N(6)-C(46)	32.6 (2)
O(3)-Y(2)-N(6)-C(46)	-57.2 (3)
O(4)-Y(2)-N(6)-C(46)	-126.5 (3)
N(11)-Y(2)-N(6)-C(46)	129.5 (3)
Y(1)-Y(2)-N(6)-C(46)	-91.4 (2)
O(5)-Y(2)-O(7)-C(16)	77.5 (4)
O(3)-Y(2)-O(7)-C(16)	175.1 (4)
O(4)-Y(2)-O(7)-C(16)	-111.1 (4)
N(11)-Y(2)-O(7)-C(16)	-11.3 (4)
N(6)-Y(2)-O(7)-C(16)	-17.5 (5)
Y(1)-Y(2)-O(7)-C(16)	-148.4 (4)
O(9)-Y(1)-N(8)-C(31)	3.7 (4)
O(10)-Y(1)-N(8)-C(31)	-94.9 (3)
O(3)-Y(1)-N(8)-C(31)	170.1 (3)
O(4)-Y(1)-N(8)-C(31)	100.1 (3)
N(13)-Y(1)-N(8)-C(31)	7.0 (3)
Y(2)-Y(1)-N(8)-C(31)	133.7 (3)
O(9)-Y(1)-N(8)-C(18)	126.6 (3)
O(10)-Y(1)-N(8)-C(18)	28.0 (2)
O(3)-Y(1)-N(8)-C(18)	-67.0 (3)
O(4)-Y(1)-N(8)-C(18)	-137.0 (3)
N(13)-Y(1)-N(8)-C(18)	129.9 (3)
Y(2)-Y(1)-N(8)-C(18)	-103.4 (2)
O(9)-Y(1)-N(8)-C(34)	-117.5 (3)
O(10)-Y(1)-N(8)-C(34)	144.0 (3)
O(3)-Y(1)-N(8)-C(34)	49.0 (3)
O(4)-Y(1)-N(8)-C(34)	-21.0 (3)
N(13)-Y(1)-N(8)-C(34)	-114.1 (3)
Y(2)-Y(1)-N(8)-C(34)	12.5 (3)
O(10)-Y(1)-O(9)-C(24)	99.8 (5)
O(3)-Y(1)-O(9)-C(24)	-156.8 (5)
O(4)-Y(1)-O(9)-C(24)	-82.6 (5)
N(13)-Y(1)-O(9)-C(24)	6.7 (5)

N (8) -Y (1) -O (9) -C (24)	9.9 (6)
Y (2) -Y (1) -O (9) -C (24)	-120.0 (5)
O (9) -Y (1) -O (10) -C (20)	-122.3 (4)
O (3) -Y (1) -O (10) -C (20)	130.4 (4)
O (4) -Y (1) -O (10) -C (20)	63.9 (6)
N (13) -Y (1) -O (10) -C (20)	-44.7 (4)
N (8) -Y (1) -O (10) -C (20)	23.0 (4)
Y (2) -Y (1) -O (10) -C (20)	116.1 (4)
O (7) -Y (2) -N (11) -C (48)	-153.8 (3)
O (5) -Y (2) -N (11) -C (48)	99.2 (3)
O (3) -Y (2) -N (11) -C (48)	-73.3 (11)
O (4) -Y (2) -N (11) -C (48)	-57.5 (3)
N (6) -Y (2) -N (11) -C (48)	22.7 (3)
Y (1) -Y (2) -N (11) -C (48)	-55.4 (3)
O (7) -Y (2) -N (11) -C (53)	-37.3 (3)
O (5) -Y (2) -N (11) -C (53)	-144.2 (3)
O (3) -Y (2) -N (11) -C (53)	43.2 (12)
O (4) -Y (2) -N (11) -C (53)	59.1 (3)
N (6) -Y (2) -N (11) -C (53)	139.2 (3)
Y (1) -Y (2) -N (11) -C (53)	61.2 (3)
O (7) -Y (2) -N (11) -C (28)	83.8 (3)
O (5) -Y (2) -N (11) -C (28)	-23.2 (3)
O (3) -Y (2) -N (11) -C (28)	164.3 (10)
O (4) -Y (2) -N (11) -C (28)	-179.9 (3)
N (6) -Y (2) -N (11) -C (28)	-99.7 (3)
Y (1) -Y (2) -N (11) -C (28)	-177.8 (2)
O (9) -Y (1) -N (13) -C (19)	-159.6 (3)
O (10) -Y (1) -N (13) -C (19)	96.1 (3)
O (3) -Y (1) -N (13) -C (19)	-65.9 (6)
O (4) -Y (1) -N (13) -C (19)	-61.9 (3)
N (8) -Y (1) -N (13) -C (19)	22.3 (3)
Y (2) -Y (1) -N (13) -C (19)	-66.0 (3)
O (9) -Y (1) -N (13) -C (33)	77.8 (3)
O (10) -Y (1) -N (13) -C (33)	-26.5 (3)
O (3) -Y (1) -N (13) -C (33)	171.4 (4)
O (4) -Y (1) -N (13) -C (33)	175.5 (3)
N (8) -Y (1) -N (13) -C (33)	-100.3 (3)
Y (2) -Y (1) -N (13) -C (33)	171.4 (2)
O (9) -Y (1) -N (13) -C (36)	-43.2 (2)
O (10) -Y (1) -N (13) -C (36)	-147.4 (2)
O (3) -Y (1) -N (13) -C (36)	50.5 (5)
O (4) -Y (1) -N (13) -C (36)	54.5 (2)
N (8) -Y (1) -N (13) -C (36)	138.7 (3)
Y (2) -Y (1) -N (13) -C (36)	50.5 (3)
Y (2) -O (7) -C (16) -C (17)	31.5 (7)
Y (2) -O (7) -C (16) -C (29)	-148.4 (4)
O (7) -C (16) -C (17) -C (59)	-177.6 (4)
C (29) -C (16) -C (17) -C (59)	2.4 (7)
O (7) -C (16) -C (17) -C (53)	2.7 (7)
C (29) -C (16) -C (17) -C (53)	-177.4 (4)
C (31) -N (8) -C (18) -C (22)	53.4 (5)
C (34) -N (8) -C (18) -C (22)	172.9 (4)
Y (1) -N (8) -C (18) -C (22)	-69.0 (4)
C (33) -N (13) -C (19) -C (31)	73.4 (5)
C (36) -N (13) -C (19) -C (31)	-167.3 (3)
Y (1) -N (13) -C (19) -C (31)	-50.6 (4)
Y (1) -O (10) -C (20) -C (22)	-37.5 (7)
Y (1) -O (10) -C (20) -C (14)	141.4 (4)
C (32) -C (14) -C (20) -O (10)	-175.7 (4)
C (40) -C (14) -C (20) -O (10)	5.7 (7)
C (32) -C (14) -C (20) -C (22)	3.2 (6)

C (40) -C (14) -C (20) -C (22)	-175.4 (4)
O (10) -C (20) -C (22) -C (50)	175.4 (4)
C (14) -C (20) -C (22) -C (50)	-3.6 (7)
O (10) -C (20) -C (22) -C (18)	-7.7 (6)
C (14) -C (20) -C (22) -C (18)	173.4 (4)
N (8) -C (18) -C (22) -C (50)	-118.5 (5)
N (8) -C (18) -C (22) -C (20)	64.5 (5)
Y (1) -O (9) -C (24) -C (57)	12.7 (8)
Y (1) -O (9) -C (24) -C (12)	-168.5 (3)
C (51) -C (12) -C (24) -O (9)	179.9 (4)
C (27) -C (12) -C (24) -O (9)	-1.3 (7)
C (51) -C (12) -C (24) -C (57)	-1.3 (7)
C (27) -C (12) -C (24) -C (57)	177.5 (4)
C (58) -C (21) -C (25) -C (70)	-96.3 (5)
C (35) -C (21) -C (25) -C (70)	82.6 (5)
C (58) -C (21) -C (25) -C (71)	143.4 (4)
C (35) -C (21) -C (25) -C (71)	-37.6 (6)
C (58) -C (21) -C (25) -C (60)	23.8 (6)
C (35) -C (21) -C (25) -C (60)	-157.2 (4)
C (51) -C (12) -C (27) -C (66)	0.6 (7)
C (24) -C (12) -C (27) -C (66)	-178.2 (4)
C (51) -C (12) -C (27) -C (65)	120.0 (5)
C (24) -C (12) -C (27) -C (65)	-58.9 (6)
C (51) -C (12) -C (27) -C (72)	-119.8 (5)
C (24) -C (12) -C (27) -C (72)	61.4 (6)
O (7) -C (16) -C (29) -C (49)	177.7 (4)
C (17) -C (16) -C (29) -C (49)	-2.2 (7)
O (7) -C (16) -C (29) -C (61)	-1.5 (7)
C (17) -C (16) -C (29) -C (61)	178.6 (4)
C (18) -N (8) -C (31) -C (19)	-156.6 (3)
C (34) -N (8) -C (31) -C (19)	85.6 (4)
Y (1) -N (8) -C (31) -C (19)	-35.8 (4)
N (13) -C (19) -C (31) -N (8)	59.6 (5)
C (20) -C (14) -C (32) -C (42)	-0.3 (7)
C (40) -C (14) -C (32) -C (42)	178.2 (4)
C (38) -C (15) -C (35) -C (21)	1.1 (7)
C (46) -C (15) -C (35) -C (21)	-172.4 (4)
C (58) -C (21) -C (35) -C (15)	-0.5 (6)
C (25) -C (21) -C (35) -C (15)	-179.5 (4)
C (19) -N (13) -C (36) -C (57)	-169.5 (4)
C (33) -N (13) -C (36) -C (57)	-49.9 (5)
Y (1) -N (13) -C (36) -C (57)	72.7 (4)
C (57) -C (23) -C (37) -C (51)	-1.2 (7)
C (57) -C (23) -C (37) -C (30)	177.5 (4)
C (81) -C (30) -C (37) -C (23)	147.8 (5)
C (52) -C (30) -C (37) -C (23)	-92.3 (5)
C (77) -C (30) -C (37) -C (23)	25.8 (7)
C (81) -C (30) -C (37) -C (51)	-33.6 (6)
C (52) -C (30) -C (37) -C (51)	86.3 (5)
C (77) -C (30) -C (37) -C (51)	-155.6 (5)
Y (2) -O (5) -C (38) -C (15)	-28.2 (6)
Y (2) -O (5) -C (38) -C (26)	151.5 (3)
C (35) -C (15) -C (38) -O (5)	179.2 (4)
C (46) -C (15) -C (38) -O (5)	-7.5 (6)
C (35) -C (15) -C (38) -C (26)	-0.5 (6)
C (46) -C (15) -C (38) -C (26)	172.8 (4)
C (58) -C (26) -C (38) -O (5)	179.8 (4)
C (47) -C (26) -C (38) -O (5)	1.2 (7)
C (58) -C (26) -C (38) -C (15)	-0.6 (6)
C (47) -C (26) -C (38) -C (15)	-179.1 (4)
C (32) -C (14) -C (40) -C (45)	121.4 (5)

C (20) -C (14) -C (40) -C (45)	-60.1 (5)
C (32) -C (14) -C (40) -C (64)	-117.3 (5)
C (20) -C (14) -C (40) -C (64)	61.2 (5)
C (32) -C (14) -C (40) -C (44)	0.8 (6)
C (20) -C (14) -C (40) -C (44)	179.4 (4)
C (14) -C (32) -C (42) -C (50)	-2.2 (7)
C (14) -C (32) -C (42) -C (39)	176.2 (4)
C (68) -C (39) -C (42) -C (50)	66.9 (5)
C (62) -C (39) -C (42) -C (50)	-172.9 (4)
C (63) -C (39) -C (42) -C (50)	-53.4 (6)
C (68) -C (39) -C (42) -C (32)	-111.4 (5)
C (62) -C (39) -C (42) -C (32)	8.9 (6)
C (63) -C (39) -C (42) -C (32)	128.4 (5)
Y (1) -O (3) -C (43) -C (78)	-74.2 (5)
Y (2) -O (3) -C (43) -C (78)	111.0 (4)
Y (1) -O (3) -C (43) -C (76)	48.8 (5)
Y (2) -O (3) -C (43) -C (76)	-126.1 (3)
C (79) -N (6) -C (46) -C (15)	51.4 (5)
C (54) -N (6) -C (46) -C (15)	170.5 (4)
Y (2) -N (6) -C (46) -C (15)	-69.6 (4)
C (35) -C (15) -C (46) -N (6)	-124.6 (4)
C (38) -C (15) -C (46) -N (6)	61.9 (6)
C (58) -C (26) -C (47) -C (73)	2.9 (6)
C (38) -C (26) -C (47) -C (73)	-178.6 (4)
C (58) -C (26) -C (47) -C (56)	121.5 (5)
C (38) -C (26) -C (47) -C (56)	-59.9 (6)
C (58) -C (26) -C (47) -C (74)	-117.8 (5)
C (38) -C (26) -C (47) -C (74)	60.7 (6)
C (53) -N (11) -C (48) -C (79)	-167.2 (4)
C (28) -N (11) -C (48) -C (79)	73.9 (5)
Y (2) -N (11) -C (48) -C (79)	-52.4 (4)
C (16) -C (29) -C (49) -C (55)	0.0 (7)
C (61) -C (29) -C (49) -C (55)	179.1 (4)
C (20) -C (22) -C (50) -C (42)	0.9 (7)
C (18) -C (22) -C (50) -C (42)	-175.9 (4)
C (32) -C (42) -C (50) -C (22)	1.9 (7)
C (39) -C (42) -C (50) -C (22)	-176.5 (4)
C (24) -C (12) -C (51) -C (37)	0.2 (7)
C (27) -C (12) -C (51) -C (37)	-178.7 (5)
C (23) -C (37) -C (51) -C (12)	1.1 (7)
C (30) -C (37) -C (51) -C (12)	-177.6 (4)
C (48) -N (11) -C (53) -C (17)	-169.9 (4)
C (28) -N (11) -C (53) -C (17)	-50.7 (5)
Y (2) -N (11) -C (53) -C (17)	74.6 (4)
C (16) -C (17) -C (53) -N (11)	-61.1 (6)
C (59) -C (17) -C (53) -N (11)	119.1 (5)
C (29) -C (49) -C (55) -C (59)	2.2 (7)
C (29) -C (49) -C (55) -C (69A)	-175.8 (5)
C (37) -C (23) -C (57) -C (24)	0.0 (7)
C (37) -C (23) -C (57) -C (36)	175.6 (4)
O (9) -C (24) -C (57) -C (23)	-179.9 (4)
C (12) -C (24) -C (57) -C (23)	1.3 (7)
O (9) -C (24) -C (57) -C (36)	4.6 (7)
C (12) -C (24) -C (57) -C (36)	-174.2 (4)
N (13) -C (36) -C (57) -C (23)	130.8 (4)
N (13) -C (36) -C (57) -C (24)	-53.6 (6)
C (35) -C (21) -C (58) -C (26)	-0.7 (7)
C (25) -C (21) -C (58) -C (26)	178.4 (4)
C (38) -C (26) -C (58) -C (21)	1.2 (7)
C (47) -C (26) -C (58) -C (21)	179.8 (4)
C (16) -C (17) -C (59) -C (55)	-0.2 (7)

C (53) -C (17) -C (59) -C (55)	179.6 (4)
C (49) -C (55) -C (59) -C (17)	-2.0 (7)
C (69A) -C (55) -C (59) -C (17)	176.0 (4)
C (49) -C (29) -C (61) -C (67)	123.2 (5)
C (16) -C (29) -C (61) -C (67)	-57.7 (6)
C (49) -C (29) -C (61) -C (75)	3.4 (6)
C (16) -C (29) -C (61) -C (75)	-177.5 (4)
C (49) -C (29) -C (61) -C (41)	-114.7 (5)
C (16) -C (29) -C (61) -C (41)	64.4 (6)
C (54) -N (6) -C (79) -C (48)	86.3 (4)
C (46) -N (6) -C (79) -C (48)	-156.3 (4)
Y (2) -N (6) -C (79) -C (48)	-37.7 (4)
N (11) -C (48) -C (79) -N (6)	63.1 (5)
C (49) -C (55) -C (69A) -C (141)	14.1 (10)
C (59) -C (55) -C (69A) -C (141)	-163.8 (8)
C (49) -C (55) -C (69A) -C (80A)	-130.1 (6)
C (59) -C (55) -C (69A) -C (80A)	52.0 (7)
C (49) -C (55) -C (69A) -C (151)	125.4 (7)
C (59) -C (55) -C (69A) -C (151)	-52.5 (8)

Computational details

In view of the good performance of density functional theory (DFT), we were instigated to perform DFT calculations at the B3PW91 level of theory on all stationary points of the potential energy surfaces (PES) we studied using the GAUSSIAN09 program suite.⁶ The equilibrium and transition structures were fully optimized at the Becke's 3-parameter hybrid functional⁷ combined with the non-local correlation functional provided by Perdew/Wang.⁸ RECP (augmented by a *f* polarization function, $\alpha = 1.0$) was used to represent the yttrium.⁹ For the rest of non-metal atoms the 6-31G(d,p) basis set was used.¹⁰ In all computations no constraints were imposed on the geometry. Full geometry optimization was performed for each structure using Schlegel's analytical gradient method¹¹ and the attainment of the energy minimum was verified by calculating the vibrational frequencies that result in absence of imaginary eigenvalues. All stationary points have been identified for minimum (number of imaginary frequencies Nimag=0) or transition states (Nimag=1). The vibrational modes and the corresponding frequencies are based on a harmonic force field. This was achieved with the SCF convergence on the density matrix of at least 10^{-9} and the rms force less than 10^{-4} au. All bond lengths and bond angles were optimized to better than 0.001 Å and 0.1°, respectively. Gibbs free energies were obtained at T = 298.15K within the harmonic approximation. Intrinsic Reaction Paths (IRPs)¹² were traced from the various transition structures to ensure that no further intermediates exist.

Cartesian coordinates of all optimized complexes as well as their energies

R_BBL.xyz

12

scf done: -306.370296

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.450000
C	1.450000	0.000000	0.000000
O	1.450000	0.000000	1.450000
O	2.227817	0.000000	-0.777817
H	-0.544500	-0.544500	-0.770039
H	-0.195852	1.065231	-0.113343
C	-0.666874	-0.666874	1.994500
H	-0.231407	1.029676	1.718588
H	-0.536631	-0.536631	2.985529
H	-1.699399	-0.441930	1.731418
H	-0.441930	-1.699399	1.731418

S_BBL.xyz

12

scf done: -306.370297

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.450000
C	1.450000	0.000000	0.000000
O	1.450000	0.000000	1.450000
O	2.227817	0.000000	-0.777817
H	-0.544500	-0.544500	-0.770039
H	-0.195852	1.065231	-0.113343
H	-0.666874	-0.666874	1.994500
C	-0.231407	1.029676	1.718588
H	-0.251410	1.118684	2.722451
H	0.531222	1.691399	1.310617
H	-1.203832	1.301468	1.310617

YComp.xyz

104

scf done: -1819.879843

C	0.783246	2.267294	-0.147083
C	0.247891	1.859378	1.103554
C	0.456096	0.526907	1.536364
C	1.201101	-0.363495	0.765757
C	1.756680	0.012533	-0.458436
C	1.520523	1.327570	-0.877030
O	-0.443737	2.679059	1.889358
Y	-0.802151	3.076162	3.946889
N	0.225655	0.749108	4.055968
C	-0.472492	0.115308	5.192521
C	-0.294856	0.870691	6.502770
N	-0.688727	2.294037	6.390656
C	-2.061861	2.543027	6.934467

C	-3.184719	1.724803	6.359785
C	-3.868509	0.818789	7.169122
C	-4.990859	0.125312	6.711576
C	-5.413683	0.409195	5.407437
C	-4.774874	1.312250	4.548525
C	-3.607541	1.964932	5.027231
O	-2.891846	2.797017	4.273479
C	-0.205229	0.056266	2.800240
O	0.022161	4.903488	4.373620
C	0.466008	6.225611	4.271881
C	0.249866	3.147668	7.141430
C	1.685245	0.674812	4.205565
C	1.535525	6.515542	5.325308
H	0.928480	6.373233	3.279852
C	-0.709813	7.196056	4.387393
H	-0.127081	-0.924565	5.324190
H	-1.539454	0.071489	4.948111
H	-0.884367	0.364204	7.278582
H	0.750301	0.824412	6.824014
H	-2.030747	2.386685	8.024861
H	-2.261818	3.608922	6.763866
H	-0.027380	-1.024722	2.920014
H	-1.292150	0.198763	2.730777
C	0.554131	3.689558	-0.682768
H	1.932835	1.640917	-1.827370
C	2.573627	-0.996193	-1.277332
H	1.335672	-1.378507	1.136290
C	-5.329594	1.603158	3.144184
H	-6.295954	-0.096859	5.037311
C	-5.709550	-0.873763	7.629079
H	-3.516666	0.672337	8.189356
H	2.023826	-0.365026	4.339847
H	2.158623	1.075145	3.306956
H	2.016505	1.261015	5.066346
H	0.259318	2.890464	8.212403
H	1.261998	3.036396	6.743938
H	-0.037317	4.193420	7.023117
C	-6.638729	0.848053	2.866309
C	-5.628423	3.110493	3.008991
C	-4.313547	1.175129	2.066603
H	-6.008984	3.330392	2.004356
H	-6.390930	3.418094	3.733248
H	-4.730272	3.706628	3.178802
H	-4.720691	1.364754	1.066240
H	-3.376963	1.727350	2.157799
H	-4.099872	0.102188	2.140113
H	-7.000698	1.113310	1.867355
H	-6.504004	-0.239213	2.886215
H	-7.425409	1.111856	3.581541
C	-6.923502	-1.522667	6.950223

C	-4.732426	-1.995888	8.032543
C	-6.202351	-0.150418	8.898067
H	-7.397854	-2.229136	7.639736
H	-7.677623	-0.779987	6.669124
H	-6.638747	-2.079464	6.051130
H	-5.222352	-2.714774	8.699970
H	-4.377249	-2.539277	7.150241
H	-3.856479	-1.600796	8.557027
H	-6.720564	-0.850187	9.564496
H	-5.374499	0.291731	9.461451
H	-6.898409	0.655096	8.642302
C	1.182986	3.902884	-2.068322
C	-0.958727	3.957975	-0.817417
C	1.187105	4.719996	0.274078
H	1.025075	5.736511	-0.104917
H	0.753255	4.651925	1.272898
H	2.268381	4.559495	0.354035
H	0.972807	4.923937	-2.404555
H	2.271869	3.781636	-2.053234
H	0.769753	3.219338	-2.818093
H	-1.130586	4.979575	-1.177725
H	-1.409240	3.266699	-1.538365
H	-1.467936	3.836183	0.139801
C	3.091579	-0.399561	-2.593274
C	3.790268	-1.463224	-0.453599
C	1.696438	-2.216805	-1.619715
H	3.665390	-1.155108	-3.140747
H	2.272372	-0.073082	-3.242754
H	3.753174	0.456218	-2.421285
H	4.383616	-2.191773	-1.019036
H	4.439308	-0.617505	-0.202371
H	3.485632	-1.939637	0.483864
H	2.268314	-2.952360	-2.197942
H	1.328081	-2.717464	-0.718744
H	0.826213	-1.917945	-2.213215
H	1.940893	7.527243	5.212282
H	1.114939	6.428838	6.334161
H	2.362106	5.803379	5.234748
H	-0.384008	8.236044	4.271798
H	-1.457113	6.984003	3.616043
H	-1.192562	7.092653	5.366352

YBRTS1.xyz

116

scf done: -2126.251328

C	0.069024	0.059297	-0.095226
C	0.156726	0.239447	1.310900
C	1.412151	0.069416	1.946824
C	2.559781	-0.184342	1.199284
C	2.518187	-0.300490	-0.192264

C	1.258599	-0.190033	-0.792417
O	-0.888403	0.567237	2.064896
Y	-1.363279	1.841409	3.716975
O	-1.347901	2.651375	5.908141
C	-2.037085	1.855059	6.592433
O	-3.317432	2.157335	6.997312
C	-3.159299	1.398906	8.243978
C	-3.412831	2.267342	9.452087
C	1.469215	0.029528	3.448299
N	1.130702	1.274275	4.202585
C	1.997409	2.411699	3.825625
C	1.414304	3.256557	2.701548
N	0.085601	3.813142	3.020895
C	0.176897	4.884040	4.023767
C	3.805682	-0.563176	-0.984980
C	4.807117	0.581658	-0.733969
C	-1.284116	0.103494	-0.825226
C	-2.228463	-0.951993	-0.214292
O	-2.804985	3.117924	2.836583
C	-2.961902	4.359670	2.381471
C	-1.827891	5.047787	1.883058
C	-1.936397	6.361554	1.432269
C	-3.153864	7.043811	1.433868
C	-4.265632	6.336374	1.903457
C	-4.220653	5.018469	2.374064
C	-0.511653	4.332026	1.752579
C	-5.494730	4.313318	2.865493
C	-5.730727	3.026800	2.047942
C	-3.228740	8.491250	0.929775
C	-2.300069	9.381491	1.779194
O	-2.249718	0.502143	5.282384
C	-3.144793	-0.583891	5.422686
C	-4.528257	-0.239784	4.875702
C	-5.356119	3.971914	4.361617
C	-6.749163	5.187009	2.708003
C	-2.778189	8.549876	-0.543430
C	-4.648503	9.068118	1.015607
C	1.307516	0.973021	5.633539
C	-1.923513	1.500223	-0.703957
C	-1.149291	-0.211556	-2.322987
C	4.433004	-1.894636	-0.526423
C	3.554503	-0.650976	-2.496822
C	-1.704562	1.081161	7.865862
H	-3.247976	-0.808087	6.498618
H	2.122163	4.068771	2.461114
H	1.314100	2.639725	1.804002
H	2.993858	2.056111	3.522233
H	2.144043	3.031217	4.715637
H	2.479010	-0.291508	3.753801
H	0.764641	-0.731383	3.808589

H	0.214205	5.013043	1.278817
H	-0.620029	3.464392	1.089259
H	-5.224942	6.837347	1.904196
H	-1.038024	6.852470	1.061239
H	1.195401	-0.308471	-1.866461
H	3.502751	-0.309042	1.729627
H	0.848173	5.689117	3.683992
H	-0.815279	5.305489	4.191538
H	0.539754	4.488962	4.974025
H	2.352840	0.711183	5.863869
H	1.002825	1.833442	6.231076
H	0.670217	0.127613	5.904611
H	-3.203609	-0.921574	-0.715127
H	-1.815246	-1.959096	-0.339918
H	-2.379474	-0.769311	0.851022
H	-2.875843	1.527056	-1.247147
H	-2.123228	1.762451	0.336053
H	-1.270976	2.264226	-1.142556
H	-2.143082	-0.196988	-2.783222
H	-0.536224	0.528756	-2.849042
H	-0.719497	-1.203738	-2.499317
H	4.501538	-0.824340	-3.019185
H	2.882180	-1.477169	-2.751268
H	3.123375	0.274898	-2.892403
H	5.738601	0.409277	-1.286230
H	4.391562	1.541233	-1.059785
H	5.062318	0.671012	0.326847
H	5.357545	-2.098048	-1.080048
H	4.681353	-1.880460	0.539634
H	3.743909	-2.728546	-0.696017
H	-6.256958	3.456885	4.718044
H	-4.495930	3.329052	4.547922
H	-5.233379	4.884216	4.956063
H	-7.622740	4.624704	3.055595
H	-6.694618	6.104688	3.304196
H	-6.931115	5.464564	1.663846
H	-6.625063	2.506867	2.412668
H	-5.888896	3.267191	0.990588
H	-4.878475	2.349935	2.121424
H	-4.650836	10.100818	0.650389
H	-5.356434	8.500075	0.402830
H	-5.021613	9.081461	2.045332
H	-2.333733	10.420456	1.429641
H	-2.601875	9.366187	2.831881
H	-1.259121	9.046880	1.726313
H	-2.815500	9.579708	-0.918564
H	-1.752730	8.187985	-0.669123
H	-3.427478	7.933611	-1.174077
H	-3.825995	0.530580	8.229965
H	-0.955331	1.591202	8.477408

H	-1.441548	0.031744	7.737555
H	-3.239902	1.695245	10.369895
H	-2.750237	3.138188	9.451826
H	-4.447483	2.622243	9.460689
H	-5.233960	-1.061448	5.043261
H	-4.916992	0.660186	5.357999
H	-4.477418	-0.054119	3.796565
C	-2.555228	-1.823123	4.751847
H	-3.214425	-2.689008	4.879165
H	-2.419214	-1.651287	3.678719
H	-1.579541	-2.067946	5.184021

YBRTS1R.xyz

116

scf done: -2126.267395

C	0.142437	0.107395	-0.205762
C	0.172095	0.289366	1.203768
C	1.387580	0.055364	1.897099
C	2.554644	-0.252773	1.201650
C	2.572740	-0.368379	-0.190367
C	1.348813	-0.199954	-0.848039
O	-0.888100	0.670898	1.902154
Y	-1.441830	1.735483	3.679191
O	-1.242519	2.925919	5.861356
C	-1.931581	2.835267	6.856280
O	-1.679134	3.421594	8.036803
C	-2.917240	2.839533	8.627456
C	-2.608599	1.984376	9.827001
C	1.380193	-0.003966	3.400077
N	1.048403	1.239364	4.163056
C	1.911107	2.378664	3.780601
C	1.317910	3.226752	2.662112
N	0.013550	3.816033	3.013378
C	0.176763	4.927228	3.957559
C	3.882066	-0.695568	-0.921135
C	4.922319	0.404727	-0.632057
C	-1.175743	0.196221	-0.993771
C	-2.168218	-0.844496	-0.435454
O	-2.914048	3.102975	2.943714
C	-3.067911	4.339048	2.482050
C	-1.948742	5.020028	1.937532
C	-2.072426	6.330290	1.480694
C	-3.286124	7.019351	1.520537
C	-4.384050	6.320390	2.032688
C	-4.324520	5.005157	2.508183
C	-0.637195	4.301117	1.762495
C	-5.587129	4.294382	3.021686
C	-5.856569	3.036185	2.170931
C	-3.372112	8.463307	1.008497
C	-2.414490	9.356620	1.821732

O	-2.377461	0.283501	4.854825
C	-3.097321	-0.878789	5.116929
C	-4.121787	-1.153445	4.014380
C	-5.398502	3.890531	4.497329
C	-6.839362	5.180720	2.944653
C	-2.967917	8.510210	-0.478548
C	-4.786525	9.045958	1.134332
C	1.229687	0.928747	5.591120
C	-1.793176	1.603149	-0.879929
C	-0.982899	-0.101650	-2.488611
C	4.427141	-2.050159	-0.426608
C	3.697212	-0.785115	-2.442363
C	-3.203634	2.155194	7.280978
H	-3.663526	-0.756153	6.064876
H	2.041061	4.017698	2.394628
H	1.182439	2.603066	1.774850
H	2.904223	2.022144	3.468218
H	2.064832	2.996333	4.670826
H	2.369764	-0.354005	3.738034
H	0.645302	-0.752126	3.725423
H	0.062777	4.971538	1.235395
H	-0.776064	3.418812	1.126068
H	-5.341639	6.824470	2.060167
H	-1.186484	6.814693	1.072709
H	1.329291	-0.319054	-1.923698
H	3.465380	-0.422453	1.774293
H	0.829935	5.710600	3.537793
H	-0.798023	5.368767	4.170168
H	0.602230	4.575513	4.898345
H	2.271300	0.646382	5.814467
H	0.958106	1.795004	6.197310
H	0.578007	0.095001	5.865913
H	-3.123010	-0.783144	-0.971706
H	-1.774763	-1.859619	-0.559820
H	-2.354780	-0.671761	0.626180
H	-2.711428	1.661304	-1.476803
H	-2.047656	1.840129	0.153910
H	-1.101528	2.364289	-1.259360
H	-1.954098	-0.051012	-2.992508
H	-0.324441	0.627338	-2.974249
H	-0.575114	-1.103614	-2.661465
H	4.657931	-1.009853	-2.918376
H	2.997215	-1.579649	-2.721867
H	3.331414	0.157073	-2.864379
H	5.871722	0.181769	-1.133728
H	4.569285	1.378071	-0.989337
H	5.126491	0.496645	0.439490
H	5.365899	-2.298368	-0.936299
H	4.626942	-2.039160	0.649567
H	3.709526	-2.853523	-0.623283

H	-6.291888	3.370974	4.866762
H	-4.537222	3.227188	4.593410
H	-5.237086	4.777416	5.121859
H	-7.702796	4.616989	3.314990
H	-6.747743	6.083082	3.559552
H	-7.064105	5.486276	1.917195
H	-6.741314	2.506360	2.545568
H	-6.046504	3.312558	1.128030
H	-5.003704	2.355939	2.196400
H	-4.796773	10.075990	0.761761
H	-5.515276	8.476035	0.548216
H	-5.127141	9.068177	2.175201
H	-2.452694	10.392505	1.463490
H	-2.685457	9.353054	2.882968
H	-1.377602	9.015131	1.741918
H	-3.012516	9.537646	-0.859519
H	-1.948642	8.142706	-0.633697
H	-3.639302	7.892385	-1.084030
H	-3.592401	3.665156	8.866088
H	-3.135743	1.066157	7.251337
H	-4.089137	2.479943	6.732235
H	-3.532621	1.533913	10.203230
H	-1.913193	1.180428	9.567820
H	-2.169134	2.582861	10.629733
H	-4.731477	-2.036488	4.239127
H	-4.789151	-0.294268	3.894533
H	-3.609557	-1.321031	3.060155
C	-2.157001	-2.071421	5.308472
H	-2.707282	-2.983243	5.568237
H	-1.598040	-2.258944	4.384495
H	-1.437615	-1.866913	6.109086

YBRTS1P.xyz

116

scf done: -2126.258284

C	0.021738	-0.001744	0.032594
C	0.126710	0.233239	1.430437
C	1.398972	0.123462	2.047707
C	2.538660	-0.140360	1.290849
C	2.476019	-0.318833	-0.092976
C	1.204206	-0.255151	-0.674533
O	-0.915655	0.558498	2.189649
Y	-1.318325	2.005272	3.732579
O	-1.556970	2.331423	5.907861
C	-2.223423	1.295109	6.373682
O	-3.556072	1.546943	6.841292
C	-3.259743	1.021852	8.161762
C	-3.414453	2.072755	9.238672
C	1.486149	0.174564	3.546690
N	1.178681	1.475723	4.218379

C	2.051251	2.569083	3.736444
C	1.429716	3.364402	2.597596
N	0.108843	3.929278	2.937018
C	0.218007	5.003380	3.936103
C	3.753728	-0.598475	-0.895772
C	4.750430	0.561456	-0.701602
C	-1.342529	-0.003513	-0.677563
C	-2.264153	-1.047218	-0.014457
O	-2.764098	3.262159	2.843886
C	-2.934932	4.498141	2.378242
C	-1.815908	5.170341	1.829117
C	-1.931332	6.477472	1.360896
C	-3.144452	7.166478	1.396469
C	-4.241927	6.474844	1.921248
C	-4.188403	5.164772	2.412520
C	-0.510356	4.441665	1.674546
C	-5.444226	4.478252	2.972635
C	-5.721851	3.174972	2.195748
C	-3.229331	8.607041	0.874400
C	-2.271795	9.504583	1.683214
O	-2.278451	0.358539	5.225202
C	-3.155696	-0.786770	5.251013
C	-4.402704	-0.502818	4.427731
C	-5.245903	4.170105	4.469740
C	-6.698878	5.356870	2.846790
C	-2.823166	8.643569	-0.612363
C	-4.643478	9.191317	0.994960
C	1.387376	1.279459	5.664532
C	-1.996603	1.389596	-0.598182
C	-1.227469	-0.371930	-2.164848
C	4.398023	-1.908001	-0.399212
C	3.480084	-0.742239	-2.399374
C	-1.835540	0.652218	7.725946
H	-3.449639	-0.949116	6.294384
H	2.124642	4.169092	2.301421
H	1.302063	2.711394	1.729245
H	3.021679	2.173186	3.402465
H	2.259817	3.233262	4.580905
H	2.498038	-0.137261	3.854023
H	0.778712	-0.549342	3.970516
H	0.212397	5.109904	1.179199
H	-0.639498	3.566730	1.024046
H	-5.196661	6.983568	1.951665
H	-1.043955	6.956967	0.950451
H	1.125084	-0.417372	-1.741860
H	3.492861	-0.223410	1.809333
H	0.906871	5.793987	3.599061
H	-0.766030	5.447747	4.095595
H	0.573082	4.607509	4.890362
H	2.440868	1.045881	5.887209

H	1.082267	2.171336	6.213951
H	0.768217	0.449150	6.010783
H	-3.247463	-1.046186	-0.500032
H	-1.840355	-2.053084	-0.111657
H	-2.399331	-0.828287	1.046027
H	-2.961049	1.384440	-1.120386
H	-2.176009	1.692461	0.434487
H	-1.362996	2.142342	-1.081829
H	-2.228794	-0.387478	-2.608450
H	-0.633545	0.356240	-2.728473
H	-0.786967	-1.364238	-2.311390
H	4.420335	-0.925923	-2.930333
H	2.812002	-1.583081	-2.613773
H	3.033877	0.164959	-2.820733
H	5.673012	0.377058	-1.264673
H	4.322046	1.506689	-1.051827
H	5.025119	0.688321	0.350536
H	5.317524	-2.123399	-0.956655
H	4.658359	-1.854164	0.662712
H	3.713837	-2.752690	-0.531100
H	-6.134554	3.670375	4.874241
H	-4.384868	3.524222	4.642314
H	-5.095035	5.095518	5.037038
H	-7.560714	4.808149	3.241847
H	-6.614865	6.286481	3.420542
H	-6.921523	5.613203	1.805036
H	-6.606024	2.673170	2.607407
H	-5.918613	3.390578	1.139476
H	-4.874083	2.491228	2.253974
H	-4.652778	10.217872	0.613038
H	-5.372513	8.616550	0.414026
H	-4.984097	9.223570	2.035439
H	-2.310512	10.538411	1.319409
H	-2.542781	9.506574	2.744351
H	-1.234561	9.163463	1.604905
H	-2.866972	9.668537	-0.999727
H	-1.803567	8.275262	-0.764228
H	-3.494086	8.022425	-1.214960
H	-3.900755	0.154955	8.375491
H	-1.034568	1.193151	8.233676
H	-1.608953	-0.416290	7.697764
H	-3.150452	1.660259	10.219034
H	-2.768403	2.930829	9.030428
H	-4.449296	2.425734	9.283354
H	-5.089497	-1.355185	4.468375
H	-4.915979	0.379160	4.815914
H	-4.142357	-0.331470	3.377571
C	-2.366053	-1.986599	4.749667
H	-2.993233	-2.883976	4.747504
H	-2.012831	-1.810117	3.728967

H -1.497445 -2.176289 5.387983

YBRTS2.xyz

116

scf done: -2126.255066

C	-2.997149	-1.089744	2.077853
C	-3.718690	-1.827149	3.014307
C	-3.168488	-2.999595	3.591156
C	-1.836821	-3.367386	3.260347
C	-1.164863	-2.589092	2.308834
C	-1.708834	-1.460314	1.685027
C	-5.040863	-1.313117	3.511713
N	-6.260073	-2.142210	3.242993
C	-7.419807	-1.367104	3.715761
O	-3.931415	-3.715001	4.410667
Y	-5.986358	-4.241450	4.694619
N	-6.380902	-4.927377	2.288394
C	-5.836748	-3.833825	1.457946
C	-6.414055	-2.469973	1.808800
C	-1.144240	-4.556005	3.946710
C	0.311374	-4.730312	3.486619
C	-0.949208	-0.630340	0.641410
C	0.439289	-1.208180	0.333870
O	-6.335094	-2.822650	6.544999
O	-5.787539	-6.346783	4.837244
C	-6.024466	-7.461719	4.147755
C	-5.982266	-7.405257	2.732586
C	-6.251843	-8.538727	1.968339
C	-6.552254	-9.769612	2.553927
C	-6.569307	-9.807981	3.952122
C	-6.317124	-8.703005	4.773924
C	-5.543767	-6.142612	2.044436
C	-6.831735	-10.995971	1.674685
C	-7.140072	-12.251199	2.502468
C	-6.366513	-8.831127	6.304206
C	-6.630362	-10.272026	6.768826
C	-7.790632	-5.198392	1.972929
C	-8.043843	-10.713637	0.765206
C	-5.598764	-11.293349	0.798283
C	-5.018969	-8.397249	6.915610
C	-7.510945	-7.955199	6.851584
C	-1.752169	-0.594836	-0.673883
C	-0.764162	0.809233	1.160899
C	-1.124550	-4.321375	5.471137
C	-1.886751	-5.870843	3.638451
H	-6.020665	-4.038246	0.389098
H	-4.752843	-3.812922	1.602938
H	-5.928067	-1.709824	1.180976
H	-7.480686	-2.442306	1.565071
H	-5.212767	-0.314411	3.078496

H	-5.003201	-1.193880	4.602004
H	-5.507941	-6.326246	0.958359
H	-4.527952	-5.876792	2.361096
H	-6.791802	-10.751258	4.433981
H	-6.207740	-8.448362	0.884091
H	-0.156271	-2.879878	2.044288
H	-3.458101	-0.193865	1.663904
H	-7.927084	-5.416454	0.901736
H	-8.128205	-6.063303	2.546879
H	-8.416714	-4.343090	2.238666
H	-7.501237	-0.403141	3.188677
H	-8.337675	-1.935266	3.550111
H	-7.319923	-1.179225	4.787521
H	-0.649975	-5.169859	5.978658
H	-0.553865	-3.418582	5.716104
H	-2.137882	-4.206860	5.859994
H	-1.370393	-6.715801	4.109738
H	-2.909818	-5.846261	4.016716
H	-1.910749	-6.058000	2.558332
H	0.760037	-5.570719	4.026976
H	0.384135	-4.954554	2.416509
H	0.919551	-3.843306	3.695114
H	0.936892	-0.592069	-0.422853
H	1.081599	-1.221995	1.220797
H	0.377398	-2.228812	-0.058778
H	-1.229206	0.002353	-1.430266
H	-1.890198	-1.604997	-1.074128
H	-2.743725	-0.153531	-0.530915
H	-0.230096	1.420806	0.423897
H	-1.724634	1.294395	1.361753
H	-0.187738	0.816340	2.091852
H	-7.523422	-7.985511	7.948562
H	-7.409091	-6.918246	6.528248
H	-8.479553	-8.324123	6.495593
H	-6.638767	-10.300209	7.863969
H	-7.600458	-10.648803	6.426450
H	-5.851806	-10.963731	6.428660
H	-5.062754	-8.460008	8.009948
H	-4.213308	-9.056451	6.573702
H	-4.765392	-7.375288	6.631123
H	-7.332904	-13.096743	1.833255
H	-6.301335	-12.527739	3.150055
H	-8.027932	-12.117812	3.129784
H	-8.251150	-11.574541	0.118317
H	-8.940192	-10.512211	1.361486
H	-7.871193	-9.846783	0.119421
H	-5.781017	-12.164811	0.158056
H	-5.350827	-10.448865	0.147633
H	-4.721324	-11.503437	1.418791
O	-8.085024	-4.190447	5.634165

C	-7.902092	-3.462556	6.684502
C	-7.383938	-4.025513	8.028016
C	-6.134754	-3.149514	7.941491
C	-4.791617	-3.786475	8.225277
O	-8.749682	-2.401370	6.904863
C	-9.951093	-2.301253	6.118895
C	-11.023448	-3.218175	6.694651
C	-10.356321	-0.836806	6.144440
H	-9.727279	-2.618625	5.096048
H	-11.267670	-0.684196	5.557736
H	-10.551241	-0.510582	7.171021
H	-9.566843	-0.202298	5.731973
H	-11.952313	-3.128397	6.121201
H	-10.697384	-4.260581	6.653435
H	-11.235473	-2.953773	7.735911
H	-6.243191	-2.229865	8.530790
H	-7.163160	-5.092820	7.939628
H	-8.054995	-3.851343	8.871536
H	-3.974290	-3.118589	7.937619
H	-4.694402	-4.005116	9.294509
H	-4.672338	-4.731960	7.682843

YBRTS2R.xyz

116

scf done: -2126.257327

C	-3.058289	-1.067092	2.038470
C	-3.783199	-1.823566	2.957163
C	-3.210831	-2.972890	3.558683
C	-1.858393	-3.297591	3.268413
C	-1.184891	-2.502759	2.331970
C	-1.747343	-1.395888	1.685810
C	-5.140231	-1.354306	3.402987
N	-6.317206	-2.229514	3.091950
C	-7.527135	-1.481577	3.482071
O	-3.971041	-3.710684	4.360896
Y	-6.018320	-4.299051	4.585176
N	-6.333791	-5.031470	2.190050
C	-5.773344	-3.946143	1.359492
C	-6.388035	-2.586204	1.657335
C	-1.147246	-4.459733	3.980778
C	0.325654	-4.589421	3.562258
C	-0.984608	-0.544609	0.661750
C	0.422469	-1.090109	0.380977
O	-6.268255	-2.940779	6.605847
O	-5.837931	-6.402368	4.768270
C	-6.050946	-7.529767	4.090320
C	-5.949617	-7.499344	2.677944
C	-6.191512	-8.645541	1.923718
C	-6.522292	-9.864114	2.518930
C	-6.598430	-9.876670	3.915737

C	-6.374524	-8.757713	4.726822
C	-5.486696	-6.246777	1.987512
C	-6.768650	-11.106131	1.651635
C	-7.126398	-12.342141	2.488266
C	-6.475265	-8.857872	6.256434
C	-6.785718	-10.283938	6.737185
C	-7.734893	-5.311303	1.844542
C	-7.932856	-10.834319	0.678630
C	-5.496443	-11.428489	0.842627
C	-5.133996	-8.444638	6.895436
C	-7.613006	-7.946659	6.758358
C	-1.759071	-0.520470	-0.670793
C	-0.843981	0.896120	1.191883
C	-1.177603	-4.216966	5.503662
C	-1.837684	-5.799639	3.659852
H	-5.911200	-4.175649	0.288749
H	-4.696522	-3.904699	1.546496
H	-5.880116	-1.830011	1.042681
H	-7.440111	-2.579531	1.356448
H	-5.330589	-0.364472	2.957725
H	-5.147134	-1.225843	4.493123
H	-5.414467	-6.444358	0.905821
H	-4.481972	-5.975195	2.334256
H	-6.845131	-10.810061	4.405081
H	-6.102028	-8.574848	0.840829
H	-0.160175	-2.761654	2.098226
H	-3.536112	-0.189029	1.605950
H	-7.845990	-5.542734	0.773308
H	-8.082622	-6.170812	2.420612
H	-8.369612	-4.454952	2.085304
H	-7.623353	-0.552716	2.897549
H	-8.414969	-2.096998	3.320867
H	-7.484729	-1.233322	4.544735
H	-0.691439	-5.047474	6.029676
H	-0.642742	-3.295306	5.758806
H	-2.204915	-4.131921	5.862282
H	-1.305138	-6.625632	4.146524
H	-2.869607	-5.806404	4.013902
H	-1.831004	-5.990666	2.580246
H	0.786102	-5.411398	4.120785
H	0.435358	-4.817839	2.496160
H	0.899038	-3.681945	3.780778
H	0.920575	-0.461503	-0.365067
H	1.047913	-1.090934	1.279902
H	0.390848	-2.111240	-0.014111
H	-1.231179	0.089671	-1.413284
H	-1.868048	-1.531655	-1.077336
H	-2.762055	-0.098990	-0.549452
H	-0.311491	1.524897	0.468303
H	-1.819865	1.355774	1.377753

H	-0.285168	0.911613	2.133427
H	-7.663291	-7.969749	7.854325
H	-7.469904	-6.915058	6.433635
H	-8.578951	-8.290775	6.371771
H	-6.832233	-10.291406	7.831663
H	-7.751249	-10.646369	6.367501
H	-6.011132	-10.998160	6.436973
H	-5.208563	-8.477029	7.989486
H	-4.337878	-9.133996	6.592940
H	-4.843955	-7.437930	6.591129
H	-7.296984	-13.198758	1.827211
H	-6.320830	-12.613834	3.178617
H	-8.040297	-12.188392	3.072033
H	-8.115178	-11.707038	0.040151
H	-8.855719	-10.614252	1.225815
H	-7.721877	-9.982656	0.024256
H	-5.652110	-12.312754	0.213040
H	-5.212531	-10.599276	0.187091
H	-4.651485	-11.629188	1.509539
O	-8.022021	-4.014915	5.543021
C	-7.748970	-3.293036	6.608426
C	-7.548506	-3.950723	8.004147
C	-6.152521	-3.323746	8.015709
C	-4.952345	-4.194814	8.296904
O	-8.409708	-2.054433	6.689097
C	-9.798304	-2.056256	6.331219
C	-10.652678	-2.824148	7.335947
C	-10.205967	-0.594236	6.237825
H	-9.895915	-2.536669	5.349286
H	-11.251590	-0.508467	5.925974
H	-10.094996	-0.101815	7.209433
H	-9.584299	-0.059138	5.514425
H	-11.709019	-2.763325	7.053395
H	-10.378041	-3.882112	7.364420
H	-10.543781	-2.402137	8.340994
H	-6.109245	-2.404008	8.609897
H	-7.532922	-5.041164	7.939676
H	-8.237198	-3.623260	8.783224
H	-4.022689	-3.673854	8.048483
H	-4.922823	-4.453140	9.361142
H	-4.993071	-5.130461	7.728692

YBRTS2P.xyz

116

scf done: -2126.297175

C	-2.547797	-1.054462	2.049704
C	-3.210483	-1.772080	3.043349
C	-2.708806	-3.021380	3.490605
C	-1.468985	-3.486455	2.973937
C	-0.854567	-2.723981	1.972696

C	-1.364301	-1.520284	1.471652
C	-4.389889	-1.160073	3.747280
N	-5.711019	-1.857502	3.643324
C	-6.709840	-0.995431	4.294994
O	-3.422447	-3.707794	4.371166
Y	-5.448366	-4.032258	4.995952
N	-6.272173	-4.594865	2.613227
C	-5.699418	-3.521618	1.778451
C	-6.096459	-2.125188	2.240547
C	-0.803902	-4.757791	3.526850
C	0.556419	-5.037257	2.869538
C	-0.668375	-0.705921	0.372740
C	0.589039	-1.403902	-0.164299
O	-5.590386	-3.092487	6.870984
O	-5.561045	-6.172524	5.094636
C	-5.964972	-7.221941	4.388791
C	-6.068928	-7.107258	2.977767
C	-6.539302	-8.172157	2.211956
C	-6.903439	-9.392599	2.783968
C	-6.753053	-9.500176	4.170777
C	-6.289458	-8.467975	4.994705
C	-5.568144	-5.869584	2.282988
C	-7.421573	-10.536629	1.902298
C	-7.754966	-11.796047	2.714031
C	-6.114604	-8.685447	6.506412
C	-6.468374	-10.115238	6.942859
C	-7.711622	-4.738865	2.374599
C	-8.703204	-10.085289	1.174362
C	-6.351615	-10.912388	0.857982
C	-4.645086	-8.433331	6.901836
C	-7.034446	-7.725048	7.284490
C	-1.635816	-0.496015	-0.808818
C	-0.250637	0.667461	0.934791
C	-0.562261	-4.584619	5.040844
C	-1.693337	-5.992962	3.287056
H	-6.002895	-3.649873	0.724431
H	-4.610356	-3.611017	1.813070
H	-5.638417	-1.388134	1.565259
H	-7.180318	-1.997581	2.154897
H	-4.521010	-0.130008	3.376413
H	-4.175941	-1.094903	4.822402
H	-5.626494	-6.029712	1.193423
H	-4.511037	-5.706453	2.526733
H	-7.005489	-10.442747	4.639367
H	-6.604715	-8.036294	1.133354
H	0.079385	-3.089445	1.565106
H	-2.966751	-0.097983	1.739547
H	-7.920133	-4.946148	1.311748
H	-8.093909	-5.567809	2.971427
H	-8.241983	-3.831184	2.668124

H	-6.801978	-0.023216	3.784322
H	-7.685062	-1.488032	4.297041
H	-6.411487	-0.818938	5.331575
H	-0.103608	-5.489943	5.456757
H	0.116431	-3.745182	5.228922
H	-1.499536	-4.397010	5.568071
H	-1.186324	-6.897532	3.643859
H	-2.641725	-5.905862	3.818963
H	-1.895741	-6.125478	2.217685
H	0.994217	-5.935478	3.318196
H	0.466544	-5.220753	1.792808
H	1.265402	-4.216007	3.021314
H	1.039699	-0.795345	-0.955787
H	1.345349	-1.540822	0.615728
H	0.357553	-2.385467	-0.591669
H	-1.156666	0.090877	-1.601626
H	-1.944372	-1.456226	-1.235928
H	-2.540331	0.039036	-0.502111
H	0.241749	1.269552	0.161498
H	-1.113175	1.234313	1.299364
H	0.446338	0.549469	1.771019
H	-6.898400	-7.856675	8.365244
H	-6.804076	-6.691023	7.024338
H	-8.087085	-7.921035	7.049259
H	-6.310089	-10.210968	8.022573
H	-7.516615	-10.364040	6.742581
H	-5.836747	-10.863098	6.451354
H	-4.515100	-8.568965	7.982630
H	-3.984024	-9.142551	6.391681
H	-4.333521	-7.421768	6.636849
H	-8.125467	-12.580280	2.044893
H	-6.874099	-12.192011	3.230348
H	-8.532565	-11.605200	3.461468
H	-9.084085	-10.884519	0.527020
H	-9.488164	-9.826783	1.893336
H	-8.522840	-9.206386	0.547289
H	-6.707428	-11.725900	0.214133
H	-6.098807	-10.065271	0.212520
H	-5.429435	-11.243020	1.347083
O	-7.890552	-3.881929	5.446449
C	-8.427399	-3.755194	6.550843
C	-7.702194	-3.726790	7.861908
C	-6.484140	-2.763058	7.864233
C	-5.822308	-2.787487	9.242853
O	-9.741537	-3.626930	6.686276
C	-10.589308	-3.700760	5.501838
C	-10.967810	-5.153168	5.263730
C	-11.776390	-2.798177	5.781300
H	-10.005666	-3.322595	4.657756
H	-12.451154	-2.795614	4.920140

H	-12.334890	-3.149965	6.653916
H	-11.453320	-1.770447	5.968677
H	-11.610983	-5.231186	4.381719
H	-10.080400	-5.767689	5.093397
H	-11.513771	-5.554283	6.123102
H	-6.883443	-1.739026	7.707203
H	-7.318056	-4.739681	8.039872
H	-8.413231	-3.487250	8.656695
H	-4.967936	-2.105133	9.242912
H	-6.513911	-2.483313	10.037093
H	-5.449111	-3.793498	9.463379

YBSTS1.xyz

116

scf done: -2126.254475

C	-4.268467	5.106866	2.370469
C	-3.013379	4.441325	2.353980
C	-1.876498	5.137716	1.873763
C	-1.980027	6.465192	1.464300
C	-3.193976	7.154070	1.491174
C	-4.308729	6.439205	1.942260
O	-2.866563	3.185365	2.768800
Y	-1.427769	1.894220	3.642729
O	-2.459958	0.637548	5.177089
C	-3.154845	-0.574323	5.386461
C	-2.210003	-1.667650	5.883149
C	-0.566244	4.415546	1.715975
N	0.033952	3.861324	2.966963
C	0.165083	4.914432	3.984073
C	-3.263061	8.615348	1.027365
C	-4.678344	9.198558	1.139605
C	-5.544501	4.386180	2.833769
C	-6.794356	5.273535	2.729419
O	-0.949633	0.616428	1.995009
C	0.099574	0.251878	1.262933
C	0.030757	0.059235	-0.142652
C	1.222476	-0.242090	-0.815294
C	2.466408	-0.388461	-0.191307
C	2.489194	-0.247292	1.198311
C	1.338725	0.056186	1.922591
C	-1.305433	0.146375	-0.899583
C	-1.151601	-0.176543	-2.393853
C	1.375103	0.044163	3.425299
N	1.054195	1.310157	4.150972
C	1.235921	1.040505	5.590049
C	3.755865	-0.717474	-0.955785
C	3.526772	-0.830692	-2.469443
O	-1.416941	2.701908	5.830400
C	-2.118000	1.915774	6.515506
C	-3.467903	2.116362	7.193899

C	-2.862290	1.239485	8.299774
C	-2.688291	1.835154	9.675481
O	-1.588547	1.195937	7.567911
C	1.934941	2.425838	3.741383
C	1.343864	3.273731	2.623419
C	4.796994	0.393120	-0.712951
C	4.323001	-2.061425	-0.457059
C	-2.297428	-0.874244	-0.305582
C	-1.899481	1.564404	-0.794097
C	-5.789300	3.141946	1.955341
C	-5.400163	3.965205	4.309399
C	-2.322405	9.477052	1.892737
C	-2.823330	8.709900	-0.447268
C	-3.875525	-0.984609	4.104412
H	-3.924011	-0.405041	6.160454
H	2.062790	4.069404	2.361088
H	1.210743	2.652937	1.732648
H	2.915070	2.046595	3.415471
H	2.118357	3.049761	4.621183
H	2.374044	-0.291616	3.749457
H	0.652999	-0.696639	3.793463
H	0.161916	5.101466	1.252759
H	-0.687924	3.565262	1.032924
H	-5.265301	6.945373	1.960223
H	-1.080525	6.962138	1.104170
H	1.174124	-0.374070	-1.888464
H	3.419062	-0.392013	1.746287
H	0.865309	5.698833	3.654009
H	-0.811278	5.369743	4.156428
H	0.512622	4.494915	4.929364
H	2.281684	0.777506	5.816428
H	0.938391	1.912210	6.173199
H	0.595743	0.208490	5.891190
H	-3.261088	-0.811424	-0.825338
H	-1.916859	-1.895305	-0.421116
H	-2.462799	-0.683283	0.756043
H	-2.836489	1.623757	-1.360841
H	-2.116000	1.832579	0.240992
H	-1.210191	2.305543	-1.215419
H	-2.134583	-0.126923	-2.874419
H	-0.500969	0.539726	-2.907895
H	-0.755000	-1.184095	-2.560188
H	4.474404	-1.056663	-2.970256
H	2.824404	-1.633845	-2.716453
H	3.142542	0.102698	-2.894657
H	5.731730	0.169274	-1.240744
H	4.426964	1.359504	-1.071905
H	5.034240	0.500298	0.350329
H	5.248219	-2.311840	-0.989741
H	4.553297	-2.033120	0.612677

H	3.605164	-2.871875	-0.621156
H	-6.302900	3.438033	4.643382
H	-4.540468	3.307100	4.442480
H	-5.265624	4.844410	4.949807
H	-7.669244	4.702312	3.058842
H	-6.726272	6.163201	3.365317
H	-6.983467	5.599100	1.700763
H	-6.684248	2.607060	2.297041
H	-5.950792	3.434509	0.911917
H	-4.938000	2.460341	1.991514
H	-4.676359	10.241057	0.803545
H	-5.394458	8.652776	0.516176
H	-5.043875	9.185386	2.172089
H	-2.350624	10.524587	1.569406
H	-2.617519	9.437951	2.946731
H	-1.284291	9.136630	1.824694
H	-2.857711	9.749267	-0.795364
H	-1.800970	8.345702	-0.589850
H	-3.480725	8.113588	-1.088589
H	-3.284428	0.230253	8.351439
H	-3.625529	3.159817	7.478364
H	-4.341595	1.736019	6.666417
H	-3.658133	1.905887	10.179224
H	-2.030796	1.211086	10.288067
H	-2.254274	2.837647	9.612496
H	-4.452098	-1.903947	4.255636
H	-4.563348	-0.198241	3.778499
H	-3.152807	-1.166376	3.301020
H	-2.757380	-2.589525	6.109803
H	-1.464002	-1.897742	5.113694
H	-1.685888	-1.340964	6.785091

YBSTS1R.xyz

116

scf done: -2126.267468

C	-4.258675	4.994269	2.627915
C	-3.014761	4.307030	2.565272
C	-1.888048	4.988040	2.036411
C	-1.990848	6.317359	1.632624
C	-3.190843	7.026875	1.711693
C	-4.297373	6.328414	2.205813
O	-2.879670	3.051710	2.978020
Y	-1.422033	1.642502	3.665250
O	-2.372624	0.171673	4.804646
C	-3.108985	-0.986691	5.037556
C	-2.184297	-2.192780	5.220628
C	-0.591689	4.252428	1.823429
N	0.063916	3.719358	3.052009
C	0.256910	4.798648	4.027010
C	-3.254886	8.490812	1.255623

C	-4.656461	9.094281	1.420423
C	-5.530883	4.285763	3.120581
C	-6.766742	5.197690	3.088950
O	-0.901235	0.621342	1.853507
C	0.146345	0.244911	1.133657
C	0.100577	0.105521	-0.280199
C	1.296346	-0.199125	-0.943244
C	2.523985	-0.404132	-0.303232
C	2.520686	-0.330543	1.091754
C	1.364677	-0.027379	1.807599
C	-1.223425	0.235553	-1.052207
C	-1.048902	-0.023119	-2.556611
C	1.370280	-0.132746	3.308209
N	1.063999	1.091297	4.111999
C	1.252686	0.733574	5.528186
C	3.821762	-0.724510	-1.057152
C	3.618886	-0.772608	-2.578036
O	-1.187469	2.764569	5.878419
C	-1.866049	2.657610	6.878939
C	-3.142549	1.984227	7.300535
C	-2.813145	2.600239	8.670199
C	-3.724515	3.660422	9.227523
O	-1.582326	3.194427	8.075715
C	1.942269	2.227454	3.756995
C	1.354005	3.118202	2.669613
C	4.875257	0.358523	-0.751199
C	4.359908	-2.096473	-0.604754
C	-2.226044	-0.805981	-0.513916
C	-1.819499	1.647573	-0.893555
C	-5.827455	3.069020	2.220132
C	-5.342005	3.817954	4.577140
C	-2.271454	9.335155	2.090012
C	-2.866844	8.585730	-0.233355
C	-4.122461	-1.230970	3.917964
H	-3.685717	-0.873693	5.980345
H	2.088419	3.904123	2.418527
H	1.198947	2.523924	1.765394
H	2.926934	1.864475	3.425897
H	2.112774	2.815725	4.663873
H	2.357695	-0.506740	3.625971
H	0.627469	-0.879806	3.617609
H	0.113838	4.926269	1.308269
H	-0.752911	3.391440	1.163286
H	-5.245125	6.848620	2.261622
H	-1.099626	6.800481	1.234556
H	1.264997	-0.285528	-2.021721
H	3.434217	-0.529897	1.650151
H	0.919956	5.582366	3.623663
H	-0.707346	5.251197	4.263177
H	0.685679	4.411302	4.952226

H	2.291402	0.427266	5.732715
H	1.001363	1.584805	6.163729
H	0.589662	-0.097416	5.783343
H	-3.184127	-0.716587	-1.040261
H	-1.848103	-1.822767	-0.668964
H	-2.401709	-0.659668	0.553494
H	-2.741612	1.735045	-1.480782
H	-2.062128	1.859725	0.148579
H	-1.120229	2.409094	-1.257999
H	-2.023905	0.054178	-3.049638
H	-0.385202	0.710122	-3.028511
H	-0.656538	-1.025314	-2.761050
H	4.571628	-0.995236	-3.070759
H	2.906951	-1.552073	-2.869589
H	3.258802	0.183976	-2.971644
H	5.816357	0.141740	-1.270897
H	4.526251	1.344355	-1.076772
H	5.093406	0.418911	0.319857
H	5.290714	-2.339483	-1.131296
H	4.571934	-2.115958	0.468947
H	3.632943	-2.888031	-0.814521
H	-6.242761	3.299806	4.930297
H	-4.492596	3.135938	4.642161
H	-5.162753	4.676568	5.235575
H	-7.638290	4.635565	3.442310
H	-6.653181	6.071772	3.739985
H	-6.992420	5.549665	2.076674
H	-6.719834	2.539891	2.577251
H	-6.016949	3.391984	1.190631
H	-4.986537	2.373546	2.213226
H	-4.651167	10.137955	1.087902
H	-5.402327	8.561067	0.821429
H	-4.984801	9.082198	2.465376
H	-2.291822	10.383671	1.769044
H	-2.532113	9.299559	3.153263
H	-1.242633	8.975992	1.987468
H	-2.897768	9.627085	-0.576036
H	-1.856111	8.206496	-0.413521
H	-3.555729	8.001996	-0.852800
H	-2.501191	1.876626	9.427669
H	-4.033848	2.366236	6.798385
H	-3.106018	0.898472	7.202144
H	-4.638815	3.194329	9.608537
H	-3.243373	4.193437	10.052152
H	-4.001211	4.384555	8.455762
H	-4.743985	-2.111229	4.119952
H	-4.779325	-0.362746	3.805335
H	-3.600230	-1.387311	2.967293
H	-2.747806	-3.102455	5.458577
H	-1.616279	-2.371634	4.300420

H -1.472532 -2.009472 6.033079

YBSTS1P.xyz

116

scf done: -2126.261990

C	-4.314165	5.326688	2.444300
C	-3.063767	4.659450	2.351588
C	-1.965454	5.340183	1.772044
C	-2.096775	6.655488	1.332403
C	-3.306664	7.345482	1.427210
C	-4.385036	6.645850	1.980431
O	-2.881239	3.415400	2.787523
Y	-1.404306	2.149822	3.626264
O	-2.694476	0.587186	4.958529
C	-3.290295	-0.726273	4.989594
C	-2.236725	-1.783821	4.695783
C	-0.669808	4.609373	1.555317
N	-0.005381	4.081893	2.786244
C	0.184044	5.156731	3.771221
C	-3.408654	8.795440	0.934692
C	-4.817835	9.376811	1.113418
C	-5.549512	4.624550	3.030099
C	-6.805485	5.508307	2.982952
O	-0.933404	0.717540	2.099114
C	0.130259	0.275829	1.433131
C	0.089495	-0.056648	0.052064
C	1.289751	-0.439013	-0.560784
C	2.518623	-0.535633	0.101436
C	2.516072	-0.246032	1.467774
C	1.356607	0.147688	2.133022
C	-1.227348	-0.019441	-0.741895
C	-1.046787	-0.475844	-2.197980
C	1.379592	0.336492	3.624296
N	1.102286	1.709379	4.150977
C	1.344442	1.674293	5.607429
C	3.817672	-0.961381	-0.596131
C	3.622336	-1.202645	-2.099271
O	-1.638662	2.326670	5.809309
C	-2.326151	1.275008	6.207406
C	-3.455054	1.434832	7.247857
C	-2.615026	0.494814	8.122555
C	-2.015231	1.063868	9.389329
O	-1.626779	0.349083	7.066426
C	1.969928	2.731961	3.523253
C	1.279693	3.473138	2.387081
C	4.882267	0.140476	-0.425452
C	4.336793	-2.268390	0.035506
C	-2.249898	-0.967481	-0.083631
C	-1.796820	1.412146	-0.776410
C	-5.856967	3.346556	2.223118

C	-5.294589	4.265204	4.507605
C	-2.424428	9.678399	1.727364
C	-3.052719	8.859265	-0.563904
C	-4.442751	-0.737267	3.997253
H	-3.681982	-0.882344	6.001577
H	1.963393	4.247430	1.997416
H	1.077994	2.775920	1.567834
H	2.890972	2.276805	3.133656
H	2.274849	3.442362	4.297317
H	2.365324	0.018860	4.001571
H	0.632480	-0.318578	4.091443
H	0.035499	5.279009	1.036724
H	-0.830177	3.742307	0.901751
H	-5.337044	7.155566	2.055414
H	-1.224808	7.140771	0.896396
H	1.261128	-0.679336	-1.615750
H	3.433994	-0.340824	2.046225
H	0.901856	5.910120	3.409256
H	-0.772837	5.650569	3.950293
H	0.546087	4.752639	4.719387
H	2.398900	1.438355	5.823421
H	1.089697	2.636924	6.054086
H	0.704231	0.926044	6.077025
H	-3.202391	-0.933830	-0.626209
H	-1.886285	-2.000974	-0.102689
H	-2.429954	-0.682682	0.954358
H	-2.722909	1.437836	-1.363261
H	-2.024259	1.772912	0.227661
H	-1.085269	2.100192	-1.247971
H	-2.017528	-0.450475	-2.704610
H	-0.369871	0.179960	-2.756736
H	-0.667444	-1.501253	-2.264925
H	4.575823	-1.491934	-2.554149
H	2.907476	-2.009149	-2.293769
H	3.270231	-0.302024	-2.613634
H	5.822512	-0.153324	-0.906972
H	4.547624	1.080054	-0.878144
H	5.098549	0.336020	0.629744
H	5.269496	-2.586077	-0.445635
H	4.537645	-2.149016	1.104872
H	3.603278	-3.073561	-0.077098
H	-6.169548	3.753868	4.928254
H	-4.427088	3.612511	4.613619
H	-5.117581	5.170259	5.099714
H	-7.652573	4.950751	3.397211
H	-6.693053	6.421065	3.578338
H	-7.069938	5.794444	1.959076
H	-6.727129	2.831867	2.649043
H	-6.090822	3.595733	1.182031
H	-5.007202	2.662456	2.229898

H	-4.839581	10.409989	0.750360
H	-5.566299	8.812300	0.547232
H	-5.122771	9.390452	2.165297
H	-2.471499	10.717795	1.380894
H	-2.662775	9.664918	2.796253
H	-1.391074	9.336124	1.612176
H	-3.110638	9.890920	-0.931040
H	-2.038469	8.495415	-0.755858
H	-3.742634	8.247668	-1.154665
H	-3.091560	-0.474503	8.324962
H	-3.541315	2.461986	7.606146
H	-4.436626	1.061683	6.948371
H	-2.788804	1.195933	10.154059
H	-1.251084	0.390519	9.790425
H	-1.550593	2.034130	9.189440
H	-4.944565	-1.710264	4.007982
H	-5.176818	0.035401	4.241635
H	-4.078262	-0.556809	2.980994
H	-2.683827	-2.783585	4.716571
H	-1.802508	-1.621967	3.704039
H	-1.444989	-1.740510	5.447173

YBTS2.xyz

116

scf done: -2126.256554

C	-4.794466	2.465435	1.282066
C	-4.691177	1.055302	1.156164
C	-5.537631	0.380795	0.243068
C	-6.410086	1.095558	-0.575021
C	-6.495434	2.488638	-0.517548
C	-5.686067	3.128285	0.428609
O	-3.823608	0.331505	1.857692
Y	-2.569560	-1.373114	1.702252
N	-4.350858	-1.865969	-0.157114
C	-5.582802	-1.121402	0.253602
C	-7.466116	3.241269	-1.437943
C	-7.136112	2.924491	-2.909870
C	-3.981351	3.233603	2.336658
C	-4.311617	2.682803	3.739399
O	-3.160537	-2.652533	3.422476
C	-2.897215	-3.866641	3.025428
O	-3.967274	-4.749024	2.958019
C	-5.193092	-4.386041	3.620242
C	-6.252080	-5.333241	3.078580
O	-2.278990	-3.777115	1.537503
C	-1.255017	-4.734389	1.934159
C	0.138048	-4.377571	1.470327
O	-0.685238	-0.556338	2.231421
C	0.492548	-0.204855	1.718177
C	0.553074	0.167263	0.352315

C	1.775461	0.459693	-0.248706
C	2.974744	0.424223	0.465592
C	2.881403	0.125693	1.829336
C	1.683399	-0.170038	2.492277
C	-0.721852	0.384842	-0.415659
N	-1.600792	-0.806110	-0.608168
C	-0.860029	-1.879458	-1.282105
C	4.302207	0.740269	-0.236384
C	4.515188	-0.243372	-1.404162
C	1.656418	-0.386208	4.015196
C	0.741099	0.675849	4.658917
C	-1.596989	-4.604239	3.417258
C	-2.769359	-0.378727	-1.403184
C	-3.860886	-1.434644	-1.485639
C	-4.710070	-3.295113	-0.208671
C	-5.044127	-4.492574	5.133270
C	4.264842	2.179950	-0.786857
C	5.505975	0.622408	0.708510
C	1.131399	-1.791830	4.360419
C	3.047331	-0.247169	4.652608
C	-2.470766	3.090491	2.066081
C	-4.306180	4.735473	2.343280
C	-8.910809	2.795324	-1.135799
C	-7.387333	4.762644	-1.251650
H	-5.443148	-3.350688	3.359588
H	-2.454708	-0.111805	-2.427380
H	-3.177293	0.527046	-0.945334
H	-4.686730	-1.037074	-2.092861
H	-3.482953	-2.317241	-2.010472
H	-6.410269	-1.449577	-0.396531
H	-5.815213	-1.469586	1.269249
H	-0.472788	0.799948	-1.406334
H	-1.334687	1.133526	0.101598
H	3.791670	0.131011	2.414889
H	1.776126	0.739246	-1.301087
H	-5.754957	4.205221	0.512943
H	-7.048415	0.537794	-1.258710
H	-0.596525	-1.596981	-2.314539
H	0.063406	-2.072808	-0.733544
H	-1.448236	-2.799559	-1.307053
H	-5.505122	-3.477653	-0.949459
H	-3.833167	-3.895203	-0.452207
H	-5.059413	-3.623806	0.771279
H	-3.721330	3.208855	4.499300
H	-5.371781	2.832761	3.972403
H	-4.090432	1.616145	3.806653
H	-1.899199	3.665851	2.804114
H	-2.150061	2.049649	2.130506
H	-2.217516	3.480249	1.072962
H	-3.720425	5.225530	3.128239

H	-4.049831	5.220165	1.394535
H	-5.363694	4.927537	2.555108
H	-8.086035	5.255459	-1.936245
H	-7.656850	5.063836	-0.233958
H	-6.384763	5.146926	-1.468162
H	-7.828071	3.446569	-3.581310
H	-6.117567	3.241070	-3.158708
H	-7.214597	1.853447	-3.122209
H	-9.621058	3.314692	-1.790311
H	-9.042707	1.719542	-1.288863
H	-9.178185	3.018284	-0.097601
H	1.119618	-1.935536	5.447796
H	0.115750	-1.925084	3.985836
H	1.775358	-2.565283	3.926352
H	2.960600	-0.390105	5.735009
H	3.751895	-0.998393	4.278295
H	3.480193	0.745138	4.486438
H	0.694870	0.528377	5.744727
H	1.128750	1.683093	4.471060
H	-0.272347	0.615578	4.258191
H	6.429089	0.838059	0.159772
H	5.443592	1.333440	1.539074
H	5.597248	-0.385741	1.126741
H	5.454804	-0.026472	-1.926278
H	4.558237	-1.276158	-1.041891
H	3.706268	-0.181720	-2.139041
H	5.203901	2.422867	-1.298405
H	3.449789	2.319135	-1.504139
H	4.121139	2.902385	0.023326
H	-5.990573	-4.246810	5.626607
H	-4.763064	-5.512223	5.418268
H	-4.282339	-3.797458	5.493189
H	-7.226274	-5.103962	3.521310
H	-6.339713	-5.252867	1.991263
H	-5.999500	-6.370298	3.321910
H	-1.541603	-5.717281	1.538265
H	-0.917259	-3.942406	3.958253
H	-1.750420	-5.531344	3.972062
H	0.206129	-4.396094	0.377873
H	0.439564	-3.388264	1.826726
H	0.854415	-5.110376	1.858234

YBSTS2R.xyz

116

scf done: -2126.257342

C	-4.837119	2.560389	1.243172
C	-4.735631	1.148786	1.136404
C	-5.581395	0.461962	0.232087
C	-6.457103	1.166339	-0.591677
C	-6.545255	2.559854	-0.549297

C	-5.732524	3.212101	0.385279
O	-3.868669	0.434585	1.849375
Y	-2.623585	-1.271409	1.691727
N	-4.381841	-1.775463	-0.166967
C	-5.617327	-1.040796	0.253178
C	-7.520603	3.300278	-1.474679
C	-7.192178	2.970988	-2.944236
C	-4.015451	3.342292	2.280791
C	-4.339752	2.816000	3.694320
O	-3.203608	-2.623047	3.331012
C	-2.893039	-3.827736	2.905243
O	-3.982912	-4.696925	2.731754
C	-5.003705	-4.637956	3.742157
C	-6.180847	-5.427912	3.192712
O	-2.244687	-3.732303	1.520131
C	-1.198323	-4.668883	1.937583
C	0.193991	-4.250189	1.532621
O	-0.742943	-0.452167	2.242290
C	0.453047	-0.161597	1.734818
C	0.544673	0.165951	0.358988
C	1.785125	0.387147	-0.235397
C	2.973733	0.321437	0.494741
C	2.851971	0.073167	1.866583
C	1.634774	-0.148740	2.523546
C	-0.713528	0.413483	-0.427109
N	-1.626240	-0.753239	-0.613291
C	-0.916912	-1.848092	-1.286197
C	4.322006	0.554334	-0.200276
C	4.501512	-0.472856	-1.335727
C	1.578498	-0.305648	4.052997
C	0.700799	0.818565	4.641319
C	-1.619352	-4.560043	3.403278
C	-2.787381	-0.297683	-1.404781
C	-3.898636	-1.332871	-1.494690
C	-4.727603	-3.209022	-0.216693
C	-4.515214	-5.190581	5.077341
C	4.358145	1.976834	-0.793816
C	5.508755	0.409231	0.762136
C	0.989735	-1.672662	4.447835
C	2.966009	-0.199813	4.703885
C	-2.507027	3.188064	2.003175
C	-4.333551	4.845421	2.264446
C	-8.963042	2.851861	-1.165618
C	-7.447232	4.823594	-1.302528
H	-5.287880	-3.587260	3.876849
H	-2.468015	-0.027774	-2.426670
H	-3.178237	0.611912	-0.938824
H	-4.722364	-0.909191	-2.086136
H	-3.542503	-2.212929	-2.038498
H	-6.447185	-1.378503	-0.388704

H	-5.837638	-1.386973	1.272016
H	-0.441531	0.807424	-1.420380
H	-1.308272	1.187066	0.074431
H	3.755067	0.059808	2.463182
H	1.809104	0.634076	-1.295686
H	-5.801489	4.290006	0.456217
H	-7.095814	0.599876	-1.267788
H	-0.660575	-1.580484	-2.324348
H	0.008957	-2.054524	-0.746615
H	-1.523658	-2.756206	-1.294980
H	-5.538110	-3.395478	-0.939400
H	-3.851201	-3.797194	-0.491122
H	-5.040023	-3.552031	0.771137
H	-3.742015	3.351069	4.442021
H	-5.397659	2.975435	3.931273
H	-4.123920	1.749406	3.777479
H	-1.928445	3.773126	2.728017
H	-2.190089	2.147008	2.082593
H	-2.258617	3.560496	1.002157
H	-3.740935	5.345685	3.037721
H	-4.080616	5.312910	1.306207
H	-5.388875	5.045925	2.479268
H	-8.150036	5.307341	-1.989380
H	-7.714623	5.132855	-0.286683
H	-6.446929	5.209994	-1.525704
H	-7.887503	3.483880	-3.619280
H	-6.175376	3.289269	-3.198018
H	-7.266748	1.897656	-3.146122
H	-9.676383	3.362886	-1.823317
H	-9.091534	1.774334	-1.308868
H	-9.229186	3.083062	-0.128917
H	0.954293	-1.767231	5.540078
H	-0.024512	-1.783374	4.061740
H	1.609700	-2.489560	4.060991
H	2.860705	-0.295952	5.789792
H	3.642269	-0.994378	4.368887
H	3.442833	0.765949	4.504854
H	0.635402	0.716813	5.731408
H	1.132166	1.800677	4.418792
H	-0.309484	0.783718	4.229600
H	6.446846	0.561915	0.217664
H	5.472644	1.149283	1.568506
H	5.546297	-0.587976	1.213590
H	5.455200	-0.314110	-1.853130
H	4.494230	-1.495033	-0.942228
H	3.703709	-0.397090	-2.081309
H	5.312555	2.159521	-1.302055
H	3.557720	2.132470	-1.524078
H	4.241091	2.729587	-0.007287
H	-5.326802	-5.168814	5.812201

H	-4.179539	-6.227889	4.969612
H	-3.692235	-4.590877	5.475741
H	-7.016824	-5.403820	3.898624
H	-6.523819	-5.011206	2.241256
H	-5.900770	-6.473315	3.026166
H	-1.441504	-5.650293	1.512743
H	-0.977178	-3.898172	3.987962
H	-1.790920	-5.497152	3.933774
H	0.308018	-4.258952	0.443916
H	0.437283	-3.251638	1.906133
H	0.923038	-4.955576	1.946581

YBSTS2P.xyz

116

scf done: -2126.298286

C	-4.902664	2.053338	1.149114
C	-4.738958	0.675935	0.832634
C	-5.429537	0.150295	-0.289938
C	-6.190126	0.977329	-1.113152
C	-6.317207	2.345866	-0.863359
C	-5.673516	2.835314	0.279805
O	-3.971319	-0.140789	1.538709
Y	-2.480967	-1.676303	1.173217
N	-4.137863	-1.999171	-0.840317
C	-5.433563	-1.336416	-0.504203
C	-7.154730	3.228222	-1.799009
C	-6.592759	3.143458	-3.231891
C	-4.276786	2.657379	2.416962
C	-4.767602	1.876855	3.653875
O	-3.287336	-2.679951	3.223203
C	-3.119843	-3.825699	3.652936
O	-3.809242	-4.293539	4.681065
C	-4.772615	-3.408604	5.338678
C	-5.846061	-4.318402	5.904630
O	-2.090177	-3.745906	0.914352
C	-2.261042	-4.958567	1.541847
C	-1.238616	-5.989753	1.060026
O	-0.681485	-0.818037	1.927446
C	0.465271	-0.268609	1.542913
C	0.520451	0.388906	0.288738
C	1.710943	0.951609	-0.165983
C	2.884372	0.909612	0.589761
C	2.803676	0.274807	1.834038
C	1.639968	-0.313577	2.342483
C	-0.735233	0.566016	-0.519925
N	-1.443966	-0.686674	-0.921716
C	-0.517732	-1.616010	-1.584680
C	4.173019	1.548774	0.055186
C	4.567334	0.881441	-1.277229
C	1.630827	-0.984074	3.725227

C	0.581628	-0.304511	4.628420
C	-2.145492	-4.812409	3.086461
C	-2.561241	-0.308695	-1.808341
C	-3.535365	-1.448016	-2.072872
C	-4.417467	-3.432401	-1.032526
C	-4.046047	-2.587511	6.389985
C	3.942368	3.054558	-0.181075
C	5.348923	1.395254	1.029798
C	1.302822	-2.482242	3.569154
C	2.986343	-0.882497	4.440878
C	-2.738697	2.594156	2.345286
C	-4.666932	4.130279	2.617652
C	-8.616707	2.738808	-1.799959
C	-7.146830	4.703157	-1.374157
H	-5.184899	-2.749809	4.569386
H	-2.172914	0.058473	-2.774499
H	-3.097037	0.520435	-1.337729
H	-4.317138	-1.088962	-2.759543
H	-3.018212	-2.263172	-2.588417
H	-6.160100	-1.578793	-1.298223
H	-5.783933	-1.825104	0.414967
H	-0.489441	1.135753	-1.431194
H	-1.465116	1.161445	0.043522
H	3.696084	0.236083	2.445825
H	1.704979	1.446005	-1.136488
H	-5.781639	3.886901	0.513093
H	-6.705849	0.526959	-1.960422
H	-0.138587	-1.196361	-2.530618
H	0.331559	-1.805917	-0.926140
H	-1.010510	-2.568998	-1.787555
H	-5.081140	-3.599224	-1.896593
H	-3.482293	-3.977868	-1.163831
H	-4.911701	-3.831246	-0.142469
H	-4.312398	2.287213	4.563700
H	-5.855964	1.958610	3.754064
H	-4.503233	0.820865	3.575539
H	-2.299100	3.040566	3.245603
H	-2.382591	1.565408	2.272437
H	-2.368294	3.158743	1.481544
H	-4.221967	4.495998	3.549418
H	-4.299657	4.771651	1.808663
H	-5.751667	4.262668	2.696596
H	-7.744226	5.294030	-2.077008
H	-7.578360	4.842835	-0.377410
H	-6.133543	5.119065	-1.369015
H	-7.184388	3.762354	-3.917114
H	-5.555977	3.494955	-3.265298
H	-6.609709	2.117690	-3.613899
H	-9.229952	3.351159	-2.472143
H	-8.695244	1.698975	-2.132944

H	-9.048100	2.798829	-0.795261
H	1.251630	-2.965936	4.553148
H	0.348371	-2.614666	3.056993
H	2.079417	-2.988192	2.984466
H	2.913454	-1.367487	5.420739
H	3.786993	-1.384434	3.886535
H	3.284621	0.157768	4.610911
H	0.549184	-0.797033	5.608511
H	0.840223	0.747824	4.790156
H	-0.411097	-0.347578	4.178045
H	6.244294	1.863298	0.606355
H	5.146325	1.879968	1.990764
H	5.584925	0.342841	1.220532
H	5.481217	1.333242	-1.681671
H	4.750053	-0.189441	-1.137834
H	3.781627	0.989477	-2.031616
H	4.851165	3.529339	-0.570164
H	3.138922	3.232834	-0.902633
H	3.667393	3.557364	0.752005
H	-4.756833	-1.931956	6.902178
H	-3.579649	-3.239209	7.135537
H	-3.277585	-1.959685	5.932967
H	-6.618176	-3.717113	6.393387
H	-6.319276	-4.906536	5.113510
H	-5.425630	-5.006157	6.644673
H	-3.271570	-5.371468	1.334656
H	-1.138614	-4.433795	3.304407
H	-2.271371	-5.771882	3.594509
H	-1.327279	-6.109821	-0.023664
H	-0.223368	-5.641472	1.278320
H	-1.386940	-6.968585	1.530440

YBRRRTS1S.xyz

128

scf done: -2432.650152

C	-3.924899	4.203069	0.348351
C	-4.129855	2.849980	0.741765
C	-5.248632	2.159967	0.209543
C	-6.059989	2.751914	-0.755264
C	-5.834978	4.049838	-1.216983
C	-4.773534	4.742634	-0.626141
O	-3.328823	2.218863	1.592781
Y	-2.760946	0.305253	2.393348
C	-5.649981	0.831084	0.784153
N	-4.660280	-0.278205	0.669543
C	-4.256176	-0.434012	-0.731666
C	-6.749051	4.660322	-2.287638
C	-6.317881	6.078494	-2.685782
C	-2.835305	5.068307	1.000616

C	-2.821516	6.508113	0.465350
O	-4.289005	0.333949	3.899204
C	-5.265412	-0.387543	4.429914
C	-6.382054	0.202731	5.084889
C	-7.422022	-0.641559	5.495778
C	-7.416890	-2.031132	5.335472
C	-6.268691	-2.588491	4.766860
C	-5.202880	-1.803293	4.332936
C	-6.423039	1.711203	5.386419
C	-7.684660	2.117973	6.163205
C	-3.922907	-2.477913	3.911040
N	-3.386324	-2.240273	2.533685
C	-2.183831	-3.080222	2.404632
C	-8.574247	-2.934518	5.781091
C	-9.755363	-2.134770	6.348569
O	-0.555537	1.169206	2.789382
C	-4.353607	-2.618681	1.486454
C	-5.326349	-1.502057	1.154022
C	-9.087370	-3.749429	4.577430
C	-8.083861	-3.903262	6.875538
C	-5.204022	2.078979	6.257720
C	-6.392936	2.543179	4.090304
C	-3.085977	5.141681	2.520764
C	-1.448971	4.457747	0.739848
C	-6.721118	3.781719	-3.554077
C	-8.193498	4.731560	-1.753546
H	-6.050905	-1.864852	0.404032
H	-5.893270	-1.245723	2.051099
H	-4.923018	-3.512691	1.788548
H	-3.786153	-2.896777	0.591693
H	-4.055832	-3.566372	4.031629
H	-3.120704	-2.164689	4.586475
H	-6.586849	0.510786	0.298143
H	-5.857379	0.939086	1.854169
H	-4.597306	5.765079	-0.934618
H	-6.902917	2.177467	-1.136716
H	-8.282189	-0.186863	5.970441
H	-6.180942	-3.669763	4.669583
H	-5.129659	-0.628292	-1.375830
H	-3.772327	0.481793	-1.074943
H	-3.551024	-1.260268	-0.832578
H	-2.427617	-4.149487	2.516117
H	-1.729384	-2.928013	1.422692
H	-1.466888	-2.798597	3.178098
H	-5.198512	3.155683	6.467520
H	-5.238305	1.546618	7.215027
H	-4.274143	1.818891	5.748405
H	-6.450676	3.612317	4.328518
H	-5.474684	2.370867	3.527575
H	-7.250766	2.300577	3.452496

H	-7.646161	3.192357	6.373125
H	-8.600031	1.929744	5.591008
H	-7.765169	1.597760	7.123950
H	-10.562939	-2.818259	6.632806
H	-9.473407	-1.569382	7.243095
H	-10.160386	-1.431077	5.613375
H	-9.909761	-4.409456	4.878952
H	-9.455017	-3.087050	3.786394
H	-8.299964	-4.376921	4.147668
H	-8.897653	-4.561529	7.203051
H	-7.265856	-4.537555	6.519216
H	-7.719416	-3.351024	7.748047
H	-0.667235	5.076752	1.198406
H	-1.391957	3.455055	1.162752
H	-1.245117	4.403588	-0.336390
H	-2.037557	7.074735	0.979926
H	-2.603618	6.549008	-0.607883
H	-3.770534	7.025563	0.643433
H	-2.302207	5.737036	3.006099
H	-4.050217	5.617226	2.731113
H	-3.091471	4.143456	2.962112
H	-6.987876	6.465322	-3.461457
H	-6.361203	6.771069	-1.838591
H	-5.299377	6.095444	-3.088603
H	-7.373536	4.199689	-4.330357
H	-5.706151	3.717109	-3.960769
H	-7.063029	2.762621	-3.347076
H	-8.865732	5.159298	-2.507365
H	-8.576173	3.740631	-1.489591
H	-8.245432	5.356610	-0.855967
O	-1.420728	-0.512522	0.519195
O	-1.461298	-0.620163	4.200779
C	0.686684	0.946777	2.203958
C	-0.191669	-0.556596	0.383988
C	0.770958	-0.453714	1.517043
C	-0.696137	0.315514	4.514715
C	-0.878953	1.556034	5.385713
C	0.625369	1.391901	5.636869
O	0.607618	0.113975	4.903852
C	1.085308	2.064472	1.243544
O	0.388550	-0.674335	-0.798919
C	-0.436342	-0.716442	-2.004521
C	0.316864	-1.590639	-2.989314
C	1.115254	1.211944	7.051462
C	-0.663780	0.703166	-2.495246
H	1.453755	0.891716	2.993102
H	1.238289	2.110474	5.081974
H	-1.496494	1.340267	6.262563
H	-1.217264	2.462057	4.886208
H	1.058821	2.164360	7.588935

H	0.504001	0.476012	7.582227
H	2.155732	0.873686	7.064952
H	-1.389417	-1.175543	-1.729147
H	-0.256414	-1.681459	-3.916535
H	1.291339	-1.154879	-3.229328
H	0.475890	-2.593460	-2.583498
H	-1.267902	0.686827	-3.407622
H	-1.194086	1.300132	-1.749380
H	0.289478	1.189140	-2.724561
H	1.785561	-0.643737	1.159307
H	0.508655	-1.203588	2.269207
H	2.091252	1.893386	0.842785
H	0.388229	2.150073	0.404852
H	1.080086	3.021490	1.770155

YBRRS1SR.xyz

128

scf done: -2432.670080

C	-4.085823	4.267689	-0.213052
C	-4.313206	2.974409	0.335019
C	-5.483879	2.273112	-0.050106
C	-6.360785	2.813110	-0.988293
C	-6.144773	4.063944	-1.569156
C	-5.005759	4.758071	-1.147435
O	-3.475103	2.406399	1.194887
Y	-2.918988	0.552930	2.109375
C	-5.850076	0.987214	0.637153
N	-4.869659	-0.131776	0.527688
C	-4.532719	-0.378053	-0.878430
C	-7.136493	4.622507	-2.598107
C	-6.725428	6.008263	-3.114742
C	-2.874075	5.110491	0.214661
C	-2.856871	6.498935	-0.443639
O	-4.109897	0.516656	3.892613
C	-5.062265	-0.205475	4.468683
C	-6.130724	0.377122	5.203094
C	-7.130496	-0.477243	5.686171
C	-7.129673	-1.866552	5.518051
C	-6.029999	-2.414665	4.852789
C	-5.006455	-1.617793	4.344306
C	-6.171557	1.887949	5.489752
C	-7.361802	2.280600	6.379066
C	-3.767335	-2.265710	3.787931
N	-3.404439	-2.017242	2.357055
C	-2.204621	-2.830669	2.086141
C	-8.247426	-2.777526	6.043266
C	-9.356706	-1.991773	6.756230
O	-0.988760	0.850421	2.909340
C	-4.482763	-2.429599	1.434297
C	-5.482490	-1.321365	1.146739

C	-8.885550	-3.538665	4.864150
C	-7.663121	-3.794157	7.044247
C	-4.883855	2.302427	6.231359
C	-6.291846	2.690544	4.179869
C	-2.896775	5.325135	1.741644
C	-1.575536	4.390051	-0.193931
C	-7.219028	3.668933	-3.806587
C	-8.532677	4.748004	-1.956474
H	-6.284930	-1.719322	0.500887
H	-5.948905	-1.010674	2.085355
H	-5.021757	-3.300880	1.838085
H	-4.015946	-2.759662	0.500475
H	-3.856049	-3.356194	3.926503
H	-2.893794	-1.944919	4.367613
H	-6.819920	0.642189	0.240759
H	-5.989952	1.164954	1.711198
H	-4.823012	5.739519	-1.565871
H	-7.244768	2.234840	-1.253426
H	-7.954752	-0.030824	6.227513
H	-5.947454	-3.494185	4.734862
H	-5.423923	-0.670001	-1.458461
H	-4.120389	0.533052	-1.315195
H	-3.784934	-1.169625	-0.959599
H	-2.428523	-3.907000	2.162650
H	-1.835553	-2.621386	1.079449
H	-1.430054	-2.596705	2.819976
H	-4.891584	3.381328	6.428441
H	-4.811716	1.784266	7.194574
H	-3.999022	2.063787	5.638450
H	-6.342048	3.764241	4.397741
H	-5.434613	2.519925	3.527203
H	-7.206898	2.418893	3.640768
H	-7.324548	3.357807	6.573760
H	-8.324249	2.069240	5.899847
H	-7.339843	1.769467	7.347869
H	-10.131164	-2.681845	7.108394
H	-8.976448	-1.450682	7.629283
H	-9.836993	-1.268889	6.088210
H	-9.680498	-4.206384	5.217719
H	-9.323932	-2.841051	4.142340
H	-8.149811	-4.150671	4.332555
H	-8.449276	-4.457540	7.424168
H	-6.894135	-4.421665	6.582928
H	-7.207050	-3.282314	7.898088
H	-0.698793	4.958512	0.140134
H	-1.536628	3.395029	0.252497
H	-1.518511	4.291728	-1.284258
H	-1.981953	7.054230	-0.088021
H	-2.784839	6.440324	-1.535416
H	-3.745153	7.086929	-0.188185

H	-2.025012	5.913241	2.054118
H	-3.797441	5.874219	2.037808
H	-2.884160	4.372152	2.272210
H	-7.458056	6.361781	-3.848440
H	-6.683964	6.747449	-2.307691
H	-5.747821	5.985854	-3.608264
H	-7.935988	4.043387	-4.547225
H	-6.243318	3.574144	-4.295331
H	-7.541314	2.665926	-3.509519
H	-9.257305	5.139555	-2.680626
H	-8.904934	3.781094	-1.603635
H	-8.506881	5.427239	-1.098039
O	-1.413495	-0.179350	0.309354
O	-0.127174	-2.234660	4.775191
C	0.352033	0.802336	2.592090
C	-0.178526	-0.251156	0.329196
C	0.647045	-0.340639	1.575531
C	-0.010406	-1.306142	5.530029
C	-0.843007	-0.137489	6.010270
C	0.408565	0.200144	6.832938
O	1.094599	-0.976398	6.256139
C	0.877699	2.149545	2.092489
O	0.542451	-0.283744	-0.780578
C	-0.133049	-0.240110	-2.076009
C	0.701073	-1.101317	-3.005959
C	0.327809	0.113116	8.335861
C	-0.248512	1.207202	-2.520366
H	0.948527	0.528830	3.482826
H	0.932307	1.101626	6.502073
H	-1.737163	-0.408494	6.576682
H	-1.101641	0.544551	5.193581
H	-0.227280	0.970789	8.729602
H	-0.184704	-0.803014	8.645375
H	1.326902	0.118079	8.781126
H	-1.128822	-0.670008	-1.936590
H	0.237828	-1.131383	-3.996584
H	1.711182	-0.694245	-3.111410
H	0.777689	-2.125655	-2.631027
H	-0.736965	1.255788	-3.498593
H	-0.844384	1.790017	-1.814574
H	0.742229	1.663585	-2.608315
H	1.705867	-0.372734	1.307853
H	0.389872	-1.284097	2.069913
H	1.958974	2.121005	1.914211
H	0.378792	2.450714	1.165818
H	0.669370	2.919090	2.840967

YBRRRTS1SP.xyz

128

scf done: -2432.661854

C	-3.870792	4.200330	0.197746
C	-4.226066	2.911691	0.683536
C	-5.313787	2.230077	0.078699
C	-5.962842	2.775533	-1.026993
C	-5.593752	4.008902	-1.567989
C	-4.559420	4.691608	-0.918091
O	-3.585834	2.331944	1.692497
Y	-3.140955	0.416869	2.505177
C	-5.849773	0.968272	0.702015
N	-4.929044	-0.206236	0.710654
C	-4.511487	-0.518027	-0.658889
C	-6.331093	4.566268	-2.793153
C	-5.770382	5.920927	-3.247468
C	-2.795770	5.047523	0.899772
C	-2.634338	6.436530	0.262408
O	-4.603652	0.344974	4.064070
C	-5.498142	-0.446205	4.639081
C	-6.634864	0.050108	5.332636
C	-7.567113	-0.883279	5.804141
C	-7.435637	-2.269889	5.664867
C	-6.270176	-2.727850	5.045697
C	-5.310043	-1.848746	4.549723
C	-6.811020	1.554269	5.598624
C	-8.069914	1.857304	6.426086
C	-4.000093	-2.383886	4.041811
N	-3.633704	-2.113322	2.614304
C	-2.408258	-2.878004	2.333078
C	-8.480121	-3.270098	6.178542
C	-9.693753	-2.575896	6.812273
O	0.414300	1.538050	2.798180
C	-4.708038	-2.505354	1.675373
C	-5.635446	-1.350172	1.318151
C	-8.984965	-4.134092	5.005771
C	-7.841846	-4.184233	7.243101
C	-5.595369	2.071281	6.395740
C	-6.926085	2.337695	4.276882
C	-3.195998	5.264381	2.373880
C	-1.424105	4.349945	0.830344
C	-6.199058	3.577970	-3.968862
C	-7.823670	4.755540	-2.457209
H	-6.421924	-1.722965	0.638185
H	-6.134108	-0.998597	2.224755
H	-5.310784	-3.321916	2.098406
H	-4.238516	-2.900242	0.768735
H	-3.990367	-3.475979	4.191668
H	-3.179637	-1.965974	4.640423
H	-6.778508	0.684387	0.178880
H	-6.112596	1.156001	1.749629
H	-4.276009	5.666008	-1.295069
H	-6.791930	2.217386	-1.459708

H	-8.443767	-0.503917	6.313238
H	-6.084326	-3.797430	4.957059
H	-5.375082	-0.804941	-1.282313
H	-4.044274	0.363149	-1.100842
H	-3.787545	-1.335299	-0.664702
H	-2.578466	-3.963082	2.419735
H	-2.052660	-2.656077	1.324244
H	-1.632124	-2.593014	3.048288
H	-5.694368	3.147701	6.581436
H	-5.526416	1.565661	7.365401
H	-4.667598	1.897694	5.847318
H	-7.099028	3.400844	4.482708
H	-6.011239	2.252312	3.689024
H	-7.769791	1.972743	3.679345
H	-8.127462	2.935624	6.609283
H	-8.989103	1.564941	5.905894
H	-8.052246	1.359074	7.401564
H	-10.415273	-3.328504	7.148341
H	-9.412102	-1.977129	7.684865
H	-10.205974	-1.921126	6.099238
H	-9.729947	-4.860700	5.351786
H	-9.450706	-3.510838	4.234846
H	-8.170064	-4.693653	4.535277
H	-8.572438	-4.910698	7.618831
H	-6.993198	-4.744797	6.838598
H	-7.477150	-3.596793	8.092161
H	-0.669972	4.945276	1.359336
H	-1.454102	3.360000	1.286438
H	-1.096250	4.251130	-0.211200
H	-1.874345	6.998331	0.816220
H	-2.302047	6.379595	-0.780436
H	-3.562665	7.017054	0.297425
H	-2.432579	5.860840	2.888363
H	-4.146394	5.805948	2.437599
H	-3.305542	4.312995	2.896275
H	-6.317611	6.270166	-4.129797
H	-5.874869	6.686166	-2.471142
H	-4.711456	5.852940	-3.519390
H	-6.728582	3.953902	-4.852606
H	-5.147464	3.432577	-4.238918
H	-6.619149	2.597579	-3.722658
H	-8.369297	5.146781	-3.324443
H	-8.295530	3.812164	-2.165149
H	-7.949781	5.459725	-1.628306
O	-1.620039	-0.110109	0.635013
O	-1.346872	0.352327	3.651221
C	1.309986	0.706524	2.096585
C	-0.411328	-0.244943	0.423520
C	0.624478	-0.539405	1.466317
C	-0.217963	0.975096	3.965905

C	-0.198306	2.021519	5.096658
C	0.933540	1.169683	5.684873
O	0.720827	0.140183	4.682609
C	2.031567	1.582193	1.084808
O	0.104862	-0.172033	-0.794811
C	-0.771337	0.073349	-1.938087
C	-0.107051	-0.616903	-3.114978
C	0.778977	0.633716	7.089490
C	-0.949677	1.568731	-2.128672
H	2.036520	0.286081	2.804518
H	1.925469	1.624949	5.553118
H	-1.115348	1.998732	5.689556
H	0.042788	3.040837	4.792963
H	0.901936	1.439915	7.821398
H	-0.211999	0.188952	7.222421
H	1.532190	-0.133217	7.297813
H	-1.733951	-0.391734	-1.709567
H	-0.725955	-0.499480	-4.009297
H	0.875044	-0.179218	-3.317627
H	0.022570	-1.685807	-2.923877
H	-1.581657	1.755823	-3.002341
H	-1.431210	2.025342	-1.261626
H	0.017347	2.052869	-2.296427
H	1.405631	-1.154171	1.009005
H	0.145953	-1.094834	2.273512
H	2.755725	0.998920	0.507600
H	1.329168	2.049858	0.389595
H	2.564433	2.379000	1.609915

YBRRRTS2S.xyz

128

scf done: -2432.652592

C	-5.183128	1.745117	-0.247083
C	-4.126392	2.541805	0.256563
C	-3.846665	3.784028	-0.379265
C	-4.605146	4.127379	-1.504937
C	-5.630350	3.336286	-2.037098
C	-5.902825	2.138688	-1.372185
O	-3.444125	2.105887	1.302731
Y	-2.776989	0.452243	2.480638
C	-2.767371	4.731209	0.167961
C	-3.102876	5.112172	1.624425
C	-6.446810	3.740219	-3.271947
C	-6.290561	2.669152	-4.369733
C	-5.580476	0.506811	0.501718
N	-4.515819	-0.523575	0.674663
C	-3.924506	-0.850704	-0.626821
O	-4.252856	0.395640	4.006845
C	-5.237684	-0.349914	4.495160
C	-5.086143	-1.759734	4.484128

C	-6.127829	-2.586795	4.898412
C	-7.342070	-2.069486	5.356413
C	-7.444105	-0.675255	5.420165
C	-6.432457	0.209206	5.022870
C	-3.749064	-2.360848	4.144990
N	-3.221212	-2.198815	2.758436
C	-1.960865	-2.952574	2.696191
C	-6.600209	1.729827	5.182235
C	-5.460274	2.283373	6.061911
C	-8.474181	-3.015767	5.778575
C	-8.882042	-3.894204	4.579154
O	-1.341441	2.104744	3.237439
C	-6.575521	2.428531	3.808991
C	-7.927041	2.101591	5.862348
C	-7.993904	-3.921873	6.929584
C	-9.720710	-2.259670	6.258112
C	-4.157379	-2.740576	1.755817
C	-5.156291	-1.708431	1.267020
C	-1.387107	4.047032	0.120721
C	-2.665828	6.033384	-0.641174
C	-7.935870	3.859526	-2.890995
C	-5.997045	5.086426	-3.856140
H	-5.833739	-2.184950	0.535395
H	-5.771325	-1.375703	2.106288
H	-4.704740	-3.605526	2.162908
H	-3.569468	-3.116284	0.912199
H	-3.789922	-3.440531	4.369514
H	-2.986231	-1.921779	4.795046
H	-6.436942	0.040870	-0.015137
H	-5.916618	0.769263	1.511791
H	-4.386150	5.070332	-1.989679
H	-6.704960	1.489525	-1.721251
H	-8.361862	-0.248981	5.804808
H	-5.970126	-3.664056	4.870256
H	-4.676412	-1.274968	-1.313731
H	-3.521604	0.056889	-1.078416
H	-3.110758	-1.568541	-0.508241
H	-2.120033	-4.026803	2.889206
H	-1.509980	-2.837227	1.707390
H	-1.271335	-2.550943	3.440892
H	-5.570643	3.367677	6.183146
H	-5.485178	1.827722	7.058437
H	-4.486759	2.084749	5.610669
H	-6.715051	3.509148	3.933678
H	-5.626894	2.270961	3.293701
H	-7.389457	2.061116	3.173091
H	-7.977244	3.189433	5.978672
H	-8.796980	1.797359	5.269572
H	-8.017783	1.659492	6.860748
H	-10.501557	-2.974959	6.538432

H	-9.509193	-1.640996	7.136648
H	-10.130987	-1.612851	5.475276
H	-9.683072	-4.587966	4.861556
H	-9.243547	-3.276713	3.749880
H	-8.041028	-4.489845	4.210060
H	-8.792205	-4.606518	7.240253
H	-7.131888	-4.529657	6.636595
H	-7.699414	-3.324628	7.798828
H	-0.614063	4.732010	0.490755
H	-1.372058	3.152802	0.744911
H	-1.130287	3.778205	-0.911496
H	-1.894888	6.672523	-0.196984
H	-2.381182	5.853178	-1.684297
H	-3.604471	6.598302	-0.633898
H	-2.331837	5.781076	2.026173
H	-4.064086	5.636641	1.672033
H	-3.153373	4.225704	2.257766
H	-6.603229	5.330549	-4.735548
H	-6.116403	5.902855	-3.136029
H	-4.948903	5.062507	-4.173434
H	-6.880707	2.932350	-5.256027
H	-5.242657	2.574894	-4.674729
H	-6.627257	1.685980	-4.025855
H	-8.537753	4.144026	-3.762733
H	-8.332188	2.914282	-2.507106
H	-8.078615	4.618506	-2.114769
O	-1.065351	-0.279486	0.847806
O	-0.887133	-0.229631	3.890945
C	-0.322272	1.451288	3.593105
C	0.156465	-0.365051	0.711742
C	-0.422893	-0.038070	5.238254
C	0.117227	1.384819	5.057066
O	0.652586	1.398280	2.612577
C	1.640630	0.375893	2.600030
C	1.092796	-0.833814	1.794169
O	0.782764	-0.049508	-0.406580
C	0.019590	0.504937	-1.528969
C	-0.359306	-0.635838	-2.457181
C	-1.486502	-0.192523	6.310157
C	2.900345	0.975552	1.997624
C	0.921592	1.539446	-2.173432
H	-0.873087	0.976955	-1.111858
H	-0.923427	-0.246008	-3.309767
H	0.534546	-1.139988	-2.837735
H	-0.986239	-1.369575	-1.944358
H	0.406524	1.995783	-3.023728
H	1.173201	2.331635	-1.464325
H	1.846444	1.080358	-2.536540
H	0.391899	-0.752765	5.440272
H	-0.409077	2.151316	5.631119

H	1.194293	1.500268	5.209301
H	-1.819662	-1.231187	6.398940
H	-1.080927	0.105773	7.283965
H	-2.356497	0.430950	6.084895
H	0.516224	-1.467265	2.465522
H	1.919890	-1.394838	1.350185
H	1.849251	0.028793	3.619191
H	3.225074	1.835236	2.589515
H	3.707574	0.236750	1.981879
H	2.716785	1.311241	0.973863

YBRRRTS2SR.xyz

128

scf done: -2432.662760

C	-5.087892	1.846108	-0.344873
C	-4.036383	2.571214	0.273366
C	-3.626167	3.805056	-0.302636
C	-4.235160	4.205348	-1.498331
C	-5.238474	3.480384	-2.151000
C	-5.655981	2.299551	-1.533712
O	-3.479803	2.083003	1.375404
Y	-3.079576	0.228380	2.342463
C	-2.568543	4.687968	0.380563
C	-3.033329	5.045298	1.807489
C	-5.892543	3.939548	-3.461376
C	-5.692248	2.861230	-4.544856
C	-5.671988	0.639964	0.341225
N	-4.758553	-0.528731	0.504717
C	-4.249687	-0.951450	-0.803027
O	-4.622613	0.264911	3.821840
C	-5.537245	-0.490350	4.413651
C	-5.335021	-1.893531	4.441776
C	-6.308386	-2.740994	4.966290
C	-7.501025	-2.248744	5.501582
C	-7.652110	-0.857237	5.519520
C	-6.709389	0.045947	5.011545
C	-4.001945	-2.453925	4.029616
N	-3.576829	-2.282282	2.602787
C	-2.335669	-3.053242	2.428394
C	-6.913521	1.564698	5.138649
C	-5.748451	2.163714	5.953622
C	-8.554076	-3.216529	6.057327
C	-9.019364	-4.169307	4.938121
O	-1.342282	0.205331	3.565507
C	-6.962606	2.231941	3.750320
C	-8.219457	1.919354	5.865829
C	-7.942510	-4.044321	7.205292
C	-9.789470	-2.486891	6.603040
C	-4.608723	-2.747286	1.649470
C	-5.507228	-1.619786	1.157126

C	-1.217313	3.950271	0.441936
C	-2.335159	6.009638	-0.368031
C	-7.402278	4.156847	-3.237409
C	-5.296159	5.253506	-3.984559
H	-6.258931	-2.039244	0.465164
H	-6.050023	-1.197658	2.006612
H	-5.236911	-3.523158	2.109611
H	-4.101068	-3.216715	0.800604
H	-3.993460	-3.532494	4.257266
H	-3.209249	-1.988663	4.630557
H	-6.565648	0.314276	-0.217471
H	-6.001947	0.910769	1.351046
H	-3.912189	5.139912	-1.938826
H	-6.460839	1.711905	-1.972934
H	-8.553728	-0.448885	5.958016
H	-6.111464	-3.812111	4.969048
H	-5.067331	-1.305546	-1.453204
H	-3.762283	-0.106140	-1.289806
H	-3.517854	-1.753795	-0.691609
H	-2.504101	-4.132602	2.571562
H	-1.929852	-2.889166	1.426864
H	-1.599176	-2.718533	3.163418
H	-5.866484	3.250694	6.040316
H	-5.729237	1.743619	6.965480
H	-4.790147	1.955728	5.473723
H	-7.157372	3.306148	3.854927
H	-6.016535	2.111136	3.220736
H	-7.769117	1.805732	3.141968
H	-8.299348	3.008433	5.949504
H	-9.104084	1.567083	5.323378
H	-8.251489	1.509407	6.881216
H	-10.515086	-3.217393	6.976901
H	-9.535181	-1.820124	7.433802
H	-10.286935	-1.893334	5.828550
H	-9.765903	-4.877736	5.316870
H	-9.470792	-3.608670	4.112498
H	-8.186741	-4.751389	4.530292
H	-8.682656	-4.741253	7.616593
H	-7.083643	-4.633673	6.868449
H	-7.600034	-3.392777	8.015941
H	-0.464970	4.573970	0.939843
H	-1.299929	3.012374	0.992207
H	-0.856063	3.735360	-0.570679
H	-1.590753	6.602590	0.174290
H	-1.950587	5.851545	-1.382039
H	-3.248190	6.611082	-0.436576
H	-2.279401	5.667558	2.305051
H	-3.970506	5.612034	1.775746
H	-3.194623	4.147312	2.405498
H	-5.787819	5.535123	-4.922003

H	-5.440557	6.076459	-3.276651
H	-4.223649	5.161858	-4.187601
H	-6.162480	3.166672	-5.487321
H	-4.626490	2.694429	-4.735753
H	-6.132488	1.903470	-4.249461
H	-7.888978	4.479216	-4.165820
H	-7.898431	3.240417	-2.902851
H	-7.576325	4.924875	-2.476678
O	-1.435350	-0.291546	0.585885
O	0.545330	-0.126916	4.870729
C	-0.216315	0.750134	4.007363
C	-0.207040	-0.351470	0.478174
C	0.716921	0.926679	5.855522
C	-0.255891	1.838386	5.097063
O	0.611894	1.213837	2.924931
C	1.479213	0.270142	2.335098
C	0.725619	-0.839578	1.547645
O	0.423737	-0.008956	-0.633351
C	-0.342083	0.506768	-1.767604
C	-0.756245	-0.663990	-2.643164
C	0.343326	0.469304	7.246767
C	2.481172	1.049029	1.497615
C	0.572332	1.489355	-2.474200
H	-1.221056	1.016191	-1.364001
H	-1.323632	-0.299848	-3.504999
H	0.123709	-1.199793	-3.012762
H	-1.389234	-1.362972	-2.091448
H	0.052942	1.920790	-3.334871
H	0.862269	2.304536	-1.806998
H	1.478436	0.990754	-2.831981
H	1.752263	1.295678	5.836967
H	-1.239923	1.910735	5.565568
H	0.104463	2.822566	4.795326
H	0.997131	-0.344729	7.576722
H	0.442020	1.295625	7.959695
H	-0.690565	0.111233	7.268071
H	0.140086	-1.418510	2.260682
H	1.474825	-1.487291	1.079805
H	2.011122	-0.268849	3.130400
H	3.027888	1.741455	2.142879
H	3.199824	0.374879	1.021083
H	1.984466	1.631338	0.718056

YBRRRTS2SP.xyz

128

scf done: -2432.682069

C	-5.511632	2.740343	0.211288
C	-4.587601	3.500503	0.973669
C	-4.394431	4.869893	0.639546
C	-5.090077	5.385171	-0.460313

C	-5.976441	4.641702	-1.246871
C	-6.172507	3.310479	-0.874532
O	-3.939811	2.916424	1.974720
Y	-3.357797	0.992382	2.720020
C	-3.458814	5.763003	1.470148
C	-3.923441	5.782602	2.940836
C	-6.723507	5.225033	-2.453707
C	-6.361966	4.424301	-3.720482
C	-5.863784	1.337874	0.628956
N	-4.744748	0.350981	0.641085
C	-4.065621	0.332706	-0.659946
O	-4.917872	0.535207	4.120921
C	-5.791715	-0.421437	4.399913
C	-5.421713	-1.767111	4.145113
C	-6.335001	-2.802368	4.331489
C	-7.631906	-2.565099	4.793982
C	-7.953243	-1.238139	5.103238
C	-7.078474	-0.156063	4.942225
C	-3.990420	-2.083710	3.808577
N	-3.434399	-1.572976	2.517886
C	-2.062818	-2.099695	2.399160
C	-7.479973	1.263372	5.376972
C	-6.477515	1.774076	6.432878
C	-8.614680	-3.731058	4.969898
C	-8.827912	-4.433661	3.614431
O	-1.493230	0.774463	1.126526
C	-7.491151	2.223757	4.172035
C	-8.879388	1.304800	6.010468
C	-8.042085	-4.744425	5.980700
C	-9.984511	-3.268732	5.484794
C	-4.241969	-1.995465	1.353958
C	-5.304553	-0.974396	0.967895
C	-2.017564	5.223801	1.386429
C	-3.435677	7.217571	0.976208
C	-8.243735	5.135115	-2.215060
C	-6.368391	6.696788	-2.705631
H	-5.885308	-1.366984	0.114534
H	-6.001517	-0.851870	1.801434
H	-4.733887	-2.959617	1.552517
H	-3.560953	-2.157932	0.512644
H	-3.862687	-3.178867	3.821681
H	-3.340020	-1.672875	4.592173
H	-6.657175	0.962235	-0.038726
H	-6.277195	1.343317	1.645495
H	-4.932110	6.425727	-0.713704
H	-6.870022	2.687063	-1.432086
H	-8.939508	-1.031925	5.499087
H	-6.007688	-3.820257	4.123246
H	-4.751191	0.008354	-1.460349
H	-3.709091	1.336662	-0.894887

H	-3.202689	-0.334142	-0.632434
H	-2.054661	-3.201179	2.377185
H	-1.590659	-1.722896	1.491322
H	-1.467620	-1.768622	3.252958
H	-6.738968	2.794240	6.739394
H	-6.498909	1.137556	7.324602
H	-5.460589	1.780203	6.036191
H	-7.815437	3.222649	4.488123
H	-6.498371	2.316735	3.729554
H	-8.191178	1.875151	3.403660
H	-9.098840	2.329214	6.330311
H	-9.663186	1.008229	5.304292
H	-8.950981	0.662231	6.894904
H	-10.652937	-4.131187	5.582052
H	-9.910715	-2.795658	6.469647
H	-10.458257	-2.558381	4.798843
H	-9.517216	-5.280057	3.720643
H	-9.250736	-3.740888	2.878913
H	-7.887813	-4.819531	3.207438
H	-8.731163	-5.586765	6.116645
H	-7.082085	-5.151286	5.647578
H	-7.882699	-4.273217	6.956149
H	-1.343238	5.835958	1.998498
H	-1.982907	4.193708	1.744806
H	-1.655005	5.247501	0.352156
H	-2.764855	7.803575	1.614211
H	-3.066562	7.302004	-0.052042
H	-4.425775	7.683711	1.025502
H	-3.249862	6.404879	3.543204
H	-4.931195	6.205192	3.018579
H	-3.939732	4.775732	3.360817
H	-6.918275	7.066355	-3.578091
H	-6.635812	7.331947	-1.854445
H	-5.299948	6.828817	-2.907606
H	-6.892054	4.821477	-4.594643
H	-5.286533	4.477438	-3.921036
H	-6.630424	3.367778	-3.621133
H	-8.794943	5.540613	-3.072247
H	-8.570217	4.100657	-2.068991
H	-8.532292	5.702897	-1.324339
O	1.332694	-2.135381	1.810357
O	-1.608168	1.141163	3.893476
C	-0.307081	1.060237	1.279539
C	2.229144	-1.623753	1.175238
C	-0.250493	1.292034	3.804253
C	0.165037	1.907114	2.421265
O	0.528439	0.555808	0.365550
C	1.955425	0.779366	0.352307
C	2.653239	-0.177093	1.332343
O	2.965587	-2.257540	0.249210

C	2.656594	-3.660684	0.005644
C	3.370376	-4.516623	1.039518
C	0.290019	2.189545	4.919639
C	2.384056	0.614317	-1.095090
C	3.089479	-3.945192	-1.420430
H	1.573814	-3.776601	0.115180
H	3.160729	-5.575261	0.857515
H	4.453229	-4.366582	0.983865
H	3.027115	-4.271316	2.047194
H	2.872696	-4.987071	-1.674188
H	2.558190	-3.303953	-2.129133
H	4.164546	-3.779823	-1.541488
H	0.261104	0.310977	3.881201
H	-0.345026	2.873622	2.337559
H	1.240463	2.091026	2.398752
H	0.002878	1.765270	5.885466
H	1.382670	2.279209	4.889192
H	-0.151304	3.189319	4.847025
H	2.414020	0.107814	2.359901
H	3.733861	-0.087518	1.187290
H	2.160088	1.807853	0.669379
H	1.840801	1.320054	-1.728250
H	3.455205	0.812399	-1.191547
H	2.189838	-0.399816	-1.449483

YBRRRTS1M.xyz

128

scf done: -2432.660080

C	-4.001751	4.286328	-0.318686
C	-4.337616	3.075735	0.348959
C	-5.525259	2.400191	-0.028994
C	-6.306769	2.863404	-1.084198
C	-5.967046	4.013112	-1.801198
C	-4.822487	4.697518	-1.377005
O	-3.594241	2.548832	1.310678
Y	-2.945325	0.691354	2.198224
O	-2.978613	-1.637791	2.724087
C	-3.453542	-1.788524	3.863213
O	-2.672953	-1.946658	4.992639
C	-3.676916	-2.807989	5.629620
C	-3.107306	-4.168202	5.952726
C	-5.993306	1.233809	0.793069
N	-5.129415	0.018290	0.817062
C	-4.785822	-0.442918	-0.545366
C	-3.445492	0.082396	-1.036308
N	-2.325332	-0.257885	-0.141804
C	-2.042081	-1.699335	-0.179135
C	-6.842927	4.485519	-2.969166
C	-6.922065	3.376794	-4.037332
C	-2.810451	5.145766	0.135692

C	-3.019029	5.547776	1.609618
O	-0.805695	0.741051	2.180445
C	0.264556	0.353604	1.498959
C	0.159463	0.178749	0.096417
C	1.254857	-0.241241	-0.653657
C	2.497799	-0.494177	-0.070071
C	2.587218	-0.302878	1.312659
C	1.522205	0.113120	2.120171
C	-1.130757	0.507716	-0.600737
C	1.712908	0.310677	3.631787
C	1.378989	1.767585	4.010321
C	3.680334	-0.949745	-0.935130
C	3.322488	-2.268332	-1.649069
O	-4.167731	0.009415	4.046986
C	-4.431875	0.549083	5.306202
C	-5.548816	1.591919	5.227074
C	-3.156768	1.111017	5.975813
C	-2.588379	2.281143	5.229076
O	-2.222599	3.274306	6.027392
C	-1.650908	4.488351	5.445816
C	-0.432133	4.832153	6.281586
O	-2.473167	2.323063	4.006787
C	0.797617	-0.657358	4.405758
C	3.155520	0.039681	4.086393
C	3.992702	0.129091	-1.990984
C	4.952202	-1.187884	-0.109068
C	-5.884305	-1.032700	1.514017
C	-1.485387	4.371616	0.004313
C	-2.671794	6.437775	-0.684296
C	-8.263379	4.796980	-2.457403
C	-6.290611	5.750851	-3.639781
C	-4.578285	-2.674263	4.393579
C	-2.727335	5.559902	5.467564
H	-4.783929	-0.252543	5.980399
H	-3.260945	-0.319156	-2.049195
H	-3.490605	1.170698	-1.124662
H	-5.564063	-0.145563	-1.263774
H	-4.769850	-1.536714	-0.537051
H	-6.995399	0.938441	0.438050
H	-6.102358	1.543914	1.841291
H	-0.998153	0.337095	-1.682605
H	-1.376963	1.568265	-0.471380
H	3.540143	-0.487375	1.791772
H	1.122386	-0.364713	-1.727545
H	-4.554071	5.609414	-1.894895
H	-7.210161	2.309391	-1.336138
H	-1.818340	-2.030338	-1.206944
H	-1.181342	-1.914329	0.454391
H	-2.889532	-2.265424	0.207740
H	-6.818629	-1.278463	0.982165

H	-5.268401	-1.929625	1.597247
H	-6.125337	-0.690297	2.522333
H	-2.174247	6.155351	1.958016
H	-3.932386	6.143104	1.722038
H	-3.097768	4.660545	2.241076
H	-0.644277	5.008426	0.305192
H	-1.482495	3.485217	0.640141
H	-1.313876	4.065341	-1.034089
H	-1.825967	7.018061	-0.299760
H	-2.474561	6.236272	-1.743082
H	-3.563290	7.070585	-0.614031
H	-6.939014	6.040997	-4.473748
H	-6.250628	6.596426	-2.944952
H	-5.284577	5.591767	-4.042557
H	-7.550634	3.693525	-4.878376
H	-5.926550	3.139506	-4.427420
H	-7.350209	2.454347	-3.632117
H	-8.906585	5.133513	-3.279478
H	-8.732829	3.916982	-2.006501
H	-8.239235	5.586135	-1.698587
H	0.906065	-0.502226	5.487231
H	-0.248575	-0.516163	4.134761
H	1.064679	-1.697444	4.188051
H	3.229949	0.206526	5.166922
H	3.463287	-0.994096	3.894077
H	3.874264	0.708722	3.600414
H	1.494997	1.908853	5.092881
H	2.061197	2.461221	3.505750
H	0.356535	2.018990	3.723737
H	5.765380	-1.513779	-0.767019
H	5.283915	-0.275919	0.398667
H	4.806976	-1.966382	0.647683
H	4.154319	-2.606152	-2.279108
H	3.103054	-3.057338	-0.921830
H	2.443552	-2.155153	-2.291614
H	4.830572	-0.180997	-2.627429
H	3.133081	0.318920	-2.641450
H	4.260711	1.076383	-1.511436
H	-4.066567	-2.315637	6.526872
H	-4.702862	-3.592504	3.813148
H	-5.538517	-2.180869	4.537529
H	-3.885468	-4.810716	6.378363
H	-2.711568	-4.646920	5.052004
H	-2.296435	-4.084089	6.682023
H	-1.365575	4.255674	4.417318
H	0.038952	5.738615	5.889854
H	-0.711525	5.012480	7.324442
H	0.303069	4.024339	6.249645
H	-2.331167	6.493023	5.056238
H	-3.586945	5.263962	4.861080

H	-3.064122	5.749657	6.491753
H	-3.344780	1.399632	7.013609
H	-2.401232	0.317224	5.972390
H	-5.789073	1.996259	6.217103
H	-5.262701	2.422204	4.572818
H	-6.454173	1.137374	4.814351

YBRRRTS1MR.xyz

128

scf done: -2432.667606

C	-4.008847	4.325473	-0.373915
C	-4.303508	3.104911	0.296342
C	-5.506029	2.426480	-0.029775
C	-6.339549	2.898033	-1.040934
C	-6.043259	4.058034	-1.760293
C	-4.883085	4.744307	-1.385235
O	-3.504815	2.574338	1.209574
Y	-2.957381	0.737461	2.195501
O	-2.831673	-1.818602	2.657123
C	-3.165194	-2.292123	3.717760
O	-2.460978	-2.294654	4.865334
C	-3.522907	-3.053167	5.567827
C	-3.004787	-4.361256	6.105490
C	-5.941502	1.253338	0.802975
N	-5.080350	0.034231	0.784171
C	-4.749842	-0.395467	-0.590728
C	-3.394677	0.115966	-1.056335
N	-2.295077	-0.271072	-0.156564
C	-2.015055	-1.707438	-0.266506
C	-6.981264	4.539313	-2.875077
C	-7.106851	3.444905	-3.953482
C	-2.802908	5.189243	0.031485
C	-2.948969	5.583732	1.515213
O	-0.799030	0.652455	2.250115
C	0.273124	0.277595	1.570046
C	0.185696	0.139355	0.160635
C	1.286360	-0.272793	-0.586205
C	2.520225	-0.551958	0.004560
C	2.596699	-0.388385	1.391764
C	1.526755	0.020397	2.196148
C	-1.087556	0.511132	-0.546007
C	1.710074	0.209543	3.709833
C	1.397019	1.671911	4.086202
C	3.707799	-0.998699	-0.858166
C	3.348305	-2.301721	-1.599369
O	-4.276154	0.300062	3.868860
C	-4.557174	0.766884	5.134536
C	-5.642254	1.850108	5.123803
C	-3.276043	1.257596	5.864292
C	-2.627902	2.404439	5.148515

O	-2.332868	3.418586	5.954564
C	-1.699279	4.612671	5.401050
C	-0.467483	4.884469	6.245448
O	-2.395580	2.415351	3.942862
C	0.771348	-0.740141	4.477366
C	3.144090	-0.087165	4.174708
C	4.036903	0.096810	-1.891608
C	4.970859	-1.259718	-0.025580
C	-5.820541	-1.026713	1.480659
C	-1.480773	4.423011	-0.160738
C	-2.707223	6.485481	-0.787579
C	-8.375761	4.831856	-2.286696
C	-6.473417	5.818683	-3.554492
C	-4.344352	-3.060675	4.269342
C	-2.724730	5.732516	5.441385
H	-4.938226	-0.056482	5.776060
H	-3.205654	-0.257956	-2.079048
H	-3.419874	1.206746	-1.111847
H	-5.518180	-0.056675	-1.300612
H	-4.759880	-1.489483	-0.617022
H	-6.956317	0.962265	0.482395
H	-6.008513	1.550563	1.857789
H	-0.930883	0.402027	-1.632815
H	-1.333222	1.563857	-0.361268
H	3.544219	-0.586393	1.876474
H	1.166124	-0.366164	-1.664708
H	-4.646108	5.663922	-1.905058
H	-7.251751	2.341777	-1.253417
H	-1.758190	-1.981873	-1.303627
H	-1.175667	-1.964453	0.379958
H	-2.879503	-2.291805	0.051295
H	-6.774421	-1.253724	0.975454
H	-5.212361	-1.933435	1.515691
H	-6.012691	-0.701061	2.505326
H	-2.091529	6.191718	1.830608
H	-3.858065	6.176495	1.668450
H	-2.998948	4.693629	2.145634
H	-0.629432	5.069222	0.086186
H	-1.440938	3.547442	0.487964
H	-1.363314	4.100459	-1.201644
H	-1.847992	7.068521	-0.438508
H	-2.556948	6.289818	-1.855189
H	-3.597737	7.113271	-0.673973
H	-7.165904	6.115606	-4.349794
H	-6.403844	6.654363	-2.850068
H	-5.488115	5.673560	-4.010310
H	-7.780894	3.767410	-4.756234
H	-6.130833	3.221824	-4.397454
H	-7.505633	2.513328	-3.539248
H	-9.064062	5.172511	-3.069738

H	-8.813607	3.942314	-1.822869
H	-8.318514	5.611791	-1.520148
H	0.879716	-0.591608	5.559844
H	-0.268621	-0.567504	4.201101
H	1.014874	-1.785426	4.255723
H	3.212696	0.073045	5.256661
H	3.436883	-1.124739	3.978595
H	3.877363	0.572774	3.698232
H	1.502771	1.811642	5.170139
H	2.096622	2.353717	3.589447
H	0.382053	1.940623	3.788508
H	5.788160	-1.578187	-0.682132
H	5.302849	-0.359182	0.501949
H	4.814206	-2.051113	0.715364
H	4.182094	-2.632071	-2.230899
H	3.120660	-3.103092	-0.888260
H	2.473486	-2.171529	-2.244311
H	4.878730	-0.207192	-2.525860
H	3.184801	0.304189	-2.546580
H	4.306322	1.033588	-1.392585
H	-3.934909	-2.413712	6.352294
H	-4.513011	-4.037791	3.810313
H	-5.262578	-2.471958	4.273694
H	-3.820978	-4.918310	6.576767
H	-2.581569	-4.974749	5.304293
H	-2.229030	-4.190309	6.856832
H	-1.420035	4.387302	4.369401
H	0.045046	5.777430	5.874952
H	-0.740911	5.053631	7.291840
H	0.231397	4.045563	6.196786
H	-2.283764	6.655061	5.052032
H	-3.594822	5.488862	4.826443
H	-3.058177	5.915855	6.467864
H	-3.482843	1.542313	6.899576
H	-2.557626	0.429110	5.871019
H	-5.893936	2.190427	6.135366
H	-5.320197	2.714872	4.533133
H	-6.550911	1.453705	4.660344

YBRRRTS1MP.xyz

128

scf done: -2432.667090

C	-3.967786	4.297948	-0.332997
C	-4.320247	3.095407	0.341112
C	-5.512080	2.429545	-0.040979
C	-6.282312	2.893870	-1.103905
C	-5.927298	4.036198	-1.825125
C	-4.778201	4.711425	-1.398315
O	-3.588056	2.566164	1.309957
Y	-2.912363	0.700489	2.184139

O	-3.115593	-1.457511	2.853037
C	-3.657202	-1.465811	4.035526
O	-2.786703	-1.764641	5.153783
C	-3.626092	-2.863580	5.594154
C	-2.892658	-4.186217	5.560131
C	-6.000295	1.276582	0.787752
N	-5.146486	0.056277	0.847700
C	-4.800126	-0.444345	-0.500413
C	-3.461827	0.064394	-1.012794
N	-2.332617	-0.255708	-0.120729
C	-2.074520	-1.703279	-0.086789
C	-6.792863	4.511244	-2.999742
C	-6.880454	3.397003	-4.061490
C	-2.765834	5.143998	0.118478
C	-2.964638	5.550105	1.592548
O	-0.788993	0.821178	2.131705
C	0.277802	0.402670	1.459479
C	0.159668	0.169285	0.067456
C	1.247267	-0.287725	-0.672292
C	2.492965	-0.522290	-0.086893
C	2.593847	-0.272776	1.285790
C	1.536621	0.181969	2.082880
C	-1.135570	0.473225	-0.631671
C	1.733688	0.428932	3.586329
C	1.389136	1.893187	3.924943
C	3.665600	-1.024987	-0.939283
C	3.288533	-2.366108	-1.599435
O	-4.198167	-0.078313	4.206211
C	-4.451754	0.428365	5.513295
C	-5.630156	1.388985	5.430836
C	-3.190272	1.065419	6.116233
C	-2.669663	2.228602	5.320289
O	-2.297538	3.241035	6.086669
C	-1.739868	4.445396	5.467212
C	-0.531067	4.831073	6.298559
O	-2.582556	2.243043	4.094725
C	0.831601	-0.525930	4.392295
C	3.181583	0.185049	4.039859
C	3.984337	0.007927	-2.038315
C	4.938518	-1.246047	-0.110245
C	-5.917583	-0.975238	1.557571
C	-1.451113	4.353062	-0.017578
C	-2.613818	6.433929	-0.702555
C	-8.211783	4.841806	-2.495618
C	-6.223704	5.766128	-3.675718
C	-4.637853	-2.580029	4.477590
C	-2.831435	5.501095	5.448001
H	-4.721461	-0.410934	6.166552
H	-3.286469	-0.366558	-2.015012
H	-3.502390	1.150256	-1.130861

H	-5.579787	-0.170818	-1.227189
H	-4.782353	-1.537185	-0.457948
H	-6.999034	0.983193	0.421688
H	-6.125716	1.604687	1.829145
H	-1.017504	0.246083	-1.704547
H	-1.371232	1.541203	-0.553559
H	3.548805	-0.443541	1.765863
H	1.105841	-0.457072	-1.738638
H	-4.497290	5.617275	-1.920115
H	-7.189652	2.347494	-1.358273
H	-1.915842	-2.099710	-1.103177
H	-1.180354	-1.894055	0.507508
H	-2.903811	-2.226575	0.389398
H	-6.833234	-1.243727	1.004887
H	-5.296518	-1.860412	1.698385
H	-6.202854	-0.601855	2.543500
H	-2.109292	6.143936	1.938964
H	-3.868051	6.160118	1.706681
H	-3.057463	4.664195	2.223925
H	-0.600828	4.978203	0.282072
H	-1.456730	3.464577	0.615422
H	-1.286784	4.047488	-1.057365
H	-1.761893	7.005737	-0.318765
H	-2.418777	6.229603	-1.761152
H	-3.498866	7.075843	-0.632891
H	-6.865337	6.058246	-4.514201
H	-6.177306	6.615570	-2.986016
H	-5.217794	5.593483	-4.073191
H	-7.501666	3.716068	-4.907095
H	-5.886173	3.145691	-4.445860
H	-7.321250	2.482097	-3.652788
H	-8.847926	5.180193	-3.322399
H	-8.692740	3.969962	-2.041016
H	-8.181930	5.635553	-1.741781
H	0.937337	-0.333178	5.467938
H	-0.217527	-0.413443	4.118066
H	1.114669	-1.568454	4.210210
H	3.262004	0.389193	5.113549
H	3.496158	-0.852255	3.881345
H	3.891512	0.842621	3.525913
H	1.515235	2.066658	5.001594
H	2.059014	2.578818	3.393597
H	0.361368	2.126260	3.642023
H	5.743621	-1.610400	-0.757815
H	5.285759	-0.318683	0.357656
H	4.786297	-1.990375	0.678792
H	4.114628	-2.739371	-2.216848
H	3.060139	-3.122935	-0.841462
H	2.410197	-2.267015	-2.245156
H	4.814824	-0.336655	-2.666607

H	3.123014	0.181790	-2.691006
H	4.266101	0.970118	-1.597937
H	-4.010603	-2.665422	6.605278
H	-4.741782	-3.370388	3.731532
H	-5.624283	-2.241007	4.802986
H	-3.560524	-5.002852	5.856720
H	-2.514400	-4.387087	4.553432
H	-2.042338	-4.172355	6.248842
H	-1.445692	4.182453	4.448597
H	-0.068088	5.728830	5.878351
H	-0.819035	5.044008	7.332818
H	0.213834	4.031621	6.298213
H	-2.445217	6.425015	5.007874
H	-3.682688	5.173947	4.845750
H	-3.176786	5.720249	6.463385
H	-3.375286	1.384646	7.145276
H	-2.410427	0.295823	6.131588
H	-5.863291	1.799204	6.418779
H	-5.413223	2.222259	4.754881
H	-6.517202	0.871126	5.056134

YBRRRTS2M.xyz

128

scf done: -2432.647480

C	1.591639	0.223596	2.259019
C	0.362395	0.430549	1.569976
C	0.338510	0.228740	0.167798
C	1.470880	-0.205982	-0.515726
C	2.680321	-0.445613	0.139127
C	2.697426	-0.210959	1.518377
O	-0.753257	0.812835	2.175347
Y	-2.900238	0.649855	2.144497
O	-2.600968	2.227759	3.981721
C	-2.392068	2.256993	5.190703
O	-2.108881	3.371204	5.848928
C	-2.027958	4.635604	5.120537
C	-3.373854	5.331049	5.228790
C	-0.907386	0.569166	-0.594653
N	-2.127893	-0.210141	-0.232461
C	-1.842206	-1.646210	-0.330319
C	3.905660	-0.929006	-0.647555
C	5.129354	-1.145843	0.253124
C	1.706848	0.462174	3.771711
C	3.142008	0.292155	4.293830
O	-3.506954	2.475607	1.178929
C	-4.267768	3.020587	0.239673
C	-3.964699	4.261058	-0.388562
C	-4.802226	4.690885	-1.426100
C	-5.933035	3.995870	-1.867591
C	-6.235110	2.809290	-1.195566

C	-5.435571	2.325574	-0.162715
C	-2.798226	5.139186	0.091751
C	-2.672002	6.444586	-0.708566
C	-5.863211	1.103545	0.598176
N	-4.972699	-0.098649	0.530518
C	-5.766022	-1.226089	1.038670
C	-6.831672	4.492190	-3.008076
C	-6.326791	5.805926	-3.620618
O	-2.562360	-1.151277	3.694862
C	-2.434817	1.065439	6.102628
C	-3.853715	0.501559	6.378676
C	-4.545173	-0.397030	-0.851763
C	-3.181186	0.179678	-1.187903
C	-6.879452	3.432876	-4.126785
C	-8.258217	4.731100	-2.474702
C	-3.048573	5.514403	1.565152
C	-1.453634	4.397156	-0.022602
C	1.268282	1.901965	4.107396
C	0.820019	-0.554677	4.516573
C	3.580938	-2.267687	-1.339744
C	4.279590	0.115941	-1.717495
C	-0.886724	5.410341	5.752126
H	-2.904955	-0.143148	-2.207879
H	-3.235607	1.270268	-1.197696
H	-5.275402	-0.015622	-1.579848
H	-4.525644	-1.484679	-0.974014
H	-6.860336	0.807729	0.231920
H	-5.969293	1.336130	1.665502
H	-0.713264	0.427870	-1.671336
H	-1.166283	1.623079	-0.446455
H	3.625547	-0.374454	2.051313
H	1.396491	-0.346740	-1.593159
H	-4.558875	5.627121	-1.911768
H	-7.123329	2.240006	-1.466310
H	-1.555605	-1.929127	-1.357048
H	-1.017564	-1.900278	0.337432
H	-2.718831	-2.231663	-0.044917
H	-6.646770	-1.416634	0.402840
H	-5.156547	-2.134208	1.057650
H	-6.097480	-1.001613	2.053323
H	-2.215306	6.116090	1.950480
H	-3.966719	6.104658	1.662739
H	-3.147764	4.613362	2.174022
H	-0.632736	5.052399	0.294024
H	-1.440920	3.507314	0.607985
H	-1.259081	4.101104	-1.059947
H	-1.839812	7.032734	-0.306540
H	-2.460666	6.260511	-1.767800
H	-3.573578	7.062767	-0.639119
H	-6.991307	6.114109	-4.435161

H	-6.308842	6.617776	-2.885756
H	-5.319743	5.699613	-4.037968
H	-7.527415	3.764787	-4.946860
H	-5.879480	3.252327	-4.535608
H	-7.268606	2.476847	-3.762337
H	-8.917621	5.084211	-3.276657
H	-8.695739	3.815984	-2.063356
H	-8.254923	5.484305	-1.679867
H	0.838312	-0.358367	5.597093
H	-0.212929	-0.520372	4.164406
H	1.197438	-1.572055	4.359516
H	3.160047	0.501152	5.369421
H	3.516301	-0.727890	4.154634
H	3.840808	0.984288	3.811154
H	1.310273	2.066569	5.191926
H	1.939992	2.625521	3.631372
H	0.254580	2.090568	3.751382
H	5.975388	-1.496022	-0.348301
H	5.438207	-0.219661	0.749338
H	4.937706	-1.899063	1.024913
H	4.443641	-2.626266	-1.914306
H	3.320838	-3.034305	-0.601937
H	2.738013	-2.172235	-2.031643
H	5.150127	-0.215875	-2.296397
H	3.458369	0.287433	-2.420651
H	4.524660	1.077217	-1.253804
H	-1.806209	4.397320	4.078045
H	-0.764407	6.368727	5.238898
H	-1.086863	5.609667	6.809615
H	0.052169	4.856627	5.671834
H	-3.337622	6.292716	4.709134
H	-4.162581	4.730336	4.769072
H	-3.630152	5.514120	6.277246
O	-4.651738	0.075311	3.625471
C	-4.177439	-0.870127	4.342239
C	-2.812722	-2.535750	3.969562
C	-4.328761	-2.382958	4.092812
C	-2.268836	-3.490283	2.929408
O	-4.080503	-0.738417	5.702264
H	-2.374907	-2.784996	4.947253
H	-4.841334	-2.576739	3.150507
H	-4.825336	-2.918370	4.905700
H	-1.187752	-3.363063	2.818425
H	-2.460921	-4.527090	3.228128
H	-2.738526	-3.326984	1.954478
H	-1.835563	0.269231	5.652310
H	-1.977292	1.356096	7.050477
H	-3.833462	0.167027	7.420608
C	-4.996525	1.499932	6.239687
H	-5.939704	1.015269	6.505373

H	-4.834958	2.335410	6.929583
H	-5.084164	1.879092	5.221391

YBRRRTS2MR.xyz

128

scf done: -2432.649466

C	1.605791	0.186495	2.258534
C	0.373494	0.378284	1.570078
C	0.348588	0.161980	0.169391
C	1.475236	-0.299148	-0.506787
C	2.680800	-0.546267	0.152102
C	2.704522	-0.277492	1.524962
O	-0.741767	0.763811	2.174513
Y	-2.896015	0.710273	2.101746
O	-2.614522	2.217345	3.988259
C	-2.486634	2.247222	5.209788
O	-2.254204	3.368308	5.878094
C	-2.141521	4.629905	5.150985
C	-3.496412	5.315892	5.181013
C	-0.880989	0.532409	-0.607111
N	-2.130701	-0.202113	-0.254791
C	-1.898083	-1.647251	-0.353532
C	3.896951	-1.066846	-0.625077
C	5.117389	-1.286351	0.279326
C	1.738482	0.485161	3.759890
C	3.180814	0.339084	4.269416
O	-3.479706	2.535423	1.151029
C	-4.261695	3.078785	0.225401
C	-3.964466	4.315983	-0.410776
C	-4.827100	4.754232	-1.423936
C	-5.974429	4.067828	-1.834884
C	-6.263649	2.879710	-1.160253
C	-5.440257	2.387319	-0.150154
C	-2.770954	5.178745	0.030299
C	-2.652744	6.480741	-0.776631
C	-5.851967	1.156014	0.606474
N	-4.957683	-0.038892	0.505061
C	-5.722232	-1.182284	1.025041
C	-6.902891	4.574207	-2.946718
C	-6.406766	5.886229	-3.570177
O	-2.494117	-1.150057	3.946257
C	-2.568356	1.060951	6.126095
C	-3.987146	0.444322	6.307648
C	-4.548251	-0.316043	-0.887019
C	-3.167681	0.229171	-1.210991
C	-6.992181	3.518642	-4.066438
C	-8.310709	4.821477	-2.369423
C	-2.963713	5.560523	1.510736
C	-1.442705	4.415710	-0.130125
C	1.301005	1.936955	4.042198

C	0.862858	-0.496435	4.561298
C	3.547699	-2.413841	-1.288573
C	4.288393	-0.051883	-1.717391
C	-1.043265	5.415796	5.842531
H	-2.894018	-0.086018	-2.233957
H	-3.192824	1.321307	-1.204710
H	-5.267640	0.106226	-1.602390
H	-4.561629	-1.400190	-1.037825
H	-6.856350	0.862823	0.258554
H	-5.938971	1.375177	1.678898
H	-0.679901	0.380201	-1.681018
H	-1.105859	1.596039	-0.469011
H	3.633350	-0.435032	2.058369
H	1.399832	-0.452839	-1.582377
H	-4.590454	5.689368	-1.915016
H	-7.160385	2.314658	-1.410683
H	-1.649941	-1.945925	-1.385871
H	-1.061768	-1.923520	0.290806
H	-2.785792	-2.202910	-0.040858
H	-6.618912	-1.376337	0.413242
H	-5.100045	-2.082098	1.015028
H	-6.014251	-0.978288	2.055539
H	-2.108066	6.148725	1.866301
H	-3.868311	6.165799	1.638016
H	-3.056503	4.662795	2.125109
H	-0.600726	5.058927	0.153634
H	-1.421600	3.528988	0.504532
H	-1.291308	4.111330	-1.172246
H	-1.799190	7.057488	-0.404124
H	-2.480020	6.292024	-1.842009
H	-3.542477	7.111917	-0.677823
H	-7.093179	6.201711	-4.363446
H	-6.360854	6.695750	-2.833974
H	-5.413517	5.774075	-4.018032
H	-7.660497	3.858964	-4.866382
H	-6.006081	3.330384	-4.504363
H	-7.379678	2.565146	-3.693668
H	-8.992010	5.180490	-3.150131
H	-8.741350	3.908397	-1.946452
H	-8.278072	5.573090	-1.573747
H	0.905205	-0.259156	5.632676
H	-0.176738	-0.461408	4.232134
H	1.229229	-1.522231	4.435176
H	3.212588	0.595030	5.334392
H	3.554938	-0.685800	4.170771
H	3.872229	1.009989	3.747812
H	1.367799	2.148039	5.117385
H	1.957439	2.642223	3.519827
H	0.277402	2.106572	3.705273
H	5.955664	-1.666384	-0.314790

H	5.445006	-0.355308	0.753890
H	4.912319	-2.017927	1.068277
H	4.402565	-2.798590	-1.857881
H	3.276922	-3.160837	-0.534627
H	2.704481	-2.318206	-1.980129
H	5.153212	-0.411418	-2.288115
H	3.470440	0.117851	-2.424744
H	4.549848	0.915019	-1.274896
H	-1.859685	4.390619	4.123252
H	-0.900403	6.374083	5.334435
H	-1.303352	5.615468	6.886796
H	-0.096715	4.869798	5.816231
H	-3.438766	6.275708	4.659740
H	-4.253981	4.706629	4.681813
H	-3.811929	5.501055	6.212804
O	-4.482368	-0.079139	3.499711
C	-3.978551	-0.995950	4.289095
C	-2.603713	-2.591861	4.115483
C	-4.132358	-2.524576	4.074906
C	-1.862678	-3.386077	3.068166
O	-4.140885	-0.818160	5.668493
H	-2.236775	-2.854025	5.116150
H	-4.539283	-2.760783	3.089797
H	-4.684281	-3.052651	4.853706
H	-0.798332	-3.132806	3.067490
H	-1.958813	-4.457810	3.274971
H	-2.265295	-3.196992	2.068940
H	-1.909164	0.283222	5.732244
H	-2.193333	1.377999	7.101334
H	-4.034800	0.157301	7.363648
C	-5.143184	1.405001	6.046620
H	-6.088101	0.903198	6.271157
H	-5.054887	2.279436	6.701308
H	-5.170253	1.727307	5.005428

YBRRTS2MP.xyz

128

scf done: -2432.687968

C	1.874589	0.191015	1.879278
C	0.612266	0.438885	1.274652
C	0.447314	0.151110	-0.103060
C	1.494719	-0.390721	-0.844158
C	2.741080	-0.660758	-0.274766
C	2.889142	-0.351428	1.081842
O	-0.416979	0.931752	1.952990
Y	-2.535879	0.773839	2.066120
O	-2.795646	1.922456	4.143709
C	-3.023507	2.211718	5.314490
O	-3.859421	3.158770	5.691205
C	-4.628236	3.892171	4.678180

C	-6.079725	3.468768	4.815417
C	-0.847480	0.499092	-0.784982
N	-2.062955	-0.184776	-0.251655
C	-1.866145	-1.640811	-0.251340
C	3.867190	-1.259333	-1.128494
C	5.144167	-1.514775	-0.315889
C	2.115998	0.507994	3.363549
C	3.558030	0.210707	3.802821
O	-3.117490	2.744379	1.281488
C	-3.833776	3.303138	0.321152
C	-3.432296	4.483240	-0.367782
C	-4.241560	4.934524	-1.418255
C	-5.432533	4.318407	-1.820678
C	-5.830394	3.195839	-1.090814
C	-5.064555	2.695423	-0.040789
C	-2.168976	5.257234	0.045545
C	-1.969788	6.538232	-0.779974
C	-5.592503	1.569433	0.801085
N	-4.808866	0.299465	0.835600
C	-5.595320	-0.671741	1.614020
C	-6.296698	4.835612	-2.978805
C	-5.682736	6.063848	-3.664146
O	-2.820425	-1.069520	3.036346
C	-2.295064	1.576844	6.472987
C	-3.055263	0.525154	7.302783
C	-4.554333	-0.231883	-0.521105
C	-3.211044	0.199276	-1.095346
C	-6.455713	3.728823	-4.040179
C	-7.689265	5.231225	-2.448776
C	-2.285514	5.672454	1.525921
C	-0.910390	4.388397	-0.139956
C	1.854183	2.004582	3.629447
C	1.182162	-0.354298	4.236837
C	3.406046	-2.603911	-1.725192
C	4.215874	-0.290491	-2.275853
C	-4.392016	5.366568	4.947116
H	-3.104127	-0.236383	-2.104756
H	-3.196839	1.286509	-1.209472
H	-5.347296	0.082048	-1.216187
H	-4.598701	-1.323857	-0.469227
H	-6.616575	1.331505	0.467038
H	-5.666374	1.898922	1.846406
H	-0.756161	0.265621	-1.859013
H	-1.041717	1.574693	-0.701863
H	3.847594	-0.543276	1.546853
H	1.322611	-0.597086	-1.899414
H	-3.924422	5.822919	-1.949120
H	-6.768419	2.695154	-1.327767
H	-1.733340	-2.023810	-1.276790
H	-0.973002	-1.880775	0.327278

H	-2.716213	-2.141831	0.213416
H	-6.571284	-0.868946	1.140008
H	-5.036672	-1.603218	1.708847
H	-5.765480	-0.284250	2.621877
H	-1.384914	6.214086	1.840465
H	-3.146716	6.334145	1.673977
H	-2.403028	4.792363	2.161083
H	-0.012563	4.961720	0.121462
H	-0.941851	3.503322	0.497380
H	-0.808969	4.071708	-1.184581
H	-1.075080	7.059949	-0.423442
H	-1.820521	6.325164	-1.844299
H	-2.814590	7.229141	-0.682545
H	-6.327181	6.388661	-4.488315
H	-5.581099	6.907885	-2.973713
H	-4.694708	5.844883	-4.083033
H	-7.078469	4.077246	-4.872954
H	-5.481322	3.434379	-4.444439
H	-6.928864	2.833658	-3.624021
H	-8.324321	5.599588	-3.263572
H	-8.201976	4.382419	-1.985307
H	-7.608948	6.022370	-1.695807
H	1.330250	-0.118180	5.298776
H	0.135399	-0.184580	3.978602
H	1.400357	-1.419258	4.097781
H	3.672675	0.466654	4.862099
H	3.815224	-0.848634	3.693017
H	4.289087	0.802563	3.241219
H	2.000740	2.231504	4.693279
H	2.553235	2.623638	3.056165
H	0.838083	2.282345	3.344824
H	5.913905	-1.949996	-0.962598
H	5.551624	-0.589208	0.104526
H	4.969099	-2.215728	0.507423
H	4.197331	-3.044142	-2.343948
H	3.156583	-3.317420	-0.932544
H	2.519641	-2.484218	-2.356275
H	5.013529	-0.704630	-2.904505
H	3.351133	-0.098398	-2.918853
H	4.557011	0.672576	-1.881994
H	-4.232475	3.610403	3.699092
H	-4.951052	5.964735	4.221785
H	-4.728508	5.639456	5.952360
H	-3.333288	5.619938	4.848598
H	-6.681549	3.973370	4.053161
H	-6.182297	2.388766	4.687689
H	-6.473263	3.743946	5.799357
O	-4.871154	0.158924	5.244634
C	-4.137153	-0.761438	5.552505
C	-2.813210	-2.129222	3.918001

C	-4.056868	-2.084876	4.852612
C	-2.763887	-3.477086	3.194753
O	-3.240120	-0.698170	6.558055
H	-1.927920	-2.074316	4.577537
H	-4.967093	-2.212423	4.261566
H	-3.987433	-2.888557	5.593026
H	-1.878712	-3.516843	2.553784
H	-2.715358	-4.314244	3.900530
H	-3.650191	-3.610810	2.563175
H	-1.391347	1.113528	6.071053
H	-1.999543	2.376005	7.161050
H	-2.342655	0.205758	8.069857
C	-4.316484	1.007827	8.005317
H	-4.753911	0.182104	8.573891
H	-4.052262	1.801550	8.711227
H	-5.058643	1.389010	7.306753

YBSSTS1S.xyz

128

scf done: -2432.656106

C	-5.155229	2.858277	-0.229964
C	-3.849752	3.337739	0.047171
C	-3.324183	4.381287	-0.766083
C	-4.080958	4.788158	-1.872633
C	-5.337326	4.269614	-2.206446
C	-5.866363	3.311847	-1.337551
O	-3.185877	2.799082	1.056347
Y	-2.812683	0.954028	2.147676
O	-3.342456	-1.326418	2.643271
C	-3.513951	-1.472495	3.867658
O	-4.714637	-1.858393	4.425483
C	-4.033641	-2.472095	5.574833
C	-4.441213	-3.913643	5.756317
C	-2.006812	5.090340	-0.407791
C	-0.814088	4.116878	-0.437743
C	-6.137782	4.732624	-3.431265
C	-7.460159	5.377635	-2.970888
C	-5.816044	1.945318	0.762090
N	-5.200758	0.614330	1.028378
C	-5.029781	-0.176342	-0.209538
C	-3.714233	0.084164	-0.930782
N	-2.528305	-0.265161	-0.127195
C	-2.343803	-1.722705	-0.086793
O	-0.711694	0.718143	1.981118
C	0.257616	0.237672	1.209241
C	1.554937	-0.047229	1.715504
C	2.508297	-0.566251	0.831273
C	2.263893	-0.821746	-0.521767
C	0.982645	-0.524222	-0.991003
C	-0.006237	0.000344	-0.162790

C	1.905033	0.215353	3.188873
C	1.007615	-0.645024	4.100775
C	-1.338536	0.374404	-0.756155
C	3.322504	-1.391476	-1.475094
C	3.579417	-0.389726	-2.618337
O	-3.400662	0.392916	4.308387
C	-3.929600	1.005228	5.441766
C	-4.282874	2.478529	5.122573
O	-2.370593	2.883927	3.719494
C	-3.063537	3.232546	4.669719
O	-2.803693	4.302198	5.409892
C	-1.643254	5.123712	5.065304
C	-0.424949	4.585042	5.795142
C	-2.985664	0.934836	6.647586
C	4.659710	-1.661964	-0.771754
C	2.820257	-2.721610	-2.070946
C	3.364220	-0.132764	3.520864
C	1.702448	1.709151	3.514963
C	-1.682618	6.245171	-1.368591
C	-2.138948	5.685282	1.009310
C	-6.120696	-0.101128	1.928157
C	-5.373359	5.763162	-4.273605
C	-6.452554	3.521676	-4.331693
C	-2.673571	-2.168622	4.929764
C	-2.012477	6.542202	5.455689
H	-4.882589	0.517466	5.715181
H	-3.714364	-0.487129	-1.876096
H	-3.648233	1.141104	-1.195959
H	-5.859367	0.020639	-0.907534
H	-5.093103	-1.233026	0.065606
H	-6.860752	1.784925	0.445290
H	-5.855616	2.451048	1.738066
H	-1.325504	0.118575	-1.829069
H	-1.498402	1.456195	-0.686368
H	3.494631	-0.781340	1.221983
H	0.734636	-0.694729	-2.037588
H	-3.666727	5.562390	-2.505350
H	-6.863166	2.907918	-1.509750
H	-2.193525	-2.123279	-1.102876
H	-1.467781	-1.961920	0.516541
H	-3.206900	-2.202651	0.372505
H	-7.110940	-0.236141	1.462196
H	-5.703498	-1.071495	2.191938
H	-6.254334	0.471484	2.850154
H	-1.205981	6.186191	1.297397
H	-2.946178	6.425910	1.043862
H	-2.353712	4.895617	1.732595
H	0.115292	4.652117	-0.207039
H	-0.934380	3.319999	0.297121
H	-0.699685	3.670227	-1.432042

H	-0.757432	6.733361	-1.043575
H	-1.524087	5.896941	-2.395377
H	-2.470258	7.006439	-1.380613
H	-5.975302	6.051036	-5.142446
H	-5.158495	6.674970	-3.706278
H	-4.425002	5.360863	-4.645706
H	-7.030921	3.832143	-5.210182
H	-5.530177	3.046384	-4.682184
H	-7.037281	2.763589	-3.800893
H	-8.050832	5.710100	-3.833116
H	-8.074241	4.675870	-2.397609
H	-7.267571	6.247508	-2.334099
H	1.239195	-0.448886	5.155653
H	-0.046364	-0.424052	3.925671
H	1.177324	-1.711138	3.910835
H	3.553192	0.080570	4.578812
H	3.584930	-1.193207	3.356024
H	4.073199	0.461684	2.934338
H	1.936912	1.899862	4.570254
H	2.370782	2.328417	2.906111
H	0.674023	2.016776	3.318496
H	5.380314	-2.066869	-1.490732
H	5.091380	-0.747028	-0.352007
H	4.554059	-2.392446	0.037651
H	3.562081	-3.141716	-2.761006
H	2.634417	-3.457169	-1.281045
H	1.887222	-2.588468	-2.627525
H	4.325798	-0.783721	-3.318913
H	2.667141	-0.181527	-3.185927
H	3.950093	0.562473	-2.224510
H	-4.244080	-1.882489	6.473219
H	-2.172042	-3.050979	4.521988
H	-1.962726	-1.550338	5.472550
H	-4.244554	-4.490473	4.847590
H	-3.877473	-4.361348	6.581592
H	-5.507151	-3.990111	5.990795
H	-1.499167	5.042735	3.984903
H	0.444860	5.210868	5.572979
H	-0.586439	4.593206	6.877893
H	-0.195487	3.566851	5.472999
H	-1.192562	7.219991	5.200741
H	-2.908138	6.873436	4.923573
H	-2.197914	6.616170	6.531850
H	-3.405702	1.461500	7.511700
H	-2.807246	-0.100932	6.946644
H	-4.731449	2.973952	5.987241
H	-2.015524	1.380064	6.404731
H	-5.010755	2.496032	4.302267

YBSSTS1SR.xyz

128

scf done: -2432.672693

C	-5.317061	2.861105	-0.237889
C	-4.038837	3.437237	-0.021651
C	-3.659927	4.566385	-0.800757
C	-4.543513	4.999079	-1.798205
C	-5.784609	4.410420	-2.062527
C	-6.153018	3.340562	-1.243474
O	-3.248464	2.900943	0.898280
Y	-2.829066	1.085882	1.999923
O	-2.985629	-1.329997	2.642979
C	-3.098394	-1.906641	3.700399
O	-3.525356	-3.172432	3.865553
C	-3.395173	-3.058791	5.342557
C	-2.446313	-4.088699	5.895595
C	-2.346001	5.320219	-0.533958
C	-1.129664	4.397715	-0.737680
C	-6.727996	4.899406	-3.169455
C	-8.065768	5.350449	-2.550362
C	-5.820743	1.791987	0.692932
N	-5.072977	0.503064	0.732146
C	-4.857645	-0.051409	-0.621170
C	-3.477160	0.274494	-1.173203
N	-2.388732	-0.178288	-0.291808
C	-2.291535	-1.642690	-0.301523
O	-0.687166	0.716354	1.988955
C	0.294122	0.156755	1.299970
C	1.528413	-0.226645	1.900513
C	2.501293	-0.829277	1.094976
C	2.346273	-1.073128	-0.273559
C	1.136498	-0.669327	-0.842265
C	0.131330	-0.063416	-0.092799
C	1.798951	0.041704	3.388767
C	0.759596	-0.698477	4.253108
C	-1.114946	0.416102	-0.783402
C	3.424377	-1.740961	-1.137465
C	3.838576	-0.790583	-2.278332
O	-4.165329	1.119608	3.719555
C	-4.714341	2.110215	4.506404
C	-4.152151	3.524183	4.157805
O	-1.933677	2.816976	3.571869
C	-2.659924	3.552233	4.238286
O	-2.186543	4.439960	5.108069
C	-0.741793	4.564269	5.265663
C	-0.310130	3.702315	6.440102
C	-4.543431	1.812813	6.000539
C	4.683190	-2.092575	-0.332861
C	2.866202	-3.044346	-1.742548
C	3.189844	-0.431987	3.836507
C	1.711112	1.557279	3.659267

C	-2.165628	6.531238	-1.462526
C	-2.348004	5.843332	0.916763
C	-5.861829	-0.431983	1.549944
C	-6.144942	6.083447	-3.953178
C	-6.992454	3.752750	-4.165366
C	-2.899475	-1.614955	5.162638
C	-0.465568	6.043482	5.461931
H	-5.804490	2.199104	4.320270
H	-3.377313	-0.180568	-2.175548
H	-3.382809	1.355834	-1.298977
H	-5.615144	0.325834	-1.322948
H	-4.990591	-1.136399	-0.571725
H	-6.869778	1.574488	0.429423
H	-5.822703	2.162598	1.726066
H	-1.019477	0.209738	-1.863329
H	-1.218663	1.502551	-0.674081
H	3.433852	-1.119376	1.562180
H	0.959025	-0.820157	-1.906331
H	-4.246095	5.848244	-2.400080
H	-7.123759	2.863573	-1.372333
H	-2.135876	-2.021416	-1.325959
H	-1.448704	-1.955666	0.314902
H	-3.195424	-2.091150	0.111139
H	-6.865276	-0.595168	1.122590
H	-5.345149	-1.391658	1.615890
H	-5.951040	-0.024526	2.559700
H	-1.418476	6.387907	1.124343
H	-3.186877	6.529095	1.080709
H	-2.428509	5.013258	1.620574
H	-0.199173	4.958382	-0.586407
H	-1.146969	3.570159	-0.027503
H	-1.113441	3.992217	-1.755785
H	-1.227261	7.038613	-1.213349
H	-2.108380	6.238952	-2.516993
H	-2.973393	7.263013	-1.351638
H	-6.847255	6.391269	-4.735535
H	-5.969335	6.950984	-3.308210
H	-5.199607	5.823005	-4.441073
H	-7.675143	4.079045	-4.959163
H	-6.059643	3.420890	-4.633733
H	-7.444724	2.885815	-3.673333
H	-8.756647	5.693552	-3.330051
H	-8.556174	4.536486	-2.007299
H	-7.910676	6.174348	-1.845854
H	0.933792	-0.494741	5.318026
H	-0.245685	-0.369913	3.984664
H	0.832772	-1.781576	4.097734
H	3.320533	-0.210128	4.901647
H	3.321020	-1.512199	3.706846
H	3.993179	0.078373	3.294412

H	1.898737	1.764695	4.720773
H	2.466714	2.092484	3.073295
H	0.724806	1.940247	3.390351
H	5.421954	-2.566577	-0.988370
H	5.149817	-1.201969	0.101576
H	4.464364	-2.794187	0.479313
H	3.616811	-3.531192	-2.377184
H	2.579203	-3.747869	-0.953558
H	1.980787	-2.856388	-2.358019
H	4.605942	-1.254828	-2.909707
H	2.990262	-0.534643	-2.920856
H	4.245211	0.144019	-1.878106
H	-4.396121	-3.139937	5.774373
H	-1.861135	-1.423628	5.441800
H	-3.541129	-0.806041	5.514271
H	-1.459444	-4.001297	5.431723
H	-2.335925	-3.945863	6.975386
H	-2.825657	-5.099464	5.721831
H	-0.279244	4.200078	4.344739
H	0.767691	3.802549	6.600122
H	-0.825310	4.010416	7.355610
H	-0.525546	2.648554	6.246758
H	0.610391	6.208248	5.572931
H	-0.814728	6.621874	4.602548
H	-0.965966	6.418812	6.360188
H	-4.995263	2.588381	6.629565
H	-5.027085	0.860706	6.243862
H	-4.583155	4.294617	4.801978
H	-3.481454	1.732832	6.260317
H	-4.410954	3.744383	3.115829

YBSSTS1SP.xyz

128

scf done: -2432.667078

C	-4.767508	3.121443	-0.107394
C	-3.406100	3.450026	0.128367
C	-2.777430	4.393381	-0.732614
C	-3.501332	4.850610	-1.841414
C	-4.815201	4.470761	-2.137625
C	-5.436953	3.614876	-1.224454
O	-2.780818	2.868730	1.138464
Y	-2.687711	1.013440	2.270162
O	-3.423201	-0.992376	3.008593
C	-3.176498	-1.097042	4.284962
O	-4.338275	-1.222660	5.151904
C	-3.842817	-2.461577	5.727931
C	-4.783099	-3.619444	5.475433
C	-1.372637	4.941280	-0.424715
C	-0.313476	3.824011	-0.462657
C	-5.576472	4.971621	-3.372628

C	-6.834529	5.745802	-2.931613
C	-5.537147	2.364010	0.941731
N	-5.103908	0.989617	1.322264
C	-5.129583	0.047469	0.185298
C	-3.874842	0.103899	-0.674341
N	-2.649940	-0.263838	0.062875
C	-2.556576	-1.723222	0.218901
O	-0.608150	0.683949	1.967208
C	0.275172	0.144115	1.131826
C	1.608849	-0.152965	1.526463
C	2.462348	-0.738862	0.584021
C	2.086306	-1.055866	-0.724466
C	0.772981	-0.748076	-1.084800
C	-0.120405	-0.152198	-0.197709
C	2.103936	0.150619	2.949588
C	1.295116	-0.685966	3.960728
C	-1.480184	0.249451	-0.705152
C	3.036103	-1.705522	-1.739399
C	3.182311	-0.790332	-2.971238
O	-2.430031	0.137731	4.635783
C	-2.489261	0.655964	5.957542
C	-3.727207	1.554999	6.136192
O	-3.546353	2.616632	3.968677
C	-3.758714	2.709767	5.177933
O	-4.064588	3.856686	5.761505
C	-4.147275	5.070863	4.944167
C	-2.813650	5.791664	5.031366
C	-1.183287	1.379782	6.250405
C	4.436567	-1.945654	-1.158670
C	2.463242	-3.065973	-2.183253
C	3.586666	-0.200149	3.147436
C	1.945993	1.653576	3.256612
C	-0.935270	6.022779	-1.425212
C	-1.384312	5.585469	0.976926
C	-6.039690	0.512889	2.356512
C	-4.725959	5.905318	-4.244489
C	-6.001517	3.767981	-4.237362
C	-2.563771	-2.381748	4.886129
C	-5.313181	5.868408	5.496700
H	-2.604302	-0.177713	6.661168
H	-4.008461	-0.562661	-1.543688
H	-3.748312	1.117145	-1.061449
H	-6.009018	0.239200	-0.451596
H	-5.247576	-0.958451	0.599215
H	-6.594885	2.316419	0.630575
H	-5.503807	2.940628	1.875258
H	-1.571395	-0.089034	-1.750744
H	-1.575358	1.340983	-0.710706
H	3.475951	-0.961102	0.892149
H	0.420995	-0.963897	-2.092627

H	-3.010380	5.548113	-2.507712
H	-6.477854	3.327281	-1.367740
H	-2.558257	-2.220197	-0.764907
H	-1.627691	-1.972075	0.733563
H	-3.383059	-2.091178	0.826298
H	-7.063541	0.422471	1.957834
H	-5.698396	-0.446634	2.746312
H	-6.062500	1.229916	3.182322
H	-0.387837	5.970507	1.226475
H	-2.089487	6.424249	1.009358
H	-1.676026	4.853181	1.732389
H	0.680876	4.241447	-0.261888
H	-0.514542	3.055976	0.285274
H	-0.279262	3.352958	-1.451656
H	0.051943	6.400159	-1.137198
H	-0.849543	5.631653	-2.445121
H	-1.622967	6.875623	-1.440020
H	-5.305851	6.228445	-5.115880
H	-4.420359	6.804765	-3.699431
H	-3.823356	5.406682	-4.613376
H	-6.555623	4.102309	-5.122829
H	-5.125752	3.204744	-4.577116
H	-6.645995	3.079335	-3.681744
H	-7.392297	6.106739	-3.804298
H	-7.510968	5.118731	-2.342221
H	-6.564248	6.611658	-2.317975
H	1.635093	-0.476395	4.983699
H	0.228799	-0.465233	3.889905
H	1.441589	-1.756017	3.773667
H	3.881860	0.050747	4.172447
H	3.782496	-1.268292	3.003069
H	4.237500	0.364157	2.470660
H	2.270346	1.867481	4.283052
H	2.565315	2.250086	2.577611
H	0.908737	1.969735	3.138972
H	5.077502	-2.407300	-1.917760
H	4.913674	-1.009853	-0.848455
H	4.409985	-2.619094	-0.295302
H	3.120826	-3.542293	-2.920647
H	2.363466	-3.742849	-1.328006
H	1.474215	-2.957833	-2.639439
H	3.853634	-1.242224	-3.711640
H	2.219572	-0.612185	-3.460455
H	3.594665	0.183189	-2.685949
H	-3.675150	-2.335196	6.807434
H	-2.438010	-3.172602	4.144446
H	-1.633146	-2.237808	5.438633
H	-4.941572	-3.755349	4.401341
H	-4.369195	-4.546073	5.888459
H	-5.754288	-3.439473	5.947318

H	-4.337270	4.757744	3.914677
H	-2.854260	6.715465	4.446946
H	-2.578659	6.048939	6.068965
H	-2.007743	5.175587	4.625118
H	-5.438524	6.786246	4.914941
H	-6.243818	5.297201	5.438523
H	-5.138890	6.144188	6.541252
H	-1.189200	1.783787	7.268073
H	-0.339843	0.694184	6.149914
H	-3.786498	1.931579	7.160558
H	-1.021349	2.207518	5.552618
H	-4.608414	0.932719	5.944395

YBSSTS2S.xyz

128

scf done: -2432.651930

C	-3.619265	-1.515121	2.333294
C	-3.831172	-2.115754	3.605223
C	-2.975503	-3.171234	4.007960
C	-1.871070	-3.524540	3.236375
C	-1.580451	-2.886344	2.028888
C	-2.488810	-1.909687	1.605965
O	-4.812829	-1.742564	4.418865
Y	-5.502239	-1.704120	6.430391
C	-3.345133	-4.011846	5.197205
N	-3.404196	-3.324003	6.517746
C	-3.724587	-4.349631	7.527157
C	-4.132659	-3.753109	8.859923
N	-5.348511	-2.919432	8.767843
C	-5.324556	-1.939453	9.866851
C	-0.342929	-3.292043	1.217864
C	-0.452009	-4.776147	0.814998
C	-4.628031	-0.517622	1.739893
C	-4.754080	0.734093	2.625878
O	-6.779576	-3.420166	6.139029
C	-7.023481	-4.638054	6.608824
C	-7.449917	-5.715899	5.781209
C	-7.583640	-6.980831	6.370154
C	-7.348228	-7.253093	7.721135
C	-6.985538	-6.165993	8.519369
C	-6.834304	-4.884322	7.995590
C	-7.790362	-5.509945	4.294068
C	-6.553526	-5.043087	3.504559
C	-6.589878	-3.737027	8.939671
C	-7.498733	-8.650156	8.337377
C	-8.599284	-8.622933	9.416516
O	-6.206681	0.465546	6.127205
C	-7.880886	-9.710963	7.295939
C	-6.166239	-9.077486	8.984145
C	-8.304414	-6.794726	3.625375

C	-8.900178	-4.448814	4.165151
C	-2.098397	-2.724746	6.813167
C	-4.231283	-0.049742	0.331330
C	-6.006527	-1.201863	1.630178
C	-0.185320	-2.461093	-0.063028
C	0.922839	-3.091035	2.074259
H	-2.856053	-5.013804	7.681081
H	-4.538609	-4.967671	7.144233
H	-4.281480	-4.564919	9.589589
H	-3.324047	-3.126847	9.250617
H	-6.588052	-4.133500	9.969012
H	-7.418131	-3.027256	8.860738
H	-2.629243	-4.847945	5.273276
H	-4.336949	-4.448428	5.040115
H	-2.313728	-1.433106	0.649758
H	-1.238582	-4.337268	3.591106
H	-7.892636	-7.800190	5.734470
H	-6.826524	-6.304588	9.587861
H	-1.327523	-3.503043	6.941760
H	-1.800493	-2.085092	5.983501
H	-2.145453	-2.120975	7.721122
H	-5.177968	-2.432524	10.841607
H	-4.524486	-1.213412	9.700340
H	-6.278610	-1.410888	9.890553
H	-9.155751	-4.294052	3.109916
H	-9.806662	-4.769451	4.691467
H	-8.566248	-3.497968	4.582475
H	-6.807171	-4.920181	2.444743
H	-6.182367	-4.086238	3.874818
H	-5.750046	-5.786028	3.567180
H	-8.554639	-6.578603	2.581172
H	-7.550921	-7.590067	3.621163
H	-9.209542	-7.179884	4.107874
H	-7.965480	-10.690142	7.779758
H	-8.845547	-9.492132	6.825912
H	-7.127083	-9.796485	6.505938
H	-6.259042	-10.070444	9.440188
H	-5.366269	-9.119820	8.237214
H	-5.853791	-8.380437	9.768344
H	-8.715288	-9.611767	9.876433
H	-8.367416	-7.910278	10.214428
H	-9.562245	-8.333946	8.982482
H	-5.453107	1.448535	2.173284
H	-5.126390	0.473556	3.617223
H	-3.783589	1.235337	2.724966
H	-4.996930	0.635929	-0.047596
H	-3.277772	0.490302	0.327621
H	-4.158240	-0.883083	-0.375965
H	-6.745951	-0.499128	1.226295
H	-5.957467	-2.065584	0.958115

H	-6.349722	-1.543427	2.608505
H	0.718247	-2.772721	-0.598380
H	-1.033114	-2.595444	-0.743204
H	-0.088847	-1.392269	0.155966
H	1.819429	-3.386941	1.516299
H	1.033876	-2.040775	2.364704
H	0.890338	-3.688042	2.991238
H	0.430133	-5.088620	0.243098
H	-0.529601	-5.428849	1.690244
H	-1.338448	-4.946078	0.194902
O	-4.221251	0.150745	7.435096
O	-7.718645	-1.066590	7.786502
C	-5.358759	1.191839	6.770323
C	-3.235027	1.169298	7.103596
C	-8.387762	-0.056921	7.578302
O	-9.482595	-0.034779	6.838313
C	-9.940438	-1.270658	6.204815
C	-11.005412	-1.890030	7.093890
C	-8.134107	1.284963	8.212903
C	-6.719990	1.484220	8.757557
O	-5.822136	2.010982	7.783414
C	-4.160965	1.912908	6.146741
C	-1.928309	0.670027	6.535598
C	-6.701624	2.481887	9.906750
C	-10.444126	-0.874290	4.830263
H	-3.044931	1.759929	8.009831
H	-4.020421	1.605443	5.110238
H	-4.197684	3.001362	6.225219
H	-2.093189	0.083976	5.626856
H	-1.304773	1.532042	6.271580
H	-1.370016	0.067820	7.257834
H	-9.079926	-1.939954	6.129866
H	-10.791133	-1.762234	4.294515
H	-11.277303	-0.168491	4.908090
H	-9.646875	-0.409729	4.244180
H	-11.379366	-2.810750	6.636529
H	-10.596171	-2.144890	8.075404
H	-11.847813	-1.203919	7.228629
H	-6.329705	0.522195	9.104365
H	-8.856986	1.364184	9.037155
H	-8.387216	2.074614	7.500731
H	-7.311745	2.122125	10.741379
H	-5.678537	2.629675	10.260864
H	-7.094095	3.451442	9.583473

YBSSTS2SR.xyz

128

scf done: -2432.651999

C	-3.638002	-1.528727	2.339205
C	-3.849731	-2.130948	3.610331

C	-2.986514	-3.178461	4.017175
C	-1.876555	-3.523872	3.249965
C	-1.587405	-2.884423	2.042751
C	-2.502067	-1.915144	1.616094
O	-4.837176	-1.766690	4.420537
Y	-5.532922	-1.723526	6.429707
C	-3.354970	-4.018712	5.206630
N	-3.422548	-3.328433	6.526193
C	-3.739103	-4.355449	7.535519
C	-4.152215	-3.760966	8.867505
N	-5.368565	-2.928340	8.771585
C	-5.349742	-1.949229	9.871665
C	-0.344147	-3.280764	1.235830
C	-0.440049	-4.766013	0.833843
C	-4.651045	-0.536938	1.743803
C	-4.783249	0.714475	2.629405
O	-6.819260	-3.428863	6.140695
C	-7.046641	-4.650517	6.610354
C	-7.464935	-5.731552	5.783103
C	-7.581846	-6.998752	6.370674
C	-7.336971	-7.270388	7.720154
C	-6.982833	-6.180513	8.518362
C	-6.848241	-4.896374	7.995773
C	-7.812678	-5.526789	4.297670
C	-6.581602	-5.048931	3.505589
C	-6.610279	-3.747635	8.939555
C	-7.468381	-8.670074	8.334840
C	-8.561325	-8.656499	9.421906
O	-6.187704	0.439132	6.148914
C	-7.846739	-9.732986	7.294203
C	-6.126715	-9.084139	8.971253
C	-8.317475	-6.815291	3.629067
C	-8.932840	-4.475819	4.173872
C	-2.121893	-2.719174	6.824362
C	-4.254588	-0.067949	0.335534
C	-6.026224	-1.227447	1.632448
C	-0.189253	-2.449542	-0.045203
C	0.917352	-3.068858	2.095910
H	-2.867579	-5.015357	7.690576
H	-4.549681	-4.977518	7.151420
H	-4.302749	-4.573753	9.595613
H	-3.345538	-3.134501	9.262017
H	-6.611059	-4.142957	9.969239
H	-7.438967	-3.038934	8.856626
H	-2.634713	-4.850520	5.287379
H	-4.343935	-4.461252	5.047006
H	-2.327389	-1.437721	0.660223
H	-1.238600	-4.331000	3.607686
H	-7.884861	-7.820455	5.735124
H	-6.817365	-6.318850	9.585899

H	-1.345750	-3.491226	6.958373
H	-1.825606	-2.080298	5.993455
H	-2.175661	-2.113073	7.730657
H	-5.208075	-2.443493	10.846492
H	-4.547125	-1.224114	9.712317
H	-6.303005	-1.419368	9.890339
H	-9.192510	-4.321546	3.119576
H	-9.834857	-4.806133	4.701769
H	-8.607562	-3.522683	4.592645
H	-6.839657	-4.923530	2.447138
H	-6.214160	-4.091512	3.878154
H	-5.773620	-5.787486	3.562513
H	-8.573572	-6.599940	2.586134
H	-7.556866	-7.603810	3.620741
H	-9.217258	-7.209364	4.114361
H	-7.918221	-10.713695	7.777014
H	-8.816689	-9.523104	6.831057
H	-7.097436	-9.809767	6.499050
H	-6.205506	-10.078716	9.426394
H	-5.331772	-9.116818	8.218475
H	-5.816124	-8.384850	9.754214
H	-8.663658	-9.647457	9.880486
H	-8.331108	-7.943218	10.219721
H	-9.530371	-8.376661	8.995515
H	-5.487891	1.424115	2.177990
H	-5.150874	0.453490	3.622520
H	-3.815657	1.222064	2.724795
H	-5.023100	0.613640	-0.044920
H	-3.303847	0.476949	0.332843
H	-4.176323	-0.901410	-0.371093
H	-6.767870	-0.528406	1.226284
H	-5.972156	-2.091712	0.961455
H	-6.369758	-1.569395	2.610467
H	0.718496	-2.754214	-0.577469
H	-1.033764	-2.591278	-0.727945
H	-0.102102	-1.379807	0.173250
H	1.817989	-3.357893	1.540902
H	1.019034	-2.017479	2.385771
H	0.886981	-3.665420	3.013253
H	0.446259	-5.071793	0.264789
H	-0.514934	-5.418642	1.709384
H	-1.323250	-4.943555	0.211272
O	-4.227923	0.210643	7.432810
O	-7.723898	-1.067772	7.802058
C	-5.328067	1.177268	6.784371
C	-3.222729	1.214976	7.080471
C	-8.368901	-0.042305	7.590417
O	-9.442638	0.009107	6.821615
C	-9.904989	-1.209750	6.159917
C	-11.002313	-1.823045	7.013195

C	-8.111122	1.282458	8.257038
C	-6.684831	1.482563	8.771763
O	-5.817875	2.020819	7.779997
C	-4.168731	1.938346	6.126811
C	-1.932799	0.684076	6.506835
C	-6.648164	2.470892	9.929179
C	-10.366712	-0.786858	4.778519
H	-3.019281	1.812331	7.978392
H	-4.032814	1.629592	5.090305
H	-4.230368	3.025054	6.204580
H	-2.116846	0.089949	5.607168
H	-1.297914	1.532107	6.225395
H	-1.377029	0.082112	7.231341
H	-9.054736	-1.893494	6.097459
H	-10.715703	-1.661600	4.222572
H	-11.189182	-0.067431	4.844844
H	-9.546909	-0.328750	4.219160
H	-11.380030	-2.730697	6.533366
H	-10.622103	-2.098524	8.000789
H	-11.836141	-1.124488	7.136897
H	-6.285471	0.519239	9.105284
H	-8.813333	1.328123	9.101791
H	-8.388088	2.090734	7.575522
H	-7.242398	2.104849	10.772660
H	-5.618920	2.618510	10.265219
H	-7.047750	3.442143	9.619850

YBSSTS2SP.xyz

128

scf done: -2432.694800

C	-3.334245	-1.421417	2.369604
C	-3.461973	-2.222063	3.537340
C	-2.729108	-3.432477	3.617491
C	-1.873689	-3.811683	2.585615
C	-1.714807	-3.038191	1.434047
C	-2.464707	-1.859250	1.364056
O	-4.243164	-1.877463	4.555244
Y	-4.485471	-2.133145	6.656320
C	-2.940529	-4.365842	4.778858
N	-2.659190	-3.807544	6.135741
C	-2.791114	-4.903663	7.115009
C	-2.824839	-4.422897	8.559329
N	-3.919897	-3.467773	8.832218
C	-3.501260	-2.530408	9.888230
C	-0.763487	-3.497909	0.320850
C	-1.227019	-4.863895	-0.222864
C	-4.128042	-0.114783	2.216552
C	-3.705767	0.874667	3.320954
O	-6.135640	-3.541212	6.777613
C	-6.345889	-4.783195	7.188525

C	-7.113667	-5.725655	6.449365
C	-7.190503	-7.034651	6.941711
C	-6.587471	-7.469531	8.128099
C	-5.896359	-6.505769	8.866153
C	-5.777906	-5.190500	8.423564
C	-7.859409	-5.313415	5.169406
C	-6.864411	-4.877696	4.076245
C	-5.158349	-4.150361	9.311771
C	-6.687749	-8.912050	8.642604
C	-7.411972	-8.925942	10.003754
O	-6.084684	-0.376813	7.151319
C	-7.464447	-9.823070	7.682093
C	-5.273455	-9.499747	8.816254
C	-8.703438	-6.459296	4.589656
C	-8.817907	-4.148050	5.488755
C	-1.320915	-3.200906	6.182440
C	-3.882410	0.572729	0.864764
C	-5.639876	-0.403533	2.315971
C	-0.716090	-2.510674	-0.853319
C	0.664344	-3.635564	0.885638
H	-1.958718	-5.619967	6.999433
H	-3.715276	-5.444518	6.893360
H	-2.902010	-5.300639	9.219173
H	-1.879527	-3.929111	8.805068
H	-4.943227	-4.603772	10.294043
H	-5.890234	-3.348813	9.479840
H	-2.311176	-5.258690	4.630394
H	-3.982998	-4.708566	4.802009
H	-2.367699	-1.244652	0.478265
H	-1.327813	-4.748054	2.689698
H	-7.759819	-7.754778	6.367884
H	-5.446850	-6.769112	9.822756
H	-0.534106	-3.955878	6.023036
H	-1.241961	-2.446256	5.398231
H	-1.159014	-2.708205	7.142994
H	-3.236657	-3.063031	10.816260
H	-2.656163	-1.934640	9.541359
H	-4.322505	-1.844075	10.112723
H	-9.343999	-3.833401	4.578751
H	-9.568750	-4.456290	6.224805
H	-8.270175	-3.293886	5.890582
H	-7.404241	-4.599747	3.162595
H	-6.272863	-4.016891	4.391797
H	-6.184995	-5.699517	3.821406
H	-9.233034	-6.100842	3.700259
H	-8.089064	-7.312271	4.280250
H	-9.456997	-6.817241	5.299833
H	-7.498844	-10.841400	8.084380
H	-8.498229	-9.487186	7.548873
H	-6.991082	-9.872111	6.695570

H	-5.325258	-10.528146	9.193706
H	-4.738038	-9.514401	7.860843
H	-4.676361	-8.916670	9.524650
H	-7.488252	-9.948896	10.391854
H	-6.882351	-8.325647	10.750279
H	-8.424849	-8.520621	9.909787
H	-4.299182	1.795794	3.256050
H	-3.844832	0.429683	4.307776
H	-2.649422	1.145337	3.212668
H	-4.480906	1.488977	0.813278
H	-2.833648	0.858763	0.728827
H	-4.178840	-0.061006	0.021795
H	-6.209474	0.530972	2.235282
H	-5.958052	-1.062165	1.500286
H	-5.886910	-0.887222	3.262175
H	-0.023483	-2.878803	-1.618000
H	-1.696951	-2.393268	-1.326340
H	-0.366640	-1.521035	-0.540032
H	1.358635	-3.971075	0.105813
H	1.024411	-2.676386	1.272692
H	0.708231	-4.362018	1.703265
H	-0.555232	-5.213081	-1.016349
H	-1.240900	-5.627628	0.561053
H	-2.238137	-4.795166	-0.637563
O	-3.308958	-0.594925	7.533663
O	-10.651439	-0.269935	7.691424
C	-5.871160	0.798297	7.467976
C	-3.406120	0.669910	8.063232
C	-10.207107	0.359127	6.753805
O	-10.817687	0.497246	5.569719
C	-12.093471	-0.181530	5.396626
C	-13.208503	0.705965	5.926104
C	-8.876254	1.081078	6.747854
C	-8.173523	1.021156	8.099853
O	-6.831396	1.577832	7.941236
C	-4.542108	1.479424	7.370149
C	-2.091311	1.440913	7.929706
C	-8.836210	1.846024	9.184132
C	-12.207354	-0.483787	3.914094
H	-3.657968	0.628751	9.144735
H	-4.287323	1.550970	6.305216
H	-4.625761	2.490160	7.777168
H	-1.821596	1.543297	6.873153
H	-2.150669	2.438686	8.379608
H	-1.292919	0.883599	8.428332
H	-12.050195	-1.106621	5.979672
H	-13.138791	-1.021641	3.713423
H	-12.210626	0.440310	3.327504
H	-11.372426	-1.104355	3.578053
H	-14.177413	0.217761	5.781605

H	-13.078335	0.891605	6.995003
H	-13.224082	1.663846	5.396296
H	-8.072457	-0.021902	8.408284
H	-9.032663	2.119286	6.433403
H	-8.254486	0.607977	5.980260
H	-9.836162	1.450016	9.371618
H	-8.260879	1.793595	10.112359
H	-8.915407	2.895845	8.884491

YBSSTS1M.xyz

128

scf done: -2432.649500

C	-5.604098	2.767980	-0.540046
C	-4.344418	3.318694	-0.199348
C	-3.899603	4.485632	-0.878563
C	-4.701810	4.979947	-1.914477
C	-5.922485	4.416381	-2.305502
C	-6.360876	3.307667	-1.577662
O	-3.634105	2.719751	0.741376
Y	-3.228147	0.936786	1.845811
O	-3.117242	-1.377686	2.625159
C	-3.582095	-1.972614	3.599821
C	-4.952121	-1.719018	4.147421
C	-5.173623	-0.274368	4.666004
C	-6.656086	-0.123617	5.025871
C	-2.604883	5.201723	-0.461440
C	-1.386512	4.276783	-0.646612
C	-6.775003	4.972550	-3.454530
C	-8.151198	5.409968	-2.914946
C	-6.172299	1.667849	0.309624
N	-5.423365	0.373990	0.362248
C	-5.078565	-0.119591	-0.989980
C	-3.652372	0.206640	-1.400864
N	-2.643930	-0.283461	-0.446159
C	-2.608685	-1.749084	-0.425049
O	-1.094730	0.882944	1.814731
C	-0.051958	0.268430	1.282267
C	1.164119	0.067054	1.993667
C	2.177962	-0.661650	1.359227
C	2.086494	-1.172069	0.058565
C	0.910419	-0.889902	-0.640962
C	-0.135818	-0.178083	-0.060004
C	1.381652	0.686615	3.384544
C	0.377938	0.114805	4.403353
C	-1.319200	0.238152	-0.886627
C	3.214663	-1.965483	-0.613941
C	3.722810	-1.194910	-1.848857
O	-4.746144	0.703629	3.761090
O	-2.933106	2.267184	3.671602
C	-3.867205	2.139644	4.498091

O	-3.614932	1.785267	5.818847
C	-4.680406	2.664239	6.310448
C	-4.145087	3.677443	7.294250
C	4.406823	-2.198124	0.324583
C	2.685506	-3.342396	-1.061068
C	2.793435	0.419691	3.929122
C	1.198825	2.215960	3.291690
C	-2.349912	6.472807	-1.286821
C	-2.709816	5.619049	1.020297
C	-6.302149	-0.594900	1.024955
C	-6.123663	6.185079	-4.133197
C	-6.974849	3.879717	-4.523570
C	-4.968577	3.132343	4.876441
O	-2.927831	-2.920369	4.243536
C	-1.580298	-3.288597	3.796205
C	-0.830133	-3.697206	5.048528
C	-1.703370	-4.400125	2.768259
H	-3.472001	-0.223498	-2.403172
H	-3.535745	1.289123	-1.487489
H	-5.762730	0.301105	-1.740116
H	-5.226943	-1.204061	-1.006504
H	-7.196805	1.456504	-0.040540
H	-6.253083	2.008148	1.351432
H	-1.150594	-0.068782	-1.933338
H	-1.405439	1.330735	-0.877278
H	3.095835	-0.828480	1.909080
H	0.798540	-1.212958	-1.675346
H	-4.353833	5.858753	-2.441724
H	-7.322990	2.850990	-1.806314
H	-2.467287	-2.160862	-1.439092
H	-1.776967	-2.074827	0.200489
H	-3.532184	-2.154492	-0.006734
H	-7.233175	-0.760536	0.457089
H	-5.788286	-1.554246	1.131486
H	-6.561401	-0.220781	2.017125
H	-1.790382	6.127800	1.334700
H	-3.546145	6.312613	1.165940
H	-2.859359	4.749099	1.662521
H	-0.464010	4.811616	-0.390865
H	-1.457505	3.400875	-0.000408
H	-1.303227	3.946827	-1.688967
H	-1.431606	6.952358	-0.931557
H	-2.214102	6.254695	-2.352209
H	-3.161761	7.201553	-1.185089
H	-6.762440	6.539242	-4.949620
H	-5.987837	7.018386	-3.435697
H	-5.146989	5.935788	-4.561527
H	-7.590533	4.254409	-5.350166
H	-6.012435	3.557676	-4.935461
H	-7.473852	2.996729	-4.111552

H	-8.775843	5.807313	-3.724157
H	-8.691618	4.574927	-2.457901
H	-8.041466	6.190529	-2.154805
H	0.530377	0.577932	5.385838
H	-0.648494	0.312453	4.092517
H	0.522655	-0.965952	4.518586
H	2.897568	0.898644	4.908830
H	2.991390	-0.649941	4.065184
H	3.571159	0.832582	3.277373
H	1.358185	2.675599	4.274854
H	1.925926	2.647216	2.594372
H	0.193535	2.468097	2.950737
H	5.177499	-2.780901	-0.191963
H	4.864947	-1.255774	0.642634
H	4.115227	-2.754999	1.221750
H	3.475795	-3.919796	-1.556039
H	2.329360	-3.920807	-0.201576
H	1.853372	-3.246405	-1.765709
H	4.526086	-1.749179	-2.349609
H	2.924820	-1.031246	-2.579947
H	4.113659	-0.213596	-1.560337
H	-4.582783	-0.174933	5.590074
H	-5.476712	2.060915	6.760960
H	-4.671693	4.163742	4.670467
H	-5.958239	2.932291	4.469221
H	-3.341671	4.266280	6.842032
H	-4.944823	4.357557	7.606680
H	-3.749896	3.181386	8.185797
H	-1.132730	-2.399832	3.344872
H	-0.707183	-4.697667	2.427758
H	-2.196960	-5.276728	3.199602
H	-2.270532	-4.066956	1.895498
H	0.196824	-3.968851	4.787894
H	-0.794074	-2.874529	5.766917
H	-1.305059	-4.560283	5.525559
H	-5.156928	-2.427169	4.953772
H	-5.658588	-1.919089	3.335160
H	-6.955350	-0.849542	5.790440
H	-6.858982	0.876898	5.414535
H	-7.292501	-0.273206	4.146581

YBSSTS1MR.xyz

128

scf done: -2432.670865

C	-5.667249	2.679107	-0.322832
C	-4.439085	3.282515	0.052941
C	-4.060948	4.503317	-0.576933
C	-4.915145	5.028828	-1.554951
C	-6.119607	4.437698	-1.951195
C	-6.473092	3.251567	-1.304309

O	-3.692132	2.682798	0.967762
Y	-3.244636	0.762698	1.881566
O	-2.971007	-1.661131	2.450160
C	-3.391617	-2.304077	3.412282
C	-4.605378	-1.946722	4.218838
C	-4.699106	-0.432363	4.544073
C	-5.940796	-0.191931	5.408356
C	-2.761986	5.234565	-0.196113
C	-1.540304	4.342942	-0.489043
C	-7.037157	5.036332	-3.025874
C	-8.409811	5.366820	-2.406777
C	-6.144642	1.450943	0.401190
N	-5.291931	0.229950	0.292330
C	-4.895375	-0.060440	-1.103281
C	-3.455483	0.338445	-1.397917
N	-2.493540	-0.245541	-0.447365
C	-2.435140	-1.703044	-0.594290
O	-1.091201	0.710959	2.041976
C	-0.033849	0.117127	1.517645
C	1.121228	-0.210695	2.285222
C	2.167836	-0.884090	1.643769
C	2.166867	-1.231446	0.287326
C	1.047753	-0.844524	-0.453399
C	-0.027037	-0.178233	0.129716
C	1.238734	0.217008	3.757801
C	0.132011	-0.441141	4.603781
C	-1.149453	0.331429	-0.729966
C	3.325675	-1.972192	-0.393374
C	3.899612	-1.104545	-1.531184
O	-4.729210	0.328780	3.393887
O	-2.713680	2.351317	3.796791
C	-3.502780	3.116527	4.297558
O	-3.320341	3.817526	5.436267
C	-4.675008	4.413552	5.328940
C	-4.616269	5.917405	5.268610
C	4.468203	-2.292547	0.580306
C	2.813642	-3.302063	-0.981797
C	2.587102	-0.177657	4.379727
C	1.113553	1.751812	3.852477
C	-2.574089	6.546739	-0.973610
C	-2.780508	5.583309	1.305112
C	-6.064701	-0.889519	0.848581
C	-6.465789	6.325588	-3.631578
C	-7.229693	4.019091	-4.168024
C	-4.894234	3.629613	4.025140
O	-2.806913	-3.416722	3.836316
C	-1.614629	-3.899470	3.141938
C	-0.779308	-4.602485	4.195080
C	-2.047708	-4.813876	2.008013
H	-3.208910	0.035746	-2.432028

H	-3.360102	1.426505	-1.347535
H	-5.552484	0.461100	-1.811564
H	-5.027754	-1.131653	-1.285272
H	-7.154237	1.203947	0.031837
H	-6.237501	1.648364	1.477274
H	-0.900949	0.146251	-1.789394
H	-1.247376	1.415954	-0.605625
H	3.038376	-1.140696	2.234341
H	1.003731	-1.049189	-1.522381
H	-4.621321	5.953660	-2.034242
H	-7.407919	2.752603	-1.555985
H	-2.208148	-1.988675	-1.635862
H	-1.651812	-2.094752	0.054091
H	-3.381924	-2.161586	-0.304047
H	-6.976538	-1.086279	0.260253
H	-5.452061	-1.795403	0.861250
H	-6.334084	-0.646054	1.877720
H	-1.860443	6.110168	1.585445
H	-3.629300	6.237623	1.537856
H	-2.851307	4.673035	1.902343
H	-0.612896	4.875647	-0.246885
H	-1.573929	3.432783	0.111504
H	-1.503577	4.069968	-1.549950
H	-1.643664	7.025027	-0.649275
H	-2.496476	6.380069	-2.053570
H	-3.389073	7.256316	-0.792175
H	-7.150083	6.710685	-4.395399
H	-6.339148	7.109503	-2.877285
H	-5.496671	6.154278	-4.112359
H	-7.889609	4.427449	-4.942785
H	-6.270432	3.770387	-4.634223
H	-7.677936	3.087174	-3.809059
H	-9.084500	5.787268	-3.162286
H	-8.890816	4.476269	-1.989995
H	-8.306089	6.097884	-1.597982
H	0.202992	-0.109529	5.647126
H	-0.853774	-0.173528	4.222944
H	0.235622	-1.532440	4.590537
H	2.616580	0.164048	5.420306
H	2.740403	-1.263074	4.386804
H	3.432424	0.284794	3.858657
H	1.192746	2.073450	4.898356
H	1.917978	2.236574	3.287831
H	0.154626	2.089164	3.456656
H	5.266545	-2.826133	0.052722
H	4.904580	-1.383333	1.007230
H	4.133323	-2.930067	1.405658
H	3.624685	-3.843711	-1.483719
H	2.412211	-3.947078	-0.192470
H	2.017645	-3.139050	-1.715420

H	4.729221	-1.618819	-2.031689
H	3.143311	-0.878899	-2.289490
H	4.273606	-0.151789	-1.142140
H	-3.814629	-0.186074	5.168295
H	-5.269076	4.056081	6.174688
H	-4.975685	4.219705	3.110214
H	-5.643445	2.835958	4.030609
H	-4.000921	6.249234	4.427499
H	-5.625694	6.322048	5.141679
H	-4.196840	6.327141	6.191785
H	-1.088984	-3.025300	2.748389
H	-1.167391	-5.194012	1.480828
H	-2.612846	-5.668024	2.394567
H	-2.667920	-4.276809	1.286325
H	0.150266	-4.964872	3.746460
H	-0.523045	-3.920114	5.009346
H	-1.317839	-5.458586	4.613517
H	-4.621555	-2.560687	5.123367
H	-5.483329	-2.213863	3.615637
H	-5.925076	-0.784529	6.330433
H	-5.999150	0.864838	5.685716
H	-6.847608	-0.441951	4.845421

YBSSTS1MP.xyz

128

scf done: -2432.658832

C	-5.525028	2.977462	-0.725486
C	-4.245592	3.477188	-0.376523
C	-3.701701	4.554541	-1.126104
C	-4.427079	5.005365	-2.236180
C	-5.663247	4.484296	-2.635805
C	-6.201607	3.471208	-1.838678
O	-3.606200	2.911007	0.637488
Y	-3.414712	1.094448	1.736137
O	-3.701805	-1.149601	2.741515
C	-4.034936	-1.885586	3.673519
C	-5.443078	-2.035269	4.181058
C	-5.868896	-0.912380	5.160329
C	-7.305389	-1.134895	5.617918
C	-2.386310	5.231090	-0.706361
C	-1.217331	4.227937	-0.746977
C	-6.432149	4.991966	-3.863465
C	-7.800787	5.549153	-3.423806
C	-6.206738	2.002518	0.193195
N	-5.579790	0.654923	0.374959
C	-5.299304	-0.011987	-0.915466
C	-3.867635	0.200068	-1.385940
N	-2.858020	-0.253834	-0.409349
C	-2.830658	-1.716651	-0.317105
O	-1.280161	1.032903	1.844348

C	-0.225904	0.439431	1.299289
C	1.027030	0.349531	1.966852
C	2.044161	-0.392357	1.353192
C	1.922102	-1.013136	0.104687
C	0.714172	-0.820994	-0.569464
C	-0.337746	-0.099208	-0.009193
C	1.280218	1.103597	3.283569
C	0.361238	0.583524	4.403340
C	-1.528742	0.248906	-0.861419
C	3.047467	-1.832250	-0.541446
C	3.450863	-1.193516	-1.885284
O	-5.790426	0.338939	4.516540
O	-4.287686	1.722529	3.592389
C	-4.653420	1.207442	4.745159
O	-3.595562	0.487612	5.447530
C	-3.769111	1.296265	6.642943
C	-2.485960	1.972603	7.068638
C	4.299517	-1.906173	0.343291
C	2.556223	-3.271563	-0.793732
C	2.728987	0.954946	3.774536
C	1.022601	2.608675	3.061976
C	-2.015700	6.407012	-1.623389
C	-2.539055	5.786358	0.725119
C	-6.520029	-0.151592	1.169383
C	-5.681122	6.106334	-4.604542
C	-6.652568	3.828825	-4.850908
C	-4.842622	2.148683	5.957111
O	-3.197004	-2.664271	4.329431
C	-1.769001	-2.640822	4.016439
C	-1.060636	-2.828626	5.344194
C	-1.482397	-3.748242	3.016802
H	-3.727818	-0.319396	-2.350627
H	-3.706338	1.265983	-1.565830
H	-5.982279	0.350605	-1.696905
H	-5.497488	-1.082021	-0.797168
H	-7.237786	1.849848	-0.165970
H	-6.275628	2.435330	1.200092
H	-1.347346	-0.116378	-1.886332
H	-1.621687	1.339686	-0.920128
H	2.989069	-0.477392	1.874817
H	0.580966	-1.221443	-1.573560
H	-4.002613	5.813963	-2.816951
H	-7.182541	3.058604	-2.070394
H	-2.692816	-2.177031	-1.309782
H	-1.996425	-2.015235	0.319401
H	-3.755233	-2.095245	0.123419
H	-7.497832	-0.241213	0.668248
H	-6.108393	-1.153067	1.311914
H	-6.660033	0.304202	2.152998
H	-1.602284	6.254509	1.051054

H	-3.327458	6.546504	0.761261
H	-2.792662	4.991399	1.429066
H	-0.279143	4.730817	-0.483061
H	-1.372839	3.411862	-0.040023
H	-1.098801	3.810671	-1.754132
H	-1.087722	6.863631	-1.263050
H	-1.843381	6.087644	-2.657491
H	-2.785461	7.186458	-1.626738
H	-6.263878	6.429949	-5.473783
H	-5.523093	6.983719	-3.968524
H	-4.705427	5.766847	-4.968236
H	-7.209702	4.169471	-5.731982
H	-5.694972	3.420149	-5.191184
H	-7.220771	3.012127	-4.394132
H	-8.365194	5.915955	-4.289555
H	-8.410375	4.785878	-2.929764
H	-7.675470	6.380097	-2.721812
H	0.542325	1.142950	5.329346
H	-0.692145	0.690675	4.140899
H	0.570289	-0.471895	4.609571
H	2.857132	1.535820	4.694426
H	2.985338	-0.085003	4.007086
H	3.452805	1.332831	3.044455
H	1.188126	3.161311	3.994956
H	1.707425	3.009628	2.306592
H	-0.001212	2.787328	2.729521
H	5.068257	-2.508814	-0.152565
H	4.726403	-0.914615	0.527770
H	4.087104	-2.372121	1.311555
H	3.339894	-3.871291	-1.272317
H	2.282593	-3.760424	0.147677
H	1.677680	-3.289959	-1.446531
H	4.252833	-1.769808	-2.362191
H	2.609853	-1.154518	-2.584600
H	3.807781	-0.169002	-1.737676
H	-5.193317	-0.943487	6.021631
H	-4.162431	0.675459	7.462181
H	-4.537230	3.173585	5.737089
H	-5.837540	2.136090	6.405434
H	-2.092603	2.591828	6.257361
H	-2.664315	2.609357	7.942540
H	-1.725213	1.232669	7.336923
H	-1.540597	-1.663164	3.586717
H	-0.421633	-3.738640	2.750092
H	-1.724884	-4.727488	3.441833
H	-2.061363	-3.611095	2.100221
H	0.021604	-2.840313	5.187663
H	-1.302638	-2.012073	6.028096
H	-1.351831	-3.777119	5.806700
H	-5.533140	-3.004263	4.679027

H	-6.120847	-2.011234	3.324159
H	-7.417759	-2.103214	6.116574
H	-7.597014	-0.348525	6.318966
H	-7.993615	-1.100333	4.767011

YBSSTS2M.xyz

128

scf done: -2432.657034

C	-7.635134	-5.663978	6.125944
C	-6.962690	-4.598081	6.790774
C	-6.654489	-4.747541	8.167846
C	-6.979976	-5.917224	8.850593
C	-7.624014	-6.984440	8.222811
C	-7.934213	-6.813364	6.870601
O	-6.586443	-3.478822	6.178037
Y	-5.204090	-1.837185	6.227277
C	-6.606376	0.387523	7.591714
O	-6.274528	1.707001	7.549547
C	-4.993176	2.070878	7.027141
C	-5.021537	3.579535	6.861526
C	-6.023894	-3.613447	8.927801
N	-4.656442	-3.188260	8.492244
C	-4.106201	-2.336238	9.558731
C	-7.961080	-8.256902	9.010767
C	-8.655057	-9.315932	8.143033
C	-8.050664	-5.574755	4.646724
C	-8.763143	-6.844748	4.154991
O	-4.584417	-1.680910	4.177662
C	-3.587769	-1.925422	3.341597
C	-2.816375	-3.101708	3.519604
C	-1.729657	-3.375170	2.693114
C	-1.363712	-2.523257	1.648475
C	-2.165556	-1.392277	1.456387
C	-3.272056	-1.066812	2.250480
C	-3.243552	-4.104453	4.553310
N	-3.208620	-3.629355	5.962575
C	-1.849009	-3.198319	6.295153
C	-4.145841	0.154798	1.923665
C	-3.656965	0.914452	0.680632
C	-0.159081	-2.860276	0.759155
C	0.087351	-1.797371	-0.319982
O	-6.692907	-0.153120	5.771417
C	-8.055028	0.241478	5.926746
C	-9.044819	-0.641991	5.201784
O	-5.822346	-0.462655	8.098013
C	-5.591017	-0.310543	1.650009
C	-4.145961	1.145989	3.103061
C	1.112434	-2.963303	1.624683
C	-0.399705	-4.209675	0.053115
C	-3.620900	-4.746758	6.826686

C	-3.757198	-4.346203	8.286667
C	-9.019313	-4.394366	4.456955
C	-6.819747	-5.361371	3.746346
C	-6.664834	-8.875273	9.571249
C	-8.901990	-7.906138	10.180280
C	-8.111647	0.232459	7.459532
C	-3.806325	1.611717	7.918058
C	-2.879783	0.712574	7.148598
O	-3.201909	-0.377561	6.678471
O	-1.675321	1.242831	6.999036
C	-0.665965	0.546573	6.202120
C	-0.017548	1.600689	5.324060
C	0.303412	-0.127183	7.157472
H	-2.890802	-5.574492	6.758362
H	-4.575194	-5.126139	6.455011
H	-4.109635	-5.216315	8.857128
H	-2.772488	-4.089356	8.689579
H	-5.971220	-3.905065	9.989886
H	-6.646485	-2.712203	8.873314
H	-2.607123	-5.002324	4.465326
H	-4.274484	-4.419141	4.362268
H	-1.924009	-0.728819	0.635807
H	-1.169333	-4.292215	2.871106
H	-8.439650	-7.622969	6.361024
H	-6.723529	-5.981745	9.907017
H	-1.146613	-4.050011	6.287912
H	-1.515622	-2.472009	5.554069
H	-1.820317	-2.727810	7.279159
H	-3.941389	-2.910884	10.485030
H	-3.151177	-1.909128	9.239165
H	-4.797552	-1.519404	9.763153
H	-9.331410	-4.320656	3.408093
H	-9.917859	-4.522821	5.070773
H	-8.533255	-3.460476	4.737204
H	-7.120191	-5.347318	2.691766
H	-6.335287	-4.410058	3.970830
H	-6.094268	-6.173046	3.875763
H	-9.038200	-6.713313	3.103007
H	-8.123160	-7.732048	4.217111
H	-9.685798	-7.045093	4.710602
H	-8.869618	-10.205134	8.745811
H	-9.607050	-8.953460	7.740754
H	-8.026688	-9.630749	7.302954
H	-6.885285	-9.784102	10.143995
H	-5.978436	-9.142802	8.760702
H	-6.140692	-8.182699	10.237549
H	-9.147909	-8.802983	10.761435
H	-8.447000	-7.181770	10.863297
H	-9.836959	-7.472084	9.810864
H	-4.754861	2.025504	2.858743

H	-4.563414	0.672909	3.992765
H	-3.127054	1.489897	3.318588
H	-4.327753	1.759179	0.489362
H	-2.647189	1.320259	0.811876
H	-3.659683	0.284181	-0.215262
H	-6.231629	0.552818	1.430801
H	-5.621136	-0.982510	0.785041
H	-5.997595	-0.836018	2.515864
H	0.960431	-2.074068	-0.921160
H	-0.765271	-1.704925	-1.000833
H	0.284210	-0.812114	0.116437
H	1.982516	-3.218496	1.007650
H	1.319971	-2.011692	2.126393
H	1.015563	-3.733158	2.396739
H	0.454663	-4.473085	-0.582253
H	-0.543633	-5.022510	0.771806
H	-1.293148	-4.163476	-0.578205
H	-8.160733	1.276325	5.566210
H	-8.418730	-0.740379	7.852860
H	-8.679402	1.033746	7.941295
H	-9.009857	-1.661702	5.591945
H	-10.064135	-0.257182	5.323483
H	-8.814827	-0.671890	4.132532
H	-1.188214	-0.193411	5.591658
H	1.075779	-0.656420	6.591515
H	0.792639	0.612759	7.798487
H	-0.209800	-0.854020	7.792434
H	0.750521	1.136014	4.699078
H	-0.754280	2.067691	4.665624
H	0.454648	2.379161	5.931260
H	-4.926008	1.594115	6.042256
H	-3.245125	2.467946	8.298121
H	-4.204476	1.035965	8.755409
H	-4.087694	3.924747	6.407625
H	-5.852765	3.875424	6.217288
H	-5.139623	4.072638	7.831784

YBSSTS2MR.xyz

128

scf done: -2432.664393

C	-7.570692	-5.628505	6.093046
C	-6.926147	-4.563986	6.784836
C	-6.585681	-4.753487	8.149525
C	-6.805736	-5.977140	8.777620
C	-7.376957	-7.059840	8.105907
C	-7.754070	-6.837643	6.778120
O	-6.609590	-3.405887	6.209106
Y	-5.148115	-1.827706	6.328022
C	-6.757353	0.446853	7.237278
O	-6.388535	1.779246	7.537655

C	-5.075237	2.158178	7.168800
C	-5.038374	3.677565	7.175235
C	-6.048489	-3.600872	8.951084
N	-4.695475	-3.083659	8.572155
C	-4.281185	-2.149037	9.631499
C	-7.586700	-8.397309	8.827919
C	-8.210612	-9.462566	7.916094
C	-8.120248	-5.454737	4.666834
C	-8.771091	-6.736583	4.122861
O	-4.551888	-1.602470	4.269986
C	-3.620720	-1.964067	3.398800
C	-2.950593	-3.201270	3.578502
C	-1.944082	-3.602399	2.703357
C	-1.559891	-2.822922	1.610398
C	-2.249442	-1.618315	1.431994
C	-3.268120	-1.161204	2.276560
C	-3.380027	-4.123874	4.684304
N	-3.223972	-3.585999	6.067573
C	-1.845728	-3.127716	6.270715
C	-3.999013	0.158786	1.985904
C	-3.496248	0.845520	0.707082
C	-0.451130	-3.304941	0.665807
C	-0.164915	-2.301250	-0.459545
O	-6.604586	0.218541	5.757472
C	-8.020410	0.541048	5.563418
C	-8.718162	-0.387637	4.605693
O	-6.083964	-0.482598	7.879683
C	-5.505182	-0.116698	1.803284
C	-3.787846	1.143082	3.152837
C	0.853029	-3.514070	1.460752
C	-0.868816	-4.640763	0.019516
C	-3.551942	-4.665886	7.015727
C	-3.699406	-4.168199	8.445717
C	-9.206285	-4.362686	4.701561
C	-7.012707	-5.051788	3.676038
C	-6.230423	-8.933253	9.327686
C	-8.524670	-8.191961	10.034050
C	-8.288763	0.426706	7.068660
C	-3.995923	1.559631	8.129952
C	-2.989792	0.752703	7.369643
O	-3.210251	-0.353145	6.869541
O	-1.825555	1.374150	7.245294
C	-0.758616	0.763404	6.456144
C	-0.110324	1.893058	5.677804
C	0.193529	0.060080	7.408368
H	-2.773271	-5.448715	6.987625
H	-4.486528	-5.129344	6.692228
H	-3.962516	-5.017758	9.092287
H	-2.738233	-3.788310	8.806087
H	-6.010663	-3.906369	10.009654

H	-6.721515	-2.738216	8.881010
H	-2.805822	-5.062330	4.605338
H	-4.439476	-4.381601	4.575169
H	-1.984076	-1.000080	0.583567
H	-1.461265	-4.561540	2.886100
H	-8.225357	-7.650988	6.241871
H	-6.527315	-6.071893	9.826245
H	-1.133706	-3.966509	6.193891
H	-1.594614	-2.391726	5.506875
H	-1.737592	-2.661578	7.251076
H	-4.158448	-2.667146	10.596489
H	-3.330238	-1.680731	9.363134
H	-5.038324	-1.370069	9.732986
H	-9.592791	-4.167614	3.693817
H	-10.045076	-4.671787	5.335023
H	-8.796834	-3.434897	5.102661
H	-7.428677	-4.957088	2.665758
H	-6.562658	-4.097023	3.949537
H	-6.228433	-5.816919	3.640045
H	-9.153207	-6.542706	3.114808
H	-8.056770	-7.564319	4.049100
H	-9.618277	-7.064711	4.734599
H	-8.329170	-10.399968	8.470220
H	-9.201981	-9.163628	7.559566
H	-7.581855	-9.670656	7.043723
H	-6.362524	-9.883256	9.859273
H	-5.546283	-9.104321	8.489630
H	-5.746897	-8.232890	10.016205
H	-8.680613	-9.137090	10.568074
H	-8.114762	-7.470684	10.748000
H	-9.501412	-7.818898	9.708857
H	-4.325691	2.080447	2.963183
H	-4.154168	0.713046	4.085862
H	-2.723088	1.381584	3.262690
H	-4.062863	1.769755	0.548370
H	-2.436676	1.118066	0.770866
H	-3.636856	0.218375	-0.179969
H	-6.043111	0.821571	1.618176
H	-5.672515	-0.776670	0.944696
H	-5.919836	-0.592227	2.693235
H	0.636034	-2.682618	-1.102379
H	-1.044323	-2.137555	-1.091199
H	0.159140	-1.331261	-0.067107
H	1.655149	-3.870316	0.803041
H	1.182618	-2.576625	1.921935
H	0.726456	-4.251943	2.259352
H	-0.083322	-5.009801	-0.651146
H	-1.055004	-5.413446	0.772004
H	-1.786998	-4.519300	-0.564613
H	-8.086928	1.579373	5.216182

H	-8.706704	-0.541820	7.353272
H	-8.829721	1.242994	7.549464
H	-8.631951	-1.423680	4.939729
H	-9.781288	-0.129033	4.545957
H	-8.290444	-0.308817	3.601968
H	-1.225576	0.045407	5.777689
H	1.009655	-0.402224	6.845004
H	0.625680	0.771382	8.119069
H	-0.319184	-0.725420	7.969663
H	0.696806	1.496134	5.055125
H	-0.836158	2.382912	5.023886
H	0.312454	2.641674	6.354994
H	-4.892581	1.798511	6.147217
H	-3.483085	2.349760	8.683016
H	-4.516985	0.891300	8.816560
H	-4.046724	4.038394	6.884470
H	-5.776427	4.076779	6.474991
H	-5.269324	4.060423	8.174626

YBSSTS2MP.xyz

128

scf done: -2432.692584

Y	-6.344603	-2.097009	5.809152
N	-5.970847	-2.873980	8.253878
N	-3.980795	-3.140573	6.029430
O	-7.385021	-3.972736	5.806716
O	-5.608703	-1.944513	3.814719
O	-5.127519	-0.023371	6.477345
C	-5.598414	1.115542	6.551392
O	-4.878963	2.196295	6.276506
C	-2.616218	2.009706	7.087871
C	-1.183085	1.641609	6.766782
O	-0.354301	2.066665	7.730856
C	1.058933	1.752105	7.577123
C	1.329211	0.366134	8.139899
C	-7.407204	-5.128424	6.454348
C	-7.675165	-6.368602	5.813420
C	-7.569124	-7.534270	6.582818
C	-7.251238	-7.555032	7.946276
C	-7.067601	-6.315637	8.563817
C	-7.150065	-5.122492	7.849386
C	-8.105636	-6.424539	4.338176
C	-6.992401	-5.882101	3.420987
C	-7.096170	-3.807503	8.575121
C	-7.128441	-8.849713	8.761273
C	-8.176998	-8.854181	9.891203
O	-7.849488	-0.650810	6.063183
C	-8.052815	0.709454	6.050634
C	-7.005829	1.433027	6.951245
O	-0.837197	1.026639	5.780019

C	-3.497703	2.030235	5.842194
C	-3.204279	3.186282	4.907357
C	-6.087616	-1.725367	9.165218
C	-4.647408	-3.516653	8.412517
C	-4.122012	-4.124948	7.118472
C	-4.523274	-2.136954	3.075014
C	-3.537561	-3.051058	3.525670
C	-2.369084	-3.249904	2.793991
C	-2.124968	-2.579815	1.593520
C	-3.123476	-1.704674	1.151799
C	-4.317063	-1.461457	1.841362
C	-3.795484	-3.887654	4.749377
C	-0.824871	-2.830124	0.817727
C	-0.742693	-4.316070	0.414950
C	-5.381077	-0.508575	1.272598
C	-5.601869	0.672147	2.238922
C	-2.835434	-2.254571	6.265501
C	-7.348612	-10.103821	7.904083
C	-5.718523	-8.937497	9.378707
C	-8.422845	-7.855752	3.877839
C	-9.383851	-5.581245	4.150354
C	-4.974724	0.082586	-0.086292
C	-6.707428	-1.269235	1.068601
C	-0.734684	-1.985002	-0.460052
C	0.384593	-2.479015	1.706798
C	-9.460453	1.071044	6.525748
C	1.812978	2.857368	8.292762
H	-3.153023	-4.613671	7.323023
H	-4.811238	-4.905972	6.785918
H	-4.689918	-4.302507	9.181072
H	-3.945357	-2.759975	8.777157
H	-7.072956	-4.006375	9.659551
H	-8.015306	-3.243794	8.366411
H	-2.960088	-4.596876	4.874454
H	-4.704852	-4.485483	4.608816
H	-2.967000	-1.182631	0.216534
H	-1.639627	-3.961438	3.178130
H	-7.750324	-8.480031	6.088231
H	-6.869274	-6.263523	9.633510
H	-1.904076	-2.832885	6.383607
H	-2.713931	-1.578298	5.419044
H	-2.994608	-1.654190	7.163012
H	-5.977185	-2.028203	10.219182
H	-5.323992	-0.981037	8.927923
H	-7.071070	-1.264766	9.039602
H	-9.696447	-5.598471	3.099147
H	-10.204685	-5.985800	4.753206
H	-9.215762	-4.543859	4.445765
H	-7.298640	-5.958254	2.370661
H	-6.778103	-4.833840	3.633495

H	-6.071511	-6.464828	3.540953
H	-8.754393	-7.831713	2.834246
H	-7.545917	-8.511185	3.926902
H	-9.226408	-8.310285	4.467646
H	-7.237941	-10.999785	8.524645
H	-8.352593	-10.128219	7.467373
H	-6.619918	-10.173781	7.089352
H	-5.610925	-9.854550	9.970402
H	-4.951119	-8.945122	8.597195
H	-5.512792	-8.089872	10.040334
H	-8.098765	-9.771156	10.487649
H	-8.046906	-8.004667	10.569327
H	-9.190921	-8.799683	9.481416
H	-6.366857	1.351384	1.842394
H	-5.927313	0.314640	3.217093
H	-4.674102	1.243289	2.361684
H	-5.773444	0.740710	-0.445645
H	-4.059871	0.682242	-0.020269
H	-4.823522	-0.693394	-0.844460
H	-7.477535	-0.590956	0.680635
H	-6.576543	-2.080067	0.343417
H	-7.061920	-1.700078	2.006334
H	0.210451	-2.190879	-0.974449
H	-1.546389	-2.214650	-1.158497
H	-0.765219	-0.912311	-0.240676
H	1.324001	-2.658211	1.169717
H	0.356814	-1.425577	2.004774
H	0.404704	-3.082129	2.619984
H	0.184302	-4.517496	-0.135627
H	-0.759993	-4.973846	1.289745
H	-1.586784	-4.593218	-0.225224
H	-7.929709	1.116490	5.028121
H	-7.149989	1.067357	7.975426
H	-7.148986	2.516190	6.942256
H	-9.613436	0.726830	7.554950
H	-9.646017	2.150438	6.482038
H	-10.191874	0.564827	5.890173
H	1.277566	1.762250	6.504791
H	2.393370	0.126382	8.051260
H	1.053733	0.318030	9.198382
H	0.765796	-0.390690	7.588667
H	2.890866	2.697878	8.194589
H	1.570315	3.834788	7.867054
H	1.563696	2.872506	9.358398
H	-3.414943	1.076199	5.319029
H	-2.644714	2.970928	7.610028
H	-2.989907	1.253299	7.788775
H	-2.182911	3.095715	4.529439
H	-3.886910	3.171015	4.054459
H	-3.310213	4.146219	5.422540

YBSRTS1S.xyz

128

scf done: -2432.654148

C	1.538337	0.129479	2.086969
C	0.259597	0.351865	1.506392
C	0.111308	0.191597	0.106562
C	1.193203	-0.188893	-0.683039
C	2.460286	-0.415702	-0.142195
C	2.588202	-0.245780	1.240138
O	-0.798483	0.705617	2.228098
Y	-2.918441	0.660349	2.293407
O	-2.615067	2.480824	4.009609
C	-3.297729	2.766494	4.987911
O	-3.104818	3.852081	5.723775
C	-2.029395	4.775240	5.360035
C	-2.573983	6.169420	5.607413
C	-1.209844	0.489199	-0.547403
N	-2.369020	-0.307026	-0.051125
C	-2.047090	-1.740612	-0.100063
C	3.627214	-0.821217	-1.052510
C	4.930629	-1.040147	-0.271670
C	1.767086	0.298393	3.596921
C	3.227559	0.046316	4.003540
O	-3.544882	2.525528	1.359309
C	-4.258196	3.049777	0.375444
C	-3.876850	4.227862	-0.327830
C	-4.667378	4.624466	-1.414472
C	-5.828244	3.963665	-1.832080
C	-6.221322	2.858864	-1.073343
C	-5.469729	2.410628	0.009309
C	-2.680533	5.080782	0.126398
C	-2.496066	6.340980	-0.733631
C	-5.993193	1.303098	0.875121
N	-5.177644	0.060485	0.981106
C	-5.985688	-0.914701	1.725358
C	-6.667181	4.417553	-3.033924
C	-6.062529	5.637420	-3.742269
O	-3.109768	-1.676018	2.693209
C	-3.480480	-1.883844	3.867397
C	-4.703717	-2.603384	4.441017
C	-3.727531	-3.048392	5.537367
C	-3.458466	-4.523422	5.710139
O	-3.777703	-0.075679	4.315981
C	-4.001333	0.432887	5.599556
C	-2.794002	0.283469	6.530642
O	-2.629357	-2.380912	4.832847
C	-4.847111	-0.500748	-0.347404
C	-3.525174	-0.001985	-0.912716
C	-6.762225	3.270338	-4.059430

C	-8.086318	4.793451	-2.563258
C	-2.928598	5.537737	1.577883
C	-1.364015	4.284640	0.064861
C	1.415906	1.739098	4.019039
C	0.893797	-0.705759	4.373967
C	3.283727	-2.134567	-1.782870
C	3.875994	0.287362	-2.094402
C	-4.428607	1.912700	5.493669
C	-0.808162	4.437483	6.197128
H	-4.859612	-0.092479	6.059714
H	-3.383253	-0.450350	-1.912615
H	-3.571298	1.080437	-1.051311
H	-5.646304	-0.275404	-1.070408
H	-4.812259	-1.589663	-0.247842
H	-6.999817	1.027204	0.517165
H	-6.111057	1.671608	1.904537
H	-1.107560	0.322606	-1.633097
H	-1.479080	1.542424	-0.408216
H	3.559622	-0.414894	1.686435
H	1.030186	-0.301917	-1.753805
H	-4.360777	5.506968	-1.961054
H	-7.142364	2.329673	-1.314594
H	-1.816485	-2.053699	-1.131757
H	-1.180082	-1.940121	0.529731
H	-2.878292	-2.331315	0.283701
H	-6.926267	-1.146602	1.198160
H	-5.410542	-1.829661	1.863996
H	-6.233011	-0.508451	2.709731
H	-2.083225	6.139173	1.935478
H	-3.833249	6.153217	1.641049
H	-3.046932	4.670508	2.230738
H	-0.523728	4.921558	0.367659
H	-1.391285	3.422199	0.732147
H	-1.165003	3.939072	-0.955997
H	-1.650206	6.919099	-0.345854
H	-2.273708	6.099222	-1.778958
H	-3.376793	6.992164	-0.710765
H	-6.686642	5.915539	-4.598565
H	-6.006976	6.507720	-3.079736
H	-5.055407	5.431076	-4.120094
H	-7.364656	3.572823	-4.924593
H	-5.767689	2.986779	-4.419989
H	-7.227012	2.378539	-3.626878
H	-8.703167	5.114539	-3.411254
H	-8.591610	3.947988	-2.085767
H	-8.051647	5.612728	-1.837473
H	1.038446	-0.578921	5.454555
H	-0.163961	-0.571908	4.147193
H	1.168209	-1.734994	4.117532
H	3.328868	0.188482	5.085253

H	3.550192	-0.976049	3.777385
H	3.919036	0.741462	3.514516
H	1.573930	1.862678	5.098284
H	2.060611	2.458772	3.501554
H	0.376950	1.974041	3.781937
H	5.731000	-1.328265	-0.962162
H	5.252920	-0.130164	0.245608
H	4.831643	-1.838717	0.471487
H	4.103608	-2.434043	-2.446986
H	3.111572	-2.944996	-1.066583
H	2.381223	-2.033934	-2.394001
H	4.702689	0.014081	-2.761450
H	2.991713	0.464447	-2.714599
H	4.131359	1.232174	-1.603247
H	-3.894701	-2.558648	6.503441
H	-5.048733	-3.415809	3.795173
H	-5.541479	-1.975023	4.740934
H	-4.314264	-5.009256	6.190900
H	-3.282438	-5.001245	4.741740
H	-2.577211	-4.684130	6.337989
H	-1.814976	4.623750	4.299796
H	0.003684	5.133009	5.963455
H	-1.034633	4.518678	7.265034
H	-0.454746	3.426329	5.982456
H	-1.816062	6.913222	5.344571
H	-3.461511	6.356574	4.997407
H	-2.837622	6.304745	6.661112
H	-3.015041	0.694069	7.522608
H	-2.512025	-0.763831	6.639547
H	-4.772066	2.295623	6.458182
H	-5.258470	1.990709	4.780594
H	-1.924217	0.804277	6.119254

YBSRTS1SR.xyz

128

scf done: -2432.672536

C	1.611111	0.070930	2.154225
C	0.338906	0.309941	1.558043
C	0.232746	0.211130	0.146016
C	1.335750	-0.134193	-0.630325
C	2.589626	-0.385586	-0.069677
C	2.682684	-0.270318	1.320985
O	-0.731050	0.627352	2.269399
Y	-2.902435	0.733107	2.228885
O	-2.275293	2.466860	3.926995
C	-3.107608	3.058846	4.611681
O	-2.776933	3.953142	5.538840
C	-1.366591	4.266392	5.739347
C	-1.300377	5.758683	6.007254
C	-1.067823	0.541654	-0.531945

N	-2.234871	-0.288162	-0.122411
C	-1.894621	-1.712755	-0.217246
C	3.778618	-0.752990	-0.967240
C	5.065848	-0.991305	-0.165455
C	1.813434	0.217944	3.669984
C	3.255214	-0.077585	4.109516
O	-3.541864	2.551918	1.243899
C	-4.348242	3.028419	0.304635
C	-4.089159	4.241330	-0.393590
C	-4.967534	4.603043	-1.423678
C	-6.098008	3.866315	-1.792194
C	-6.359519	2.713765	-1.047662
C	-5.520898	2.297243	-0.016746
C	-2.916689	5.158624	-0.004614
C	-2.859879	6.433669	-0.859889
C	-5.922216	1.123398	0.834242
N	-5.017519	-0.060992	0.852650
C	-5.712131	-1.124144	1.595696
C	-7.042134	4.284987	-2.926812
C	-6.573221	5.563470	-3.635445
O	-2.792040	-1.732086	2.690883
C	-2.821167	-2.383527	3.709771
C	-2.654773	-2.161622	5.188523
C	-2.918351	-3.673710	5.271613
C	-4.170299	-4.155490	5.955495
O	-4.263371	0.480887	3.907392
C	-4.949156	1.337907	4.742350
C	-4.753343	0.973721	6.218425
O	-3.057392	-3.706186	3.791562
C	-4.686313	-0.522338	-0.511568
C	-3.362111	0.035846	-1.011930
C	-7.119347	3.159006	-3.976876
C	-8.451067	4.542924	-2.356747
C	-3.084116	5.593610	1.465506
C	-1.567024	4.434928	-0.167507
C	1.483802	1.663867	4.091503
C	0.892247	-0.762286	4.422228
C	3.459099	-2.042317	-1.749492
C	4.044647	0.391369	-1.965274
C	-4.580255	2.832937	4.489964
C	-0.843482	3.417560	6.885822
H	-6.039373	1.290190	4.542210
H	-3.173642	-0.349971	-2.030376
H	-3.434190	1.123582	-1.088418
H	-5.478742	-0.244168	-1.221706
H	-4.646257	-1.615621	-0.500440
H	-6.921202	0.788532	0.506312
H	-6.018850	1.436780	1.881796
H	-0.927987	0.445729	-1.622248
H	-1.348503	1.584294	-0.337409

H	3.644287	-0.451988	1.783993
H	1.200418	-0.198529	-1.709141
H	-4.758760	5.516766	-1.965287
H	-7.247632	2.118778	-1.256670
H	-1.630968	-1.987719	-1.252356
H	-1.041306	-1.927179	0.426404
H	-2.730427	-2.329529	0.113652
H	-6.672764	-1.385811	1.121595
H	-5.082968	-2.015399	1.637867
H	-5.884472	-0.781658	2.618566
H	-2.258005	6.251735	1.762470
H	-4.021675	6.144064	1.602633
H	-3.087941	4.722640	2.122858
H	-0.741217	5.115073	0.074530
H	-1.503317	3.574401	0.499227
H	-1.427517	4.095530	-1.200230
H	-2.021920	7.054212	-0.524120
H	-2.697713	6.212659	-1.920690
H	-3.770887	7.034915	-0.767678
H	-7.269489	5.815623	-4.442700
H	-6.537957	6.418871	-2.952419
H	-5.580102	5.440664	-4.080723
H	-7.796247	3.436544	-4.793918
H	-6.131982	2.958405	-4.406263
H	-7.489840	2.225141	-3.542057
H	-9.144027	4.839744	-3.153308
H	-8.861652	3.650209	-1.874368
H	-8.427656	5.343080	-1.609494
H	1.017507	-0.646774	5.507116
H	-0.148132	-0.566777	4.157767
H	1.136094	-1.798722	4.160308
H	3.333252	0.042406	5.196005
H	3.560322	-1.102286	3.869160
H	3.974202	0.610440	3.651939
H	1.620601	1.783364	5.174085
H	2.154362	2.369159	3.587788
H	0.453766	1.916518	3.832847
H	5.884056	-1.248392	-0.847228
H	5.368701	-0.098351	0.391783
H	4.956531	-1.817271	0.545695
H	4.292948	-2.312987	-2.408626
H	3.280201	-2.878444	-1.064983
H	2.566667	-1.926220	-2.372563
H	4.887442	0.144567	-2.622415
H	3.173772	0.585583	-2.599126
H	4.283792	1.320347	-1.437128
H	-2.042040	-4.269411	5.540182
H	-3.421111	-1.500490	5.596876
H	-1.662308	-1.813585	5.480222
H	-4.052546	-4.071583	7.040659

H	-5.035548	-3.558083	5.653434
H	-4.366815	-5.203722	5.713737
H	-0.840227	4.012831	4.815664
H	0.207236	3.655916	7.077079
H	-1.413357	3.609720	7.800600
H	-0.908703	2.354284	6.642063
H	-0.259549	6.063780	6.151414
H	-1.710128	6.323725	5.165926
H	-1.863817	6.019693	6.908697
H	-5.306965	1.644466	6.885500
H	-5.110872	-0.046030	6.396375
H	-5.124878	3.498382	5.164423
H	-4.845745	3.077637	3.455136
H	-3.691878	1.015361	6.489008

YBSRTS1SP.xyz

128

scf done: -2432.660189

C	1.433615	0.258080	2.008748
C	0.113198	0.377314	1.496220
C	-0.103257	0.161363	0.112404
C	0.957830	-0.180033	-0.722471
C	2.265143	-0.305853	-0.249369
C	2.458903	-0.077192	1.116202
O	-0.924474	0.683309	2.272533
Y	-3.034149	0.658376	2.392557
O	-3.039364	2.403386	4.237305
C	-3.480988	2.538436	5.373946
O	-3.347333	3.646285	6.084037
C	-2.651641	4.791812	5.489952
C	-3.369389	6.024165	6.006203
C	-1.464181	0.373990	-0.496730
N	-2.583885	-0.399221	0.110178
C	-2.242916	-1.829642	0.163170
C	3.403004	-0.672694	-1.211548
C	4.759312	-0.775858	-0.500754
C	1.731974	0.479789	3.499815
C	3.228845	0.360233	3.827746
O	-3.499354	2.543880	1.399133
C	-4.119622	3.065093	0.353127
C	-3.606307	4.164017	-0.392550
C	-4.301860	4.552585	-1.545034
C	-5.490059	3.961207	-1.988898
C	-6.016523	2.944513	-1.187757
C	-5.364058	2.507959	-0.038234
C	-2.371835	4.948104	0.085672
C	-2.060215	6.156715	-0.811127
C	-6.040731	1.533689	0.883202
N	-5.356815	0.248168	1.195551
C	-6.261634	-0.511511	2.071152

C	-6.222055	4.398605	-3.264869
C	-5.495404	5.535289	-3.996190
O	-3.468864	-1.537171	2.850918
C	-3.629707	-1.662674	4.137016
C	-4.752448	-2.545334	4.743878
C	-3.619137	-3.259005	5.488809
C	-3.385020	-4.723028	5.189597
O	-3.634112	-0.250652	4.618029
C	-3.608144	0.091537	6.000815
C	-2.204734	0.054835	6.595134
O	-2.629072	-2.409672	4.856873
C	-5.081264	-0.556007	-0.013386
C	-3.785006	-0.181279	-0.718624
C	-6.329117	3.202511	-4.231706
C	-7.639509	4.889977	-2.909566
C	-2.651713	5.481754	1.505376
C	-1.114514	4.059897	0.118581
C	1.285180	1.893786	3.922857
C	0.991841	-0.583887	4.333792
C	3.106011	-2.034439	-1.870330
C	3.519260	0.405051	-2.307832
C	-4.254969	1.476116	6.116842
C	-1.187111	4.722795	5.884096
H	-4.251473	-0.611904	6.547585
H	-3.711955	-0.766027	-1.652206
H	-3.817891	0.872673	-1.001687
H	-5.914314	-0.467094	-0.730297
H	-5.036644	-1.604118	0.296607
H	-7.040901	1.303523	0.477426
H	-6.196709	2.023948	1.854908
H	-1.405223	0.123887	-1.569316
H	-1.750603	1.429770	-0.430382
H	3.462558	-0.166067	1.511310
H	0.745551	-0.340868	-1.778068
H	-3.894033	5.371327	-2.123504
H	-6.966252	2.479653	-1.449143
H	-2.055222	-2.220273	-0.850358
H	-1.344432	-1.967189	0.765218
H	-3.045864	-2.390903	0.639479
H	-7.222900	-0.722575	1.573673
H	-5.778311	-1.444418	2.358221
H	-6.470785	0.068052	2.975919
H	-1.779527	6.029868	1.883675
H	-3.507834	6.166123	1.500123
H	-2.868747	4.650439	2.179519
H	-0.247990	4.646918	0.447130
H	-1.235246	3.223048	0.807683
H	-0.886736	3.667586	-0.878946
H	-1.198688	6.694765	-0.400935
H	-1.801478	5.858108	-1.833153

H	-2.897176	6.861938	-0.859703
H	-6.049279	5.806485	-4.901561
H	-5.417392	6.434465	-3.375747
H	-4.485450	5.241972	-4.301804
H	-6.859532	3.490080	-5.147669
H	-5.334648	2.840548	-4.513922
H	-6.872825	2.365946	-3.781256
H	-8.178190	5.201623	-3.812588
H	-8.231165	4.107073	-2.424628
H	-7.595657	5.744557	-2.226252
H	1.172568	-0.423723	5.404483
H	-0.082983	-0.555308	4.153005
H	1.350187	-1.587565	4.079806
H	3.377995	0.542821	4.897830
H	3.621658	-0.638811	3.609759
H	3.831064	1.094421	3.281185
H	1.474404	2.042969	4.993814
H	1.849384	2.655713	3.373176
H	0.223131	2.043697	3.722230
H	5.537415	-1.040645	-1.225121
H	5.049189	0.173013	-0.036946
H	4.753526	-1.548561	0.275480
H	3.904868	-2.307349	-2.570575
H	3.030003	-2.824045	-1.115290
H	2.165504	-2.017590	-2.430005
H	4.323712	0.156406	-3.010660
H	2.592398	0.499490	-2.882220
H	3.739391	1.384119	-1.869433
H	-3.628422	-3.088264	6.575600
H	-5.244713	-3.155502	3.983550
H	-5.505048	-2.040900	5.355023
H	-4.167731	-5.339713	5.645597
H	-3.384059	-4.895543	4.109076
H	-2.418655	-5.046826	5.588179
H	-2.754235	4.706049	4.406008
H	-0.654766	5.584674	5.470589
H	-1.076302	4.740162	6.972957
H	-0.716212	3.818925	5.490605
H	-2.909138	6.920908	5.581578
H	-4.424291	6.013493	5.718800
H	-3.304789	6.087548	7.096937
H	-2.236441	0.333660	7.654380
H	-1.785545	-0.946389	6.498013
H	-4.351054	1.768971	7.165004
H	-5.262389	1.441668	5.684080
H	-1.539823	0.747625	6.071037

YBSRTS2S.xyz

128

scf done: -2432.654903

C	-5.550065	2.532386	0.001642
C	-4.339976	3.156867	0.393831
C	-3.994960	4.404021	-0.197687
C	-4.839136	4.912006	-1.193781
C	-6.013013	4.286818	-1.626938
C	-6.352946	3.091466	-0.989627
O	-3.578080	2.542244	1.288953
Y	-3.038112	0.664453	2.179914
O	-4.837350	0.120237	3.633958
C	-4.389160	-0.843339	4.342723
O	-4.237594	-0.670346	5.695360
C	-4.015193	0.651498	6.185139
C	-4.557354	0.688600	7.603112
C	-2.768909	5.202468	0.273890
C	-1.470449	4.399192	0.072946
C	-6.917938	4.863692	-2.724033
C	-8.316030	5.151692	-2.141978
C	-6.014530	1.300835	0.725400
N	-5.180069	0.065526	0.585046
C	-4.797680	-0.191250	-0.818551
C	-3.409421	0.322789	-1.156255
N	-2.366030	-0.161767	-0.233982
C	-2.182111	-1.611635	-0.366902
O	-0.882736	0.669379	2.167632
C	0.194039	0.237747	1.526138
C	1.418874	-0.077397	2.181555
C	2.482807	-0.545513	1.401240
C	2.427823	-0.719141	0.014239
C	1.222923	-0.382225	-0.605475
C	0.132683	0.093671	0.117976
C	1.577449	0.090653	3.699475
C	0.620813	-0.874535	4.426038
C	-1.102876	0.540593	-0.605088
C	3.607593	-1.240956	-0.816476
C	4.013028	-0.182924	-1.861976
O	-2.528602	2.201760	4.051196
C	-2.245668	2.171910	5.246911
C	-2.501301	0.985499	6.125463
O	-2.803493	-1.199305	3.654594
C	-3.112261	-2.569741	3.934549
C	-2.658395	-3.541842	2.867798
O	-1.722290	3.196046	5.899792
C	-1.475279	4.449717	5.187958
C	-0.176804	5.002772	5.743513
C	-2.672351	5.356920	5.415410
C	4.838522	-1.551899	0.046186
C	3.194089	-2.536613	-1.542201
C	3.001394	-0.217761	4.187769
C	1.267669	1.548307	4.093971
C	-2.606844	6.533573	-0.476398

C	-2.940842	5.526551	1.770509
C	-6.008504	-1.049104	1.065542
C	-6.367531	6.171368	-3.309293
C	-7.048127	3.845683	-3.874257
C	-4.615082	-2.346747	4.116864
H	-3.166837	0.024681	-2.192119
H	-3.401823	1.414493	-1.122675
H	-5.518273	0.264101	-1.512684
H	-4.842093	-1.271392	-0.991424
H	-7.032676	1.065245	0.373575
H	-6.083634	1.493080	1.803518
H	-0.942867	0.416165	-1.689399
H	-1.283320	1.606038	-0.424859
H	3.408424	-0.786315	1.908081
H	1.119742	-0.477170	-1.685562
H	-4.564963	5.853124	-1.652526
H	-7.273776	2.574945	-1.256514
H	-1.941580	-1.893442	-1.405673
H	-1.360448	-1.933675	0.274517
H	-3.088941	-2.141840	-0.068170
H	-6.905351	-1.181930	0.437727
H	-5.434546	-1.980338	1.042899
H	-6.314269	-0.848465	2.092737
H	-2.067369	6.079041	2.140081
H	-3.827672	6.149892	1.931303
H	-3.050472	4.607598	2.350141
H	-0.604171	4.996323	0.383704
H	-1.481563	3.482830	0.664482
H	-1.332108	4.139832	-0.983087
H	-1.732040	7.062597	-0.082937
H	-2.444461	6.386025	-1.549902
H	-3.473591	7.190578	-0.346000
H	-7.039349	6.537512	-4.093229
H	-6.288944	6.956539	-2.549865
H	-5.379247	6.030796	-3.760104
H	-7.699716	4.236369	-4.664977
H	-6.069528	3.629204	-4.315944
H	-7.475919	2.898682	-3.530074
H	-8.980146	5.559566	-2.913532
H	-8.784503	4.245436	-1.745374
H	-8.255067	5.878931	-1.325590
H	0.685983	-0.730013	5.512856
H	-0.413314	-0.730469	4.107399
H	0.898836	-1.913661	4.213795
H	3.053196	-0.057827	5.270671
H	3.289762	-1.257692	3.998948
H	3.747132	0.436153	3.722369
H	1.329930	1.666517	5.183349
H	1.995893	2.229169	3.638379
H	0.271412	1.837012	3.756082

H	5.650571	-1.924721	-0.587680
H	5.206983	-0.660570	0.565006
H	4.625818	-2.320864	0.796591
H	4.019877	-2.919096	-2.154377
H	2.915711	-3.313609	-0.822149
H	2.337236	-2.373146	-2.203480
H	4.851164	-0.541639	-2.471837
H	3.186975	0.054724	-2.539717
H	4.320071	0.748405	-1.374594
H	-1.374992	4.208531	4.127266
H	0.063830	5.945396	5.243064
H	-0.261923	5.195756	6.817553
H	0.647901	4.305715	5.576476
H	-2.514925	6.314061	4.910275
H	-3.584527	4.911141	5.010441
H	-2.812861	5.548874	6.484009
H	-2.649518	-2.847402	4.892968
H	-5.177458	-2.526939	3.199863
H	-5.098861	-2.850653	4.957234
H	-1.575862	-3.476113	2.723062
H	-2.901509	-4.569543	3.160627
H	-3.148956	-3.336512	1.911194
H	-1.985940	0.130513	5.677237
H	-2.089580	1.164581	7.120768
H	-4.577508	1.340471	5.546682
H	-5.623780	0.448471	7.608879
H	-4.035901	-0.035852	8.236856
H	-4.422188	1.685573	8.034057

YBSRTS2SR.xyz

128

scf done: -2432.656923

C	-5.544207	2.582752	0.008417
C	-4.322594	3.204551	0.367454
C	-3.990241	4.451507	-0.230821
C	-4.863939	4.967475	-1.196876
C	-6.053108	4.348315	-1.595198
C	-6.375197	3.149803	-0.955142
O	-3.534118	2.589267	1.241914
Y	-3.033420	0.715477	2.137777
O	-4.664871	-0.028680	3.516066
C	-4.201120	-0.972580	4.299023
O	-4.294391	-0.728620	5.678305
C	-4.119208	0.612799	6.107452
C	-4.745938	0.714326	7.487983
C	-2.741345	5.239493	0.197233
C	-1.459168	4.426256	-0.061033
C	-6.990575	4.933623	-2.659790
C	-8.370974	5.215490	-2.034110
C	-5.991538	1.343486	0.731544

N	-5.157916	0.113459	0.558113
C	-4.790132	-0.124047	-0.852734
C	-3.386911	0.357248	-1.180411
N	-2.363345	-0.159965	-0.253356
C	-2.219317	-1.613848	-0.386042
O	-0.880396	0.580970	2.178965
C	0.200769	0.165206	1.533866
C	1.429631	-0.137511	2.187819
C	2.490917	-0.612721	1.407934
C	2.432749	-0.796097	0.022368
C	1.230836	-0.451134	-0.598365
C	0.142108	0.030159	0.124215
C	1.602479	0.064875	3.700683
C	0.657531	-0.881362	4.464584
C	-1.077907	0.508230	-0.607016
C	3.608249	-1.330218	-0.806626
C	4.022430	-0.279716	-1.856330
O	-2.545729	2.203147	4.041804
C	-2.327433	2.179122	5.252769
C	-2.610721	0.998056	6.128891
O	-2.745939	-1.233611	3.910372
C	-2.953454	-2.663964	4.080832
C	-2.327730	-3.502617	2.993101
O	-1.841574	3.213110	5.921021
C	-1.559095	4.459002	5.211137
C	-0.293671	5.020744	5.831158
C	-2.767971	5.366639	5.361841
C	4.836548	-1.648275	0.057132
C	3.183521	-2.625034	-1.527292
C	3.033255	-0.226273	4.179634
C	1.289917	1.530437	4.063694
C	-2.598690	6.573128	-0.552539
C	-2.848585	5.557246	1.701224
C	-5.965108	-1.014912	1.046010
C	-6.458470	6.246640	-3.250155
C	-7.154356	3.924827	-3.813883
C	-4.474556	-2.484339	4.117352
H	-3.144285	0.061051	-2.216752
H	-3.351693	1.448430	-1.137998
H	-5.497398	0.367565	-1.534919
H	-4.866237	-1.198339	-1.049547
H	-7.018308	1.111548	0.403587
H	-6.037042	1.524039	1.813755
H	-0.909606	0.387910	-1.690470
H	-1.231719	1.577747	-0.422649
H	3.417971	-0.849539	1.913854
H	1.129300	-0.541945	-1.678952
H	-4.600926	5.909578	-1.660097
H	-7.304239	2.635898	-1.197126
H	-1.996826	-1.904942	-1.426226

H	-1.397672	-1.953594	0.246494
H	-3.136694	-2.120956	-0.077564
H	-6.874399	-1.148495	0.436783
H	-5.382352	-1.940052	0.999112
H	-6.239896	-0.833872	2.085187
H	-1.955082	6.098387	2.038031
H	-3.721735	6.188495	1.900986
H	-2.943953	4.636524	2.280332
H	-0.575006	5.015648	0.211097
H	-1.453278	3.511303	0.532401
H	-1.370395	4.163589	-1.121506
H	-1.706333	7.094455	-0.189495
H	-2.477514	6.430233	-1.632076
H	-3.455573	7.234954	-0.386397
H	-7.154565	6.619943	-4.009113
H	-6.355638	7.024935	-2.486532
H	-5.485046	6.110398	-3.733522
H	-7.828581	4.322090	-4.581999
H	-6.189116	3.711721	-4.285526
H	-7.572531	2.975255	-3.464978
H	-9.058428	5.626216	-2.783282
H	-8.825879	4.306145	-1.628905
H	-8.287080	5.938164	-1.215708
H	0.747335	-0.718122	5.546792
H	-0.381320	-0.729106	4.168577
H	0.922897	-1.926330	4.264619
H	3.096678	-0.039246	5.257503
H	3.323287	-1.269653	4.013519
H	3.771281	0.418380	3.689743
H	1.373530	1.675794	5.148277
H	2.002895	2.205471	3.576646
H	0.283769	1.803041	3.741703
H	5.644474	-2.032612	-0.575086
H	5.214295	-0.757771	0.570640
H	4.616644	-2.410865	0.811938
H	4.005366	-3.015978	-2.139395
H	2.900243	-3.397514	-0.804290
H	2.326936	-2.456964	-2.187771
H	4.858052	-0.647759	-2.464003
H	3.198852	-0.038556	-2.535847
H	4.336594	0.651235	-1.372809
H	-1.399847	4.207804	4.159959
H	-0.026528	5.958178	5.334435
H	-0.438047	5.225073	6.896701
H	0.539798	4.323059	5.718014
H	-2.583385	6.319199	4.857189
H	-3.655234	4.914889	4.910901
H	-2.968989	5.568098	6.418916
H	-2.555516	-2.961446	5.059512
H	-4.950496	-2.700481	3.159079

H	-5.020177	-2.960565	4.933232
H	-1.247852	-3.333442	2.945205
H	-2.497971	-4.565817	3.196212
H	-2.759200	-3.271281	2.014690
H	-2.045023	0.152920	5.725976
H	-2.262661	1.202960	7.143573
H	-4.653496	1.263666	5.406390
H	-5.805279	0.448613	7.441951
H	-4.250026	0.034443	8.188429
H	-4.657507	1.734771	7.874458

YBSRTS2SP.xyz

128

scf done: -2432.693315

C	-5.712891	1.714437	-0.673048
C	-4.698199	2.592185	-0.211263
C	-4.485366	3.813822	-0.909362
C	-5.237980	4.042892	-2.068216
C	-6.205523	3.163271	-2.569232
C	-6.435971	2.001573	-1.828446
O	-3.993567	2.236044	0.852062
Y	-2.976051	0.460458	1.592525
O	-3.344336	1.384752	3.803970
C	-3.633646	0.834847	4.868165
O	-3.719928	1.512038	6.003253
C	-3.411426	2.938714	5.980535
C	-4.634727	3.719040	5.531888
C	-3.484902	4.859882	-0.391038
C	-2.051158	4.295383	-0.406894
C	-7.013728	3.437947	-3.844678
C	-8.514400	3.513616	-3.499899
C	-6.084771	0.531472	0.174431
N	-5.072763	-0.553649	0.347414
C	-4.654964	-1.130488	-0.948101
C	-3.425816	-0.454726	-1.537700
N	-2.250739	-0.502656	-0.647658
C	-1.727040	-1.869977	-0.518141
O	-0.908570	0.942152	1.524437
C	0.214043	0.717486	0.851288
C	1.497101	0.788657	1.458385
C	2.614382	0.520092	0.659229
C	2.549238	0.185541	-0.698185
C	1.275219	0.127705	-1.266473
C	0.126259	0.392381	-0.524621
C	1.651683	1.150461	2.943712
C	0.948980	0.088829	3.813566
C	-1.211158	0.411125	-1.211415
C	3.790577	-0.102034	-1.553545
C	3.858499	0.903190	-2.720296
O	-0.873271	2.142980	6.993700

C	-1.669208	2.606689	7.780620
C	-2.974780	3.272915	7.395015
O	-3.154554	-1.250271	2.835675
C	-3.033320	-1.545076	4.179465
C	-3.381911	-3.007281	4.464927
O	-1.507575	2.623692	9.112054
C	-0.273586	2.058489	9.635880
C	-0.599062	1.569418	11.035044
C	0.819187	3.114729	9.598062
C	5.093820	0.014972	-0.751080
C	3.707600	-1.532531	-2.121752
C	3.121960	1.204887	3.386434
C	1.039089	2.540439	3.211985
C	-3.483507	6.139972	-1.240570
C	-3.865741	5.260749	1.049257
C	-5.699098	-1.604839	1.166779
C	-6.613243	4.757684	-4.518632
C	-6.784030	2.297780	-4.856455
C	-3.945943	-0.624901	5.030551
H	-3.189888	-0.929458	-2.506417
H	-3.654020	0.595880	-1.738676
H	-5.474607	-1.072455	-1.680666
H	-4.451588	-2.194457	-0.792495
H	-7.005375	0.079906	-0.232495
H	-6.316935	0.881888	1.189230
H	-1.064785	0.160737	-2.275026
H	-1.642135	1.420195	-1.175333
H	3.590027	0.576446	1.124915
H	1.159464	-0.118811	-2.321028
H	-5.063291	4.965402	-2.607621
H	-7.208443	1.299081	-2.139330
H	-1.489472	-2.303608	-1.503166
H	-0.814346	-1.848518	0.079734
H	-2.451340	-2.510561	-0.010772
H	-6.552094	-2.066185	0.642325
H	-4.960809	-2.363082	1.429546
H	-6.065175	-1.168690	2.099445
H	-3.148946	5.994000	1.439108
H	-4.861924	5.717453	1.070880
H	-3.867823	4.388918	1.705895
H	-1.341810	5.052395	-0.050745
H	-1.958105	3.419032	0.236212
H	-1.755427	4.018365	-1.425581
H	-2.779542	6.858635	-0.807177
H	-3.163525	5.952220	-2.271589
H	-4.468657	6.618556	-1.267041
H	-7.208400	4.904781	-5.426490
H	-6.790095	5.618955	-3.865732
H	-5.557676	4.761469	-4.810836
H	-7.364465	2.467723	-5.771303

H	-5.726311	2.229617	-5.132679
H	-7.085295	1.328033	-4.447543
H	-9.110381	3.703194	-4.400800
H	-8.874743	2.581438	-3.053412
H	-8.709293	4.320777	-2.786018
H	1.018755	0.358495	4.873864
H	-0.105664	0.004343	3.548181
H	1.418901	-0.892187	3.677479
H	3.166785	1.471831	4.447951
H	3.626512	0.239032	3.270418
H	3.691804	1.959857	2.833386
H	1.115116	2.787494	4.277467
H	1.573511	3.310423	2.643778
H	-0.012636	2.567427	2.923628
H	5.949163	-0.197286	-1.401883
H	5.231043	1.022136	-0.343330
H	5.126383	-0.697582	0.080108
H	4.580090	-1.751250	-2.749306
H	3.675358	-2.271121	-1.313659
H	2.812680	-1.672216	-2.736414
H	4.737412	0.708749	-3.346754
H	2.973066	0.841677	-3.360886
H	3.926454	1.930013	-2.345998
H	0.001219	1.221973	8.985639
H	0.284126	1.104536	11.483248
H	-0.911936	2.400375	11.675066
H	-1.403279	0.828926	11.012465
H	1.748523	2.708367	10.009305
H	1.014071	3.431470	8.570663
H	0.533158	3.987977	10.193195
H	-1.995638	-1.378782	4.527861
H	-4.981211	-0.775566	4.692968
H	-3.904352	-0.874756	6.094268
H	-2.737263	-3.654195	3.863179
H	-3.242306	-3.265627	5.521047
H	-4.422529	-3.213123	4.188630
H	-3.749560	3.006833	8.120901
H	-2.829999	4.357237	7.477845
H	-2.580091	3.079587	5.286124
H	-4.919505	3.436163	4.516423
H	-5.480206	3.543306	6.204697
H	-4.412225	4.790479	5.530907

YBSRTS1M.xyz

128

scf done: -2432.652668

C	-5.204894	-1.804222	4.264250
C	-5.242290	-0.394997	4.441376
C	-6.339447	0.179958	5.139778
C	-7.385021	-0.668593	5.528121

C	-7.402113	-2.048518	5.302444
C	-6.275059	-2.592995	4.681474
O	-4.254593	0.339808	3.941723
Y	-2.827747	0.363994	2.351427
O	-1.314802	-0.858778	3.831527
C	-0.754980	0.046254	4.482260
O	0.589880	0.011762	4.795728
C	0.368211	0.806026	6.015673
C	0.914468	0.106180	7.235541
C	-6.359438	1.674666	5.509180
C	-6.350299	2.563885	4.251256
C	-8.562672	-2.957373	5.728494
C	-8.059283	-3.993205	6.753509
C	-3.955133	-2.480965	3.757099
N	-3.494391	-2.207369	2.359755
C	-4.531902	-2.532739	1.363951
C	-5.478869	-1.377554	1.101179
N	-4.785050	-0.157741	0.656940
C	-4.348797	-0.280346	-0.737875
O	-3.243726	2.199740	1.279468
C	-4.098480	2.868814	0.514903
C	-3.809920	4.155482	-0.026944
C	-4.781410	4.776480	-0.820688
C	-6.021866	4.211281	-1.131725
C	-6.273574	2.944984	-0.602503
C	-5.352225	2.283551	0.205659
C	-2.456006	4.837516	0.217154
C	-1.360609	3.998880	-0.471682
C	-5.748052	0.968149	0.813728
C	-7.077111	4.915305	-1.994842
C	-8.349581	5.152279	-1.157161
O	-0.984676	1.468627	3.212347
C	0.076904	1.900894	2.406920
C	1.074176	2.773794	3.171422
O	-1.152689	-0.234044	0.709942
C	0.056242	0.015819	0.665309
O	0.809996	-0.349914	-0.360941
C	0.203171	-1.069028	-1.476854
C	-0.268761	-0.057619	-2.507833
C	-6.592097	6.273818	-2.519225
C	-7.428352	4.035562	-3.210773
C	-2.383261	6.254856	-0.373029
C	-2.177784	4.963912	1.728220
C	-7.601151	2.056318	6.330173
C	-5.120280	1.995504	6.369896
C	-2.325461	-3.071630	2.117579
C	-9.715047	-2.172611	6.371176
C	-9.120597	-3.695941	4.495830
C	0.836132	0.732350	1.724338
C	-1.144669	0.775316	5.763561

C	1.271733	-2.014559	-1.992600
H	-6.229076	-1.688292	0.352212
H	-6.020221	-1.140669	2.019703
H	-5.115093	-3.412252	1.681629
H	-4.026846	-2.815955	0.434204
H	-4.098356	-3.570623	3.853898
H	-3.110058	-2.199887	4.393182
H	-6.714489	0.665094	0.376896
H	-5.907468	1.077405	1.893152
H	-4.553005	5.756365	-1.219557
H	-7.221517	2.449375	-0.806727
H	-8.230279	-0.225558	6.038826
H	-6.208466	-3.668866	4.526160
H	-5.198568	-0.483346	-1.410468
H	-3.875105	0.650445	-1.053204
H	-3.622276	-1.090536	-0.836286
H	-2.602025	-4.137936	2.163117
H	-1.910584	-2.859835	1.128393
H	-1.560140	-2.865054	2.865128
H	-5.105641	3.060563	6.631918
H	-5.135713	1.417524	7.300903
H	-4.203535	1.758115	5.827588
H	-6.390363	3.621799	4.537870
H	-5.446559	2.408528	3.661009
H	-7.223738	2.358248	3.622113
H	-7.548028	3.119554	6.587969
H	-8.530262	1.902186	5.770164
H	-7.665838	1.493117	7.267505
H	-10.525392	-2.858976	6.640132
H	-9.400007	-1.661217	7.286938
H	-10.128763	-1.424249	5.686730
H	-9.943122	-4.361715	4.783779
H	-9.501494	-2.985071	3.754710
H	-8.354447	-4.307468	4.008694
H	-8.875244	-4.655719	7.066572
H	-7.262830	-4.619414	6.338917
H	-7.661773	-3.496667	7.644838
H	-0.363364	4.401078	-0.251238
H	-1.405619	2.960098	-0.137946
H	-1.497117	4.014985	-1.559249
H	-1.399830	6.684733	-0.152492
H	-2.505120	6.261780	-1.461716
H	-3.137869	6.918770	0.062612
H	-1.199337	5.432275	1.894518
H	-2.936146	5.599458	2.199547
H	-2.194808	3.991343	2.220651
H	-7.374570	6.734592	-3.132034
H	-6.361480	6.967141	-1.703542
H	-5.698266	6.172364	-3.144349
H	-8.187506	4.523364	-3.834084

H	-6.543123	3.856138	-3.830248
H	-7.825675	3.062134	-2.906605
H	-9.122911	5.647619	-1.757054
H	-8.767557	4.212115	-0.783796
H	-8.132500	5.785395	-0.290438
H	-0.352869	2.526209	1.612132
H	0.814742	1.796445	5.886202
H	-1.704013	0.129935	6.446084
H	-1.650481	1.729337	5.633384
H	0.685982	0.689780	8.133703
H	0.471964	-0.888501	7.345487
H	2.001154	-0.003784	7.168530
H	-0.649564	-1.627297	-1.080585
H	0.874984	-2.602940	-2.825215
H	2.143224	-1.457896	-2.349997
H	1.597606	-2.703292	-1.208485
H	-0.715950	-0.577272	-3.360936
H	-1.019870	0.613600	-2.084850
H	0.571661	0.540626	-2.872880
H	1.767412	1.085151	1.272865
H	1.106023	-0.001902	2.493173
H	1.768867	3.267183	2.482418
H	0.528392	3.548099	3.717277
H	1.661386	2.184520	3.880862

YBSRTS1MR.xyz

128

scf done: -2432.671550

C	-4.954176	-1.673373	4.405773
C	-5.008525	-0.264336	4.563594
C	-6.084975	0.303402	5.298000
C	-7.086710	-0.561202	5.758865
C	-7.082751	-1.946916	5.564691
C	-5.980334	-2.480453	4.892075
O	-4.047479	0.469905	4.014364
Y	-2.907221	0.544673	2.198623
O	-0.402454	-2.290422	5.072479
C	-0.274574	-1.333544	5.788371
O	0.774477	-1.065314	6.615986
C	0.147127	0.197973	7.060099
C	-0.105719	0.198354	8.546594
C	-6.138247	1.810567	5.601389
C	-6.257840	2.623455	4.297667
C	-8.201244	-2.869745	6.067083
C	-7.619003	-3.903601	7.051561
C	-3.719336	-2.308334	3.826158
N	-3.377380	-2.015382	2.398716
C	-4.467084	-2.416757	1.483309
C	-5.457696	-1.295665	1.205175
N	-4.835960	-0.117846	0.572198

C	-4.499704	-0.389233	-0.828984
O	-3.473355	2.423671	1.353766
C	-4.237061	2.983910	0.424257
C	-3.951161	4.263290	-0.127591
C	-4.789798	4.742438	-1.141191
C	-5.903181	4.051977	-1.633098
C	-6.183559	2.818684	-1.041268
C	-5.386300	2.288479	-0.029703
C	-2.776978	5.108416	0.393649
C	-1.443337	4.378957	0.140614
C	-5.802407	1.015724	0.654569
C	-6.806236	4.597751	-2.747666
C	-8.243421	4.761501	-2.214419
O	-0.938860	0.892717	2.889379
C	0.296440	1.149193	2.325716
C	1.390803	1.274019	3.386258
O	-1.505179	-0.106747	0.277893
C	-0.274677	-0.058287	0.170489
O	0.331167	-0.088600	-1.006162
C	-0.473217	-0.177253	-2.222974
C	-0.823636	1.226141	-2.685767
C	-6.334635	5.962239	-3.268393
C	-6.814859	3.613050	-3.933748
C	-2.688242	6.479653	-0.294289
C	-2.952465	5.360418	1.905312
C	-7.336656	2.185712	6.487316
C	-4.858886	2.229738	6.354151
C	-2.160843	-2.789747	2.088161
C	-9.315787	-2.100101	6.789358
C	-8.832370	-3.610275	4.871235
C	0.681275	0.029356	1.320207
C	-1.034099	-0.066552	6.116079
C	0.367460	-0.957322	-3.216275
H	-6.273772	-1.685975	0.571719
H	-5.908254	-0.975583	2.148888
H	-5.013543	-3.279879	1.893041
H	-4.013958	-2.753897	0.545518
H	-3.809174	-3.402326	3.931221
H	-2.838754	-2.011080	4.406318
H	-6.767589	0.686083	0.234344
H	-5.965737	1.203716	1.723510
H	-4.562753	5.711886	-1.565876
H	-7.054668	2.248089	-1.359864
H	-7.915693	-0.126283	6.302308
H	-5.897749	-3.557050	4.749938
H	-5.394343	-0.680474	-1.404393
H	-4.076743	0.510201	-1.278461
H	-3.760245	-1.188909	-0.896635
H	-2.349952	-3.873355	2.151382
H	-1.818072	-2.550922	1.078595

H	-1.378390	-2.543535	2.809806
H	-4.878875	3.306149	6.563612
H	-4.786521	1.701519	7.311897
H	-3.969122	2.007285	5.762591
H	-6.314373	3.695141	4.523835
H	-5.397416	2.462656	3.646541
H	-7.169755	2.351241	3.753420
H	-7.308419	3.261179	6.692890
H	-8.294776	1.972312	6.000480
H	-7.316686	1.665114	7.451119
H	-10.090181	-2.798651	7.124451
H	-8.941219	-1.574739	7.674379
H	-9.794592	-1.365912	6.132678
H	-9.625658	-4.287801	5.209552
H	-9.271376	-2.900540	4.161717
H	-8.092735	-4.209176	4.330285
H	-8.405233	-4.575925	7.415312
H	-6.846271	-4.520261	6.582063
H	-7.167972	-3.406924	7.916947
H	-0.606132	4.969592	0.533190
H	-1.438955	3.403867	0.630049
H	-1.279242	4.237755	-0.934003
H	-1.848041	7.040668	0.129286
H	-2.514100	6.393431	-1.372778
H	-3.593320	7.076658	-0.138483
H	-2.111047	5.949267	2.291099
H	-3.873113	5.922979	2.095650
H	-3.002103	4.419802	2.455959
H	-7.003473	6.305797	-4.065056
H	-6.342178	6.723226	-2.480866
H	-5.322994	5.911516	-3.685287
H	-7.466011	3.978983	-4.736765
H	-5.806655	3.488954	-4.343792
H	-7.177732	2.624090	-3.636479
H	-8.906147	5.146825	-2.998650
H	-8.657860	3.809892	-1.867008
H	-8.268404	5.461305	-1.372648
H	0.277773	2.100666	1.760297
H	0.789912	1.028136	6.753633
H	-2.009845	-0.216764	6.583333
H	-1.127247	0.590962	5.246295
H	-0.609115	1.125598	8.839213
H	-0.740603	-0.645592	8.833626
H	0.834400	0.129122	9.101498
H	-1.384216	-0.726509	-1.969362
H	-0.185405	-1.079997	-4.152217
H	1.300202	-0.428990	-3.435367
H	0.614030	-1.949926	-2.829513
H	-1.407617	1.175862	-3.610030
H	-1.418714	1.752749	-1.936286

H	0.084307	1.803590	-2.885373
H	1.693227	0.161340	0.929301
H	0.640310	-0.922777	1.865096
H	2.359719	1.530769	2.943264
H	1.116616	2.065361	4.090166
H	1.500691	0.337228	3.943043

YBSRTS1MP.xyz

128

scf done: -2432.658821

C	-5.262972	-1.793375	4.323805
C	-5.365318	-0.383343	4.462945
C	-6.452945	0.157355	5.200775
C	-7.434811	-0.729875	5.661806
C	-7.396108	-2.114250	5.468410
C	-6.273486	-2.621209	4.808585
O	-4.445893	0.384068	3.888083
Y	-2.953064	0.362460	2.365685
O	-1.421231	-0.648582	3.724929
C	-0.771806	0.338153	4.280481
O	0.622850	0.119761	4.559015
C	0.485597	0.619584	5.919516
C	0.981455	-0.379506	6.939414
C	-6.528634	1.659205	5.529341
C	-6.634881	2.504935	4.246035
C	-8.493895	-3.064621	5.964749
C	-7.895199	-4.071973	6.966651
C	-3.996558	-2.422210	3.796835
N	-3.586061	-2.156553	2.381223
C	-4.648514	-2.496309	1.416783
C	-5.564582	-1.319623	1.130229
N	-4.837185	-0.130628	0.650616
C	-4.389777	-0.307646	-0.735193
O	-3.273817	2.258054	1.344583
C	-4.083358	2.912105	0.519661
C	-3.764783	4.193173	-0.020865
C	-4.679131	4.797326	-0.891600
C	-5.891907	4.221282	-1.280635
C	-6.179106	2.966274	-0.743269
C	-5.317398	2.321574	0.141286
C	-2.433895	4.886651	0.305755
C	-1.293201	4.052280	-0.311212
C	-5.770346	1.027697	0.758531
C	-6.879634	4.896829	-2.240782
C	-8.233758	5.098675	-1.532067
O	-0.956226	1.519269	3.358091
C	0.101093	1.944468	2.493050
C	1.136820	2.793016	3.225591
O	-1.244874	-0.058394	0.681524
C	-0.030345	0.146641	0.642751

O	0.717639	-0.228483	-0.385031
C	0.094369	-0.921385	-1.508456
C	-0.355404	0.110705	-2.528754
C	-6.385297	6.268720	-2.719305
C	-7.085843	4.005235	-3.481558
C	-2.331818	6.302222	-0.284634
C	-2.252706	5.023952	1.830530
C	-7.742224	2.003601	6.407228
C	-5.262822	2.071453	6.308601
C	-2.395863	-2.984674	2.117862
C	-9.639729	-2.321052	6.665236
C	-9.087415	-3.833665	4.767795
C	0.785197	0.800346	1.718775
C	-1.027066	0.784120	5.736593
C	1.140634	-1.885966	-2.034391
H	-6.329929	-1.624165	0.394763
H	-6.089037	-1.042732	2.047807
H	-5.252712	-3.342199	1.779630
H	-4.170647	-2.831318	0.490014
H	-4.086663	-3.514699	3.918012
H	-3.145203	-2.089034	4.400480
H	-6.730898	0.744488	0.296988
H	-5.957737	1.160617	1.830448
H	-4.426727	5.771720	-1.289428
H	-7.111192	2.466759	-1.002890
H	-8.274395	-0.314897	6.204381
H	-6.159983	-3.696591	4.678900
H	-5.236557	-0.526262	-1.406348
H	-3.906337	0.608234	-1.078619
H	-3.669962	-1.127016	-0.800210
H	-2.630776	-4.058627	2.196428
H	-2.021706	-2.782002	1.110156
H	-1.616966	-2.726077	2.836468
H	-5.292370	3.143486	6.538878
H	-5.196859	1.523385	7.255165
H	-4.363530	1.866780	5.724892
H	-6.731980	3.567157	4.501269
H	-5.747384	2.387240	3.623376
H	-7.518184	2.221387	3.662207
H	-7.728871	3.075310	6.633101
H	-8.691803	1.787873	5.904728
H	-7.727599	1.466261	7.361757
H	-10.400703	-3.038356	6.991453
H	-9.293381	-1.781922	7.553407
H	-10.126588	-1.602780	5.997009
H	-9.866377	-4.529802	5.101793
H	-9.535705	-3.143443	4.045001
H	-8.323834	-4.416670	4.242972
H	-8.666193	-4.763467	7.327277
H	-7.098814	-4.669981	6.512787

H	-7.469951	-3.553600	7.832361
H	-0.312682	4.448825	-0.017075
H	-1.367555	3.009183	0.003456
H	-1.351445	4.080206	-1.405436
H	-1.368914	6.740707	0.000338
H	-2.378660	6.304287	-1.379001
H	-3.119435	6.961740	0.095459
H	-1.286573	5.492666	2.056899
H	-3.038780	5.663573	2.247364
H	-2.306077	4.055795	2.328730
H	-7.122176	6.711441	-3.398358
H	-6.246156	6.963957	-1.884662
H	-5.437968	6.193396	-3.264010
H	-7.797815	4.466862	-4.176577
H	-6.140523	3.853781	-4.013754
H	-7.477352	3.019362	-3.211143
H	-8.955794	5.576611	-2.205232
H	-8.664528	4.147662	-1.203491
H	-8.118971	5.734163	-0.647798
H	-0.415702	2.590379	1.778844
H	1.019653	1.573852	6.022047
H	-1.628601	0.056965	6.285752
H	-1.434531	1.787908	5.860529
H	0.826067	0.004593	7.953726
H	0.445907	-1.328375	6.839029
H	2.051289	-0.571383	6.808157
H	-0.770611	-1.464138	-1.116975
H	0.729583	-2.456597	-2.872374
H	2.024300	-1.345954	-2.387371
H	1.451240	-2.589719	-1.257487
H	-0.815156	-0.390190	-3.386348
H	-1.090706	0.794630	-2.098424
H	0.498115	0.692986	-2.889261
H	1.703920	1.173146	1.257910
H	1.081652	0.019067	2.428939
H	1.765322	3.324652	2.502833
H	0.624503	3.537601	3.840247
H	1.779168	2.182966	3.863234

YBSRTS2M.xyz

128

scf done: -2432.660855

C	-5.262385	2.697026	0.198806
C	-4.019637	3.307531	0.510459
C	-3.564242	4.387752	-0.293717
C	-4.330046	4.732260	-1.415389
C	-5.525428	4.102125	-1.778110
C	-5.979627	3.089668	-0.929464
O	-3.325046	2.843190	1.543021
Y	-2.894487	1.026586	2.579537

O	-2.150830	1.396874	4.718907
C	-3.161414	1.723863	5.424453
O	-3.460330	0.975081	6.539348
C	-3.045804	-0.386813	6.527134
C	-3.025098	-0.851769	7.972063
C	-2.295938	5.179160	0.071193
C	-1.048849	4.275603	0.020586
C	-6.335433	4.490966	-3.022081
C	-7.747270	4.946404	-2.602454
C	-5.881543	1.714650	1.158409
N	-5.197474	0.410012	1.405245
C	-5.024144	-0.357801	0.157723
C	-3.738066	-0.012505	-0.571216
N	-2.535924	-0.250878	0.243288
C	-2.257628	-1.686404	0.341780
O	-0.785443	0.940888	2.251565
C	0.220372	0.528163	1.496871
C	1.552457	0.422207	1.987437
C	2.533701	-0.068366	1.117423
C	2.291758	-0.448009	-0.208018
C	0.982074	-0.301487	-0.670103
C	-0.035474	0.183672	0.147166
C	1.910030	0.861783	3.416551
C	1.143297	0.005249	4.443275
C	-1.398442	0.438656	-0.430301
C	3.384400	-0.983874	-1.142811
C	3.517793	-0.057490	-2.367852
O	-3.104877	-1.284721	3.421390
C	-3.340130	-1.860241	4.486989
C	-4.030637	-1.229649	5.656771
O	-4.543867	1.621912	4.343025
C	-4.984248	2.840137	4.983748
C	-5.560370	3.895943	4.064009
O	-2.986337	-3.113038	4.718643
C	-2.250030	-3.857925	3.696562
C	-2.668103	-5.306429	3.862743
C	-0.763415	-3.620636	3.890832
C	4.755378	-1.062019	-0.457082
C	3.008870	-2.401188	-1.619078
C	3.409126	0.713324	3.719335
C	1.541924	2.347141	3.607251
C	-2.050122	6.357577	-0.884570
C	-2.446866	5.762600	1.491260
C	-6.059426	-0.347035	2.327214
C	-5.682947	5.634510	-3.810920
C	-6.453968	3.272079	-3.958577
C	-3.640780	3.157555	5.636077
H	-3.690218	-0.593249	-1.510001
H	-3.755594	1.044040	-0.847080
H	-5.876741	-0.192493	-0.520376

H	-5.033464	-1.422592	0.413012
H	-6.906138	1.497277	0.811307
H	-5.965039	2.180304	2.144070
H	-1.390811	0.143567	-1.493645
H	-1.628838	1.509931	-0.393211
H	3.544544	-0.154219	1.495429
H	0.736244	-0.555429	-1.700222
H	-3.972888	5.542343	-2.037994
H	-6.927449	2.593256	-1.132997
H	-2.105893	-2.133826	-0.655056
H	-1.351602	-1.840582	0.929708
H	-3.086375	-2.198728	0.834096
H	-7.056523	-0.526021	1.892020
H	-5.599199	-1.311985	2.552625
H	-6.167274	0.216855	3.256469
H	-1.548331	6.329290	1.763596
H	-3.304192	6.443401	1.541841
H	-2.588028	4.967169	2.225027
H	-0.152295	4.858835	0.262948
H	-1.119508	3.454973	0.735888
H	-0.910765	3.859298	-0.984002
H	-1.157354	6.902657	-0.559647
H	-1.872547	6.026963	-1.914060
H	-2.884999	7.067041	-0.889126
H	-6.291772	5.873172	-4.689830
H	-5.599114	6.546757	-3.210740
H	-4.682307	5.365710	-4.165910
H	-7.041881	3.522931	-4.849760
H	-5.464479	2.936532	-4.287316
H	-6.944847	2.428321	-3.463062
H	-8.342224	5.218624	-3.482448
H	-8.286818	4.157928	-2.068351
H	-7.695089	5.818810	-1.942752
H	1.401899	0.317421	5.463026
H	0.065957	0.119994	4.314254
H	1.415346	-1.052064	4.338312
H	3.603132	1.053824	4.742416
H	3.745901	-0.327417	3.650550
H	4.027667	1.319941	3.048772
H	1.786671	2.669262	4.627026
H	2.107036	2.975069	2.909228
H	0.476157	2.506930	3.439806
H	5.499895	-1.450085	-1.160928
H	5.098928	-0.077351	-0.122852
H	4.739935	-1.730712	0.410320
H	3.773780	-2.798199	-2.297555
H	2.919907	-3.085877	-0.768643
H	2.053765	-2.408684	-2.153882
H	4.291934	-0.427310	-3.051232
H	2.581185	0.007738	-2.930477

H	3.790551	0.957389	-2.060278
H	-2.567761	-3.470680	2.725262
H	-2.169665	-5.922048	3.108396
H	-2.386966	-5.681407	4.851466
H	-3.748730	-5.422010	3.741590
H	-0.199060	-4.185031	3.142189
H	-0.511861	-2.564043	3.775887
H	-0.445191	-3.955239	4.883111
H	-5.726766	2.577666	5.752056
H	-3.032833	3.837328	5.033122
H	-3.653709	3.482267	6.679381
H	-6.527805	3.591396	3.651418
H	-5.725567	4.820881	4.628961
H	-4.873915	4.107925	3.239804
H	-4.793962	-0.546329	5.275925
H	-4.498914	-2.011361	6.259109
H	-2.036591	-0.431006	6.104082
H	-2.339456	-0.233357	8.556786
H	-4.022252	-0.779201	8.418116
H	-2.692389	-1.892751	8.029279

YBSRTS2MR.xyz

128

scf done: -2432.663913

C	-5.204170	2.816803	0.107898
C	-3.920747	3.393917	0.282431
C	-3.554239	4.508199	-0.519702
C	-4.449493	4.912700	-1.518378
C	-5.691703	4.312653	-1.754582
C	-6.053723	3.268743	-0.899757
O	-3.110135	2.864586	1.188325
Y	-2.713449	1.087870	2.302831
O	-3.258867	1.768080	4.246328
C	-4.023899	1.888096	5.313152
O	-3.528948	1.180244	6.443906
C	-2.800924	0.004075	6.172050
C	-2.202412	-0.462088	7.488451
C	-2.245377	5.274823	-0.267467
C	-1.021356	4.363107	-0.477636
C	-6.648963	4.770162	-2.863404
C	-7.970265	5.259848	-2.238305
C	-5.708428	1.809921	1.105013
N	-4.987385	0.502996	1.223042
C	-4.825152	-0.165941	-0.086091
C	-3.485754	0.136113	-0.745993
N	-2.331871	-0.236668	0.094098
C	-2.177271	-1.692712	0.152955
O	-0.589718	0.995449	2.217281
C	0.413873	0.455809	1.534108
C	1.708207	0.285275	2.098386

C	2.683596	-0.350565	1.320909
C	2.473295	-0.806174	0.014748
C	1.208645	-0.575068	-0.530440
C	0.193911	0.046756	0.194079
C	2.038198	0.813980	3.504470
C	1.175518	0.096418	4.560161
C	-1.105184	0.379629	-0.490408
C	3.563351	-1.490422	-0.821646
C	3.909697	-0.604771	-2.035247
O	-2.824495	-1.192332	3.282668
C	-3.060466	-1.755581	4.357501
C	-3.710433	-1.096000	5.532062
O	-5.419523	1.466810	5.051335
C	-5.932849	2.637813	5.736985
C	-7.010339	3.350470	4.951645
O	-2.752513	-3.024192	4.576542
C	-2.107085	-3.803947	3.523050
C	-2.578953	-5.232113	3.722248
C	-0.601778	-3.635708	3.631188
C	4.850541	-1.729103	-0.020068
C	3.056627	-2.857324	-1.322420
C	3.509468	0.589143	3.886425
C	1.774418	2.332840	3.561062
C	-2.086496	6.480776	-1.206075
C	-2.243580	5.807958	1.180467
C	-5.784988	-0.340939	2.131584
C	-6.066423	5.916157	-3.702299
C	-6.943990	3.589510	-3.809685
C	-4.531734	3.257457	5.799736
H	-3.440776	-0.387085	-1.717618
H	-3.421283	1.206998	-0.952807
H	-5.630651	0.130777	-0.773397
H	-4.928782	-1.244484	0.069682
H	-6.763319	1.591753	0.870626
H	-5.687836	2.244076	2.112918
H	-1.031946	0.080868	-1.549626
H	-1.270577	1.463275	-0.471563
H	3.663974	-0.491014	1.757766
H	0.997979	-0.868756	-1.557617
H	-4.161596	5.748381	-2.143598
H	-7.030424	2.796782	-0.998190
H	-2.047638	-2.120801	-0.855164
H	-1.296798	-1.938454	0.748360
H	-3.051703	-2.150574	0.619096
H	-6.781227	-0.551943	1.710212
H	-5.269722	-1.288874	2.303584
H	-5.912179	0.174493	3.088135
H	-1.310517	6.347309	1.383892
H	-3.076505	6.502700	1.336555
H	-2.334052	4.990405	1.898313

H	-0.096595	4.936603	-0.341416
H	-1.016611	3.540510	0.238639
H	-1.011122	3.951455	-1.493716
H	-1.155584	7.004676	-0.963920
H	-2.028413	6.181802	-2.258816
H	-2.905275	7.200426	-1.097026
H	-6.776631	6.197724	-4.487315
H	-5.875324	6.808126	-3.096441
H	-5.129883	5.627159	-4.191097
H	-7.636773	3.893572	-4.603390
H	-6.023786	3.228123	-4.281174
H	-7.398561	2.748085	-3.277068
H	-8.670809	5.582511	-3.018030
H	-8.460179	4.472330	-1.657027
H	-7.792911	6.106957	-1.567524
H	1.380359	0.501475	5.558660
H	0.113897	0.227358	4.345079
H	1.403276	-0.975727	4.579676
H	3.687921	1.000265	4.886037
H	3.772991	-0.474046	3.918143
H	4.194865	1.093661	3.196874
H	1.997401	2.717434	4.563786
H	2.416574	2.860161	2.847000
H	0.734552	2.561570	3.323371
H	5.588678	-2.239835	-0.647993
H	5.301409	-0.790373	0.318439
H	4.670245	-2.357875	0.858660
H	3.824076	-3.354833	-1.927309
H	2.808323	-3.513734	-0.481409
H	2.160960	-2.756459	-1.943506
H	4.682605	-1.077624	-2.653249
H	3.034675	-0.431038	-2.669533
H	4.283043	0.371720	-1.709722
H	-2.459950	-3.408747	2.566938
H	-2.151470	-5.874133	2.946541
H	-2.261262	-5.613899	4.697184
H	-3.668779	-5.298988	3.662554
H	-0.106818	-4.242256	2.866491
H	-0.306716	-2.595027	3.479749
H	-0.246812	-3.966505	4.612200
H	-6.310215	2.355168	6.729774
H	-4.363252	4.034999	5.051298
H	-4.163341	3.572868	6.776808
H	-7.873255	2.695723	4.789632
H	-7.356551	4.234523	5.498609
H	-6.632527	3.676595	3.977477
H	-4.622107	-0.605158	5.179641
H	-3.986226	-1.852033	6.270689
H	-1.994291	0.243255	5.468977
H	-1.549511	0.312121	7.899431

H -2.991525 -0.670277 8.218085
H -1.614076 -1.373636 7.341510

YBSRTS2MP.xyz

128

scf done: -2432.696748

C -0.193586 0.172104 -0.140443
C -0.061646 0.721490 1.162002
C 1.225621 0.727096 1.769112
C 2.286591 0.138800 1.070780
C 2.168124 -0.441433 -0.196980
C 0.902357 -0.398618 -0.784397
O -1.133833 1.217545 1.765846
Y -3.273520 1.023002 1.778162
O -3.028928 -1.144561 2.943543
C 1.451350 1.379276 3.142792
C 1.041103 2.865240 3.087178
C 3.346976 -1.080181 -0.943569
C 3.026283 -2.556445 -1.250243
C -1.499122 0.293728 -0.879128
N -2.663662 -0.421268 -0.277894
C -2.342458 -1.839688 -0.091117
O -3.876681 2.710966 0.597815
C -4.677472 3.034614 -0.406770
C -5.858005 2.271776 -0.600779
C -6.683699 2.508148 -1.697761
C -6.400508 3.509652 -2.629772
C -5.267135 4.293026 -2.382052
C -4.401784 4.108131 -1.296622
C -6.286038 1.296953 0.461592
N -5.421055 0.101718 0.711889
C -6.122291 -0.748988 1.689509
C -3.218842 5.059341 -1.050548
C -3.376977 5.716423 0.336470
C -7.325953 3.727086 -3.834907
C -7.386704 2.437783 -4.677889
C -1.880777 4.297038 -1.107975
C -3.149828 6.187299 -2.092145
C -8.744804 4.077409 -3.344016
C -6.844591 4.865226 -4.744896
C -5.142986 -0.657262 -0.526067
C -3.823823 -0.255917 -1.175081
C 0.617240 0.649677 4.213570
C 2.920653 1.324804 3.588710
C 3.588119 -0.329762 -2.268499
C 4.647520 -1.036255 -0.129690
H -3.683152 -0.844733 -2.098601
H -3.876530 0.796053 -1.468670
H -5.951621 -0.516560 -1.257916
H -5.129327 -1.722598 -0.275657

H	-7.298567	0.936161	0.216249
H	-6.352296	1.819650	1.425137
H	-1.356433	-0.072493	-1.909663
H	-1.791401	1.348661	-0.950458
H	3.261105	0.140381	1.542185
H	0.752604	-0.806165	-1.783313
H	-5.044305	5.099266	-3.068928
H	-7.579931	1.899147	-1.808220
H	-2.132842	-2.329939	-1.056525
H	-1.458660	-1.929233	0.541635
H	-3.169854	-2.359074	0.395660
H	-7.087928	-1.103901	1.294715
H	-5.513881	-1.615787	1.954546
H	-6.311673	-0.169955	2.597004
H	-2.531355	6.385731	0.536526
H	-4.296211	6.311359	0.378932
H	-3.416480	4.961864	1.124321
H	-1.043795	4.991784	-0.967653
H	-1.824874	3.539560	-0.325064
H	-1.750959	3.812253	-2.082772
H	-2.309422	6.846796	-1.850518
H	-2.985186	5.805949	-3.106334
H	-4.057678	6.800522	-2.097998
H	-7.528296	4.973633	-5.593878
H	-6.818910	5.824868	-4.217917
H	-5.845063	4.669354	-5.147535
H	-8.052663	2.569959	-5.539191
H	-6.393113	2.170837	-5.053768
H	-7.761808	1.590399	-4.095013
H	-9.420971	4.229296	-4.194090
H	-9.167223	3.282057	-2.721866
H	-8.734469	4.995727	-2.747726
H	0.754031	1.123625	5.193625
H	-0.441566	0.681756	3.952923
H	0.928031	-0.398290	4.298600
H	3.019672	1.815259	4.563272
H	3.283427	0.296798	3.701211
H	3.581815	1.848148	2.889486
H	1.183575	3.335643	4.068024
H	1.659363	3.405527	2.361842
H	-0.004871	2.974178	2.796303
H	5.456275	-1.508280	-0.698079
H	4.955602	-0.008580	0.089854
H	4.552708	-1.574327	0.819741
H	3.853170	-3.027734	-1.795263
H	2.863435	-3.120033	-0.325130
H	2.125126	-2.655525	-1.863860
H	4.424075	-0.776848	-2.820064
H	2.707378	-0.359891	-2.917734
H	3.826420	0.722422	-2.081510

O	-4.134546	1.342465	3.671041
C	-3.080279	-1.355805	4.155838
C	-4.375362	0.720281	4.874838
C	-3.258704	-0.305281	5.209218
O	-2.957731	-2.579148	4.664312
C	-2.711535	-3.692149	3.760161
C	-3.495051	-4.863805	4.324298
C	-4.992851	-4.676559	4.191035
O	-5.523702	-3.936493	3.388148
C	-4.487718	1.734405	6.014201
C	-1.214804	-3.939252	3.689254
O	-5.648749	-5.457446	5.056718
C	-7.104153	-5.429105	5.014418
C	-7.569475	-5.766754	6.418374
C	-7.592134	-6.406764	3.957596
H	-7.400040	-4.411648	4.740787
H	-8.662065	-5.737391	6.466389
H	-7.239753	-6.769524	6.707476
H	-7.174422	-5.050205	7.143539
H	-8.686131	-6.410574	3.927111
H	-7.226719	-6.120854	2.968134
H	-7.251649	-7.422193	4.183962
H	-5.329183	0.153825	4.838508
H	-2.312137	0.248629	5.268011
H	-3.426070	-0.792777	6.173312
H	-5.275688	2.454159	5.776390
H	-4.727311	1.255618	6.970901
H	-3.548087	2.287559	6.119825
H	-3.237308	-5.046059	5.371780
H	-3.228450	-5.774033	3.772349
H	-3.110003	-3.417805	2.781894
H	-0.699055	-3.055875	3.304829
H	-0.808922	-4.178515	4.676879
H	-1.002189	-4.775438	3.015919

YBRSTS1S.xyz

128

scf done: -2432.649753

C	-0.085673	-0.152426	0.050713
C	-0.022401	0.247243	1.409002
C	1.188726	0.036222	2.126910
C	2.225800	-0.640148	1.471940
C	2.160425	-1.092770	0.148417
C	0.982765	-0.813504	-0.549219
O	-1.081107	0.823755	1.951537
Y	-3.221681	0.818331	1.977850
O	-2.882722	1.901179	3.972558
C	-3.997530	2.034460	4.536364
C	-5.007717	3.178760	4.458239
C	-5.158159	2.937913	5.966278

C	-4.771086	4.049552	6.911483
C	1.376793	0.594702	3.547903
C	1.193451	2.126508	3.514091
C	3.315911	-1.824004	-0.548087
C	2.833024	-3.198648	-1.051381
C	-1.280568	0.251059	-0.765203
N	-2.586467	-0.325744	-0.335549
C	-2.498895	-1.789765	-0.337895
O	-3.710236	2.660256	1.017837
C	-4.402986	3.235273	0.045324
C	-5.621240	2.633511	-0.355736
C	-6.356952	3.156328	-1.416745
C	-5.936635	4.291930	-2.113358
C	-4.754370	4.896726	-1.671006
C	-3.974229	4.421702	-0.608992
C	-6.174273	1.492251	0.450134
N	-5.379748	0.226782	0.491896
C	-6.218741	-0.778519	1.157763
C	-2.715088	5.174457	-0.148404
C	-2.868284	5.571243	1.334305
C	-6.770182	4.832504	-3.283595
C	-6.910216	3.743093	-4.365356
O	-3.079188	-1.491351	2.755281
C	-3.204721	-1.940580	3.899603
O	-2.796197	-3.151052	4.234005
C	-2.168067	-4.000476	3.219935
C	-2.518024	-5.424090	3.611402
O	-4.922167	0.636692	3.746721
C	-5.181839	-0.523341	4.494961
C	-6.176283	-0.313836	5.639673
C	-3.885890	-1.205413	5.011936
C	-1.464291	4.289810	-0.314187
C	-2.479158	6.463331	-0.951578
C	-8.172297	5.227971	-2.779379
C	-6.133118	6.067343	-3.935146
C	-5.025723	-0.243863	-0.865192
C	-3.615331	0.141456	-1.280149
C	0.352354	-0.015702	4.523984
C	2.777256	0.304069	4.108938
C	3.804296	-0.989929	-1.749154
C	4.511105	-2.054837	0.386943
O	-4.121871	1.898681	5.911254
C	-0.676169	-3.724599	3.184203
H	-3.422730	-0.265913	-2.289542
H	-3.540165	1.229642	-1.352379
H	-5.730940	0.155273	-1.607960
H	-5.132929	-1.333013	-0.889046
H	-7.180379	1.252557	0.066511
H	-6.291192	1.798750	1.497660
H	-1.104291	-0.023562	-1.819554

H	-1.400562	1.340232	-0.728642
H	3.140771	-0.812690	2.024815
H	0.886416	-1.099344	-1.596003
H	-4.419677	5.792756	-2.177313
H	-7.289609	2.664347	-1.689487
H	-2.339648	-2.179169	-1.358005
H	-1.658051	-2.096674	0.285098
H	-3.408635	-2.234155	0.070205
H	-7.112621	-1.023999	0.560683
H	-5.646647	-1.695537	1.325715
H	-6.540669	-0.385127	2.122996
H	-1.973998	6.106004	1.676490
H	-3.730834	6.234276	1.468523
H	-3.002481	4.687141	1.960136
H	-0.566016	4.846610	-0.021712
H	-1.525192	3.398572	0.312093
H	-1.341335	3.983634	-1.359785
H	-1.586465	6.967338	-0.566227
H	-2.307906	6.263163	-2.015246
H	-3.316513	7.164447	-0.863280
H	-6.756248	6.408062	-4.769152
H	-6.043199	6.900295	-3.229890
H	-5.136839	5.848555	-4.334062
H	-7.509623	4.109182	-5.207546
H	-5.928370	3.447388	-4.750121
H	-7.400473	2.845335	-3.975376
H	-8.785565	5.613579	-3.602774
H	-8.700718	4.374905	-2.342061
H	-8.104790	6.006059	-2.011800
H	0.501224	0.396337	5.529655
H	-0.665855	0.217805	4.210961
H	0.475728	-1.103049	4.587378
H	2.859580	0.736539	5.112036
H	2.973243	-0.770757	4.198207
H	3.568312	0.747839	3.494573
H	1.327330	2.545204	4.519110
H	1.935629	2.587929	2.852909
H	0.195476	2.389619	3.159532
H	5.303099	-2.589644	-0.148881
H	4.935671	-1.111207	0.745273
H	4.235193	-2.657366	1.259193
H	3.643661	-3.730876	-1.563641
H	2.491855	-3.821207	-0.217087
H	2.001530	-3.102315	-1.756851
H	4.629038	-1.496926	-2.264823
H	3.005479	-0.825922	-2.479262
H	4.159439	-0.007671	-1.420593
H	-5.659073	-1.243395	3.808832
H	-6.114048	2.486240	6.252449
H	-4.528897	4.124471	4.193440

H	-5.883889	3.005670	3.836644
H	-3.808013	4.482567	6.625619
H	-5.529625	4.839447	6.890860
H	-4.692527	3.678448	7.937917
H	-2.621494	-3.739544	2.259436
H	-2.103922	-6.120718	2.876635
H	-2.099621	-5.670902	4.591760
H	-3.601371	-5.568204	3.649917
H	-0.199194	-4.385315	2.453621
H	-0.465666	-2.693113	2.893292
H	-0.226275	-3.916817	4.163083
H	-3.207832	-0.437093	5.400384
H	-4.094815	-1.907926	5.822546
H	-5.728984	0.233577	6.470517
H	-7.041828	0.243999	5.269483
H	-6.531353	-1.280574	6.013753

YBRSTS1SR.xyz

128

scf done: -2432.672480

C	0.049995	-0.116167	0.254460
C	0.027457	0.125217	1.652635
C	1.193167	-0.185877	2.411425
C	2.270346	-0.785363	1.747702
C	2.288736	-1.075497	0.378304
C	1.154729	-0.710205	-0.350233
O	-1.056192	0.653369	2.195292
Y	-3.210073	0.693808	2.006626
O	-2.713666	2.345181	3.879511
C	-3.534662	3.061213	4.400830
C	-4.951475	3.510317	4.148886
C	-4.761593	4.276000	5.467911
C	-4.776865	5.781905	5.439648
C	1.288164	0.180064	3.902000
C	1.112792	1.704465	4.060692
C	3.481279	-1.734825	-0.327497
C	3.031623	-3.061952	-0.970446
C	-1.095846	0.365794	-0.590190
N	-2.410599	-0.281305	-0.321406
C	-2.277908	-1.732782	-0.482346
O	-3.709361	2.596445	1.073085
C	-4.475161	3.167348	0.155297
C	-5.680114	2.519311	-0.222817
C	-6.500488	3.056056	-1.212268
C	-6.186220	4.249795	-1.865206
C	-5.007852	4.887707	-1.463395
C	-4.140937	4.400031	-0.476774
C	-6.119604	1.282257	0.509348
N	-5.225523	0.090535	0.417149
C	-5.959435	-1.048485	0.986422

C	-2.877071	5.186949	-0.088199
C	-2.923186	5.536906	1.412223
C	-7.115800	4.806899	-2.951697
C	-7.252468	3.778979	-4.092322
O	-2.965619	-1.741591	2.502698
C	-3.186737	-2.292691	3.581741
O	-2.989335	-3.591545	3.771892
C	-2.445814	-4.388753	2.676823
C	-2.998870	-5.788174	2.872285
O	-4.678789	0.238418	3.524506
C	-4.964808	-0.727417	4.460949
C	-5.508166	-0.121363	5.758885
C	-3.718915	-1.593472	4.793876
C	-1.615226	4.348988	-0.368617
C	-2.739882	6.504535	-0.866853
C	-8.507759	5.082066	-2.349080
C	-6.591427	6.117094	-3.555217
C	-4.817159	-0.200099	-0.974711
C	-3.396201	0.258833	-1.273479
C	0.195654	-0.548490	4.707362
C	2.643115	-0.200037	4.518425
C	4.017093	-0.796855	-1.427441
C	4.635662	-2.042017	0.636354
O	-3.378764	3.744719	5.554439
C	-0.928769	-4.318579	2.716937
H	-3.137305	-0.035652	-2.306896
H	-3.348041	1.350024	-1.225736
H	-5.496922	0.283183	-1.688923
H	-4.903191	-1.278384	-1.142672
H	-7.118081	0.997161	0.136959
H	-6.224408	1.486792	1.582965
H	-0.840981	0.220326	-1.654112
H	-1.243776	1.441224	-0.437879
H	3.148986	-1.029470	2.331454
H	1.121603	-0.875300	-1.426413
H	-4.745962	5.820856	-1.945231
H	-7.415327	2.521624	-1.465022
H	-2.012947	-1.992882	-1.521649
H	-1.492243	-2.096063	0.179617
H	-3.208531	-2.237952	-0.219682
H	-6.851647	-1.296839	0.387739
H	-5.310209	-1.926417	1.035635
H	-6.264332	-0.794284	2.002690
H	-2.029416	6.104044	1.699062
H	-3.801749	6.153565	1.637043
H	-2.959022	4.625011	2.010052
H	-0.713714	4.923137	-0.123246
H	-1.613207	3.441706	0.236915
H	-1.559127	4.071848	-1.427560
H	-1.834806	7.024404	-0.534805

H	-2.644509	6.339916	-1.945733
H	-3.587390	7.177300	-0.694710
H	-7.282169	6.471224	-4.328210
H	-6.506482	6.907667	-2.802058
H	-5.610603	5.984871	-4.024408
H	-7.920996	4.156225	-4.875435
H	-6.278437	3.570509	-4.547583
H	-7.663567	2.829694	-3.734371
H	-9.190542	5.473196	-3.112982
H	-8.956822	4.173466	-1.935604
H	-8.442953	5.818485	-1.541111
H	0.254372	-0.270479	5.767023
H	-0.791017	-0.277641	4.330701
H	0.319243	-1.635485	4.636391
H	2.652653	0.094005	5.573864
H	2.830598	-1.279194	4.476505
H	3.477716	0.312898	4.028287
H	1.171196	1.984982	5.119829
H	1.906815	2.237783	3.525977
H	0.147646	2.028372	3.668136
H	5.458915	-2.514944	0.089476
H	5.028553	-1.132254	1.102551
H	4.329583	-2.728958	1.432687
H	3.866298	-3.542120	-1.495741
H	2.664297	-3.757801	-0.208275
H	2.226462	-2.907020	-1.695792
H	4.869126	-1.253998	-1.945268
H	3.252530	-0.574306	-2.178300
H	4.348294	0.154989	-0.999321
H	-5.741852	-1.428604	4.083865
H	-5.331771	3.871539	6.308734
H	-5.071425	4.114566	3.247517
H	-5.656879	2.677680	4.145294
H	-4.185642	6.161701	4.601478
H	-5.805902	6.139225	5.329032
H	-4.370285	6.192107	6.368355
H	-2.815067	-3.953749	1.743757
H	-2.647472	-6.441442	2.068152
H	-2.664786	-6.207836	3.826051
H	-4.092381	-5.784204	2.859852
H	-0.508365	-4.927784	1.910682
H	-0.576389	-3.292739	2.585848
H	-0.551346	-4.704107	3.669203
H	-2.933019	-0.921222	5.162189
H	-3.931382	-2.331666	5.571479
H	-4.757926	0.535148	6.214107
H	-6.399153	0.474468	5.537028
H	-5.785761	-0.891001	6.488508

YBRSTS1SP.xyz

128

scf done: -2432.658980

C	0.065362	0.017922	0.104816
C	0.107578	0.362096	1.480369
C	1.301017	0.110328	2.211766
C	2.363874	-0.507472	1.541925
C	2.332198	-0.881083	0.193590
C	1.158000	-0.594424	-0.505365
O	-0.963187	0.913766	2.040151
Y	-3.087424	0.963234	1.851422
O	-4.042905	1.417846	3.681370
C	-4.919041	1.439378	4.673597
C	-5.942024	2.589505	4.767434
C	-5.358203	2.820812	6.167979
C	-4.771845	4.176684	6.488282
C	1.428782	0.527258	3.686333
C	1.213684	2.049166	3.815685
C	3.511921	-1.553681	-0.521191
C	3.069145	-2.922372	-1.075333
C	-1.131704	0.393553	-0.726774
N	-2.419315	-0.252546	-0.335237
C	-2.268100	-1.710082	-0.330736
O	-3.433659	2.779872	0.772277
C	-4.200961	3.323678	-0.162175
C	-5.443924	2.707902	-0.459111
C	-6.240333	3.182056	-1.499664
C	-5.865884	4.285115	-2.270143
C	-4.667491	4.916239	-1.917228
C	-3.825750	4.490600	-0.881994
C	-5.970633	1.619654	0.436147
N	-5.194526	0.341968	0.516390
C	-6.005204	-0.618129	1.285711
C	-2.563968	5.285480	-0.507212
C	-2.678354	5.752307	0.958825
C	-6.761917	4.768013	-3.418512
C	-6.932625	3.635094	-4.450103
O	-3.204956	-1.320880	2.765465
C	-3.309332	-1.837010	3.880229
O	-3.266407	-3.153149	4.053769
C	-3.045920	-4.026878	2.908576
C	-3.828539	-5.295536	3.193041
O	-5.621190	0.187448	4.786438
C	-5.029488	-0.887909	5.498994
C	-5.246460	-0.778614	7.009553
C	-3.525670	-1.122666	5.181750
C	-1.299713	4.419906	-0.671188
C	-2.380756	6.536200	-1.381099
C	-8.145841	5.162771	-2.866034
C	-6.175239	5.986158	-4.144884
C	-4.871812	-0.201844	-0.822546

C	-3.466753	0.166139	-1.285556
C	0.384725	-0.220108	4.539469
C	2.812771	0.206051	4.271320
C	3.983942	-0.664068	-1.688260
C	4.707510	-1.784236	0.413285
O	-4.330348	1.823105	5.939175
C	-1.551129	-4.252280	2.754356
H	-3.289463	-0.283903	-2.278602
H	-3.399363	1.250278	-1.404554
H	-5.591617	0.158604	-1.570407
H	-4.978907	-1.290424	-0.783464
H	-6.996013	1.373893	0.114978
H	-6.037674	1.990857	1.467492
H	-0.921067	0.150929	-1.781870
H	-1.304634	1.474959	-0.672711
H	3.268324	-0.702325	2.104315
H	1.081414	-0.838171	-1.564006
H	-4.371220	5.794851	-2.475791
H	-7.186489	2.678101	-1.692693
H	-2.042947	-2.091248	-1.340906
H	-1.447753	-1.985865	0.332720
H	-3.180938	-2.187985	0.029156
H	-6.967997	-0.820645	0.789368
H	-5.459448	-1.558163	1.394116
H	-6.198849	-0.223736	2.287171
H	-1.777425	6.304589	1.252376
H	-3.539529	6.417926	1.085614
H	-2.796536	4.900383	1.631244
H	-0.404115	5.014687	-0.455193
H	-1.315337	3.571380	0.013949
H	-1.212994	4.046690	-1.698397
H	-1.485158	7.075011	-1.053675
H	-2.242824	6.285479	-2.438948
H	-3.226993	7.227010	-1.298308
H	-6.841918	6.287212	-4.960291
H	-6.065594	6.845871	-3.475425
H	-5.195365	5.766987	-4.582426
H	-7.577476	3.957688	-5.276355
H	-5.964341	3.341256	-4.869371
H	-7.386607	2.745084	-4.002600
H	-8.802008	5.506084	-3.674902
H	-8.640581	4.320664	-2.371972
H	-8.056696	5.971748	-2.133470
H	0.456830	0.091211	5.588687
H	-0.624756	-0.008017	4.184932
H	0.554631	-1.302489	4.496310
H	2.845509	0.533826	5.316118
H	3.030537	-0.867871	4.257674
H	3.616068	0.726973	3.739041
H	1.286601	2.353920	4.866838

H	1.979935	2.593427	3.252604
H	0.233647	2.340693	3.435287
H	5.520190	-2.269270	-0.138453
H	5.097763	-0.842948	0.814427
H	4.447007	-2.432878	1.256649
H	3.897009	-3.413909	-1.600342
H	2.740256	-3.582792	-0.265638
H	2.239581	-2.823983	-1.782902
H	4.826368	-1.130004	-2.213531
H	3.186812	-0.497830	-2.419646
H	4.308900	0.315824	-1.323505
H	-5.588338	-1.766955	5.150721
H	-6.030995	2.492451	6.973070
H	-5.722468	3.392052	4.059781
H	-6.990574	2.293561	4.709593
H	-4.106897	4.506110	5.684273
H	-5.569200	4.918326	6.611495
H	-4.194885	4.139004	7.417987
H	-3.442197	-3.517425	2.026135
H	-3.715865	-5.995924	2.360191
H	-3.461811	-5.781484	4.102085
H	-4.893186	-5.080945	3.320437
H	-1.358676	-4.908409	1.899867
H	-1.025887	-3.308906	2.586193
H	-1.140297	-4.727151	3.650573
H	-2.999139	-0.167963	5.175916
H	-3.111626	-1.754950	5.970885
H	-4.628314	0.011532	7.437389
H	-6.296986	-0.545383	7.204279
H	-5.010509	-1.731216	7.496840

YBRSTS2S.xyz

128

scf done: -2432.664356

C	-3.328280	-1.237363	2.179715
C	-3.669996	-2.026605	3.315776
C	-2.939016	-3.219116	3.546731
C	-1.875554	-3.582237	2.724617
C	-1.489353	-2.803029	1.632283
C	-2.245517	-1.649893	1.393094
O	-4.643600	-1.701729	4.153415
Y	-5.266988	-1.778332	6.225192
O	-3.432169	-0.186268	6.778901
C	-3.270463	1.036311	6.745699
O	-2.078548	1.603804	6.659967
C	-0.886035	0.768183	6.544868
C	-0.310174	0.560332	7.935439
C	-3.363058	-4.124977	4.664753
N	-3.265937	-3.533827	6.029820
C	-3.572728	-4.599883	6.997379

C	-3.714719	-4.080690	8.416859
N	-4.729012	-3.013074	8.535597
C	-4.307036	-2.063512	9.578403
C	-0.307777	-3.231281	0.752070
C	-0.605798	-4.605373	0.119820
C	-4.152750	-0.000658	1.790936
C	-4.161477	1.034002	2.932788
O	-6.680931	-3.383251	6.204295
C	-6.973528	-4.538947	6.797429
C	-7.630861	-5.605520	6.123460
C	-7.797903	-6.813392	6.814270
C	-7.387808	-7.030075	8.133151
C	-6.801133	-5.944729	8.787615
C	-6.598380	-4.720737	8.153866
C	-8.201347	-5.431552	4.706010
C	-7.097690	-5.061118	3.697355
C	-6.057621	-3.563101	8.948989
C	-7.581367	-8.364103	8.866121
C	-8.499685	-8.153870	10.086476
O	-6.497625	0.126654	5.649983
C	-7.865020	0.486580	5.404801
C	-8.354533	0.282623	6.841601
C	-6.932988	0.355378	7.392978
O	-6.329498	-0.587955	7.991780
O	-6.620208	1.653069	7.693138
C	-5.266337	1.913977	8.069498
C	-4.386438	2.035321	6.796078
C	-5.277468	3.195053	8.883904
C	-8.217866	-9.435866	7.970786
C	-6.215868	-8.894357	9.346248
C	-8.883755	-6.705740	4.183561
C	-9.268006	-4.319562	4.745524
C	-1.913799	-3.012974	6.251596
C	-3.611438	0.701928	0.536629
C	-5.598654	-0.445185	1.492009
C	-0.033299	-2.235183	-0.382882
C	0.966774	-3.336534	1.612825
C	-8.529585	-0.315016	4.308615
C	0.048305	1.498523	5.599224
H	-2.782736	-5.372392	6.977427
H	-4.502970	-5.081488	6.687894
H	-3.956092	-4.922908	9.081860
H	-2.755796	-3.679952	8.760480
H	-5.980388	-3.879505	10.002738
H	-6.752544	-2.718067	8.907589
H	-2.751104	-5.042597	4.632614
H	-4.409168	-4.425330	4.536212
H	-1.982525	-1.038115	0.539253
H	-1.347453	-4.507595	2.951502
H	-8.281503	-7.628201	6.291174

H	-6.497926	-6.037235	9.829548
H	-1.166205	-3.824648	6.253720
H	-1.662893	-2.322116	5.445539
H	-1.857590	-2.478825	7.201741
H	-4.130077	-2.575597	10.538604
H	-3.383297	-1.564021	9.271599
H	-5.081709	-1.308350	9.710857
H	-9.662728	-4.127193	3.740433
H	-10.105116	-4.611579	5.389501
H	-8.841784	-3.394230	5.135888
H	-7.525118	-4.961313	2.692288
H	-6.617010	-4.117560	3.957565
H	-6.334425	-5.847019	3.655637
H	-9.283509	-6.512207	3.182284
H	-8.184520	-7.545347	4.100056
H	-9.722775	-7.016696	4.815405
H	-8.322868	-10.371200	8.531164
H	-9.216662	-9.142041	7.631206
H	-7.604485	-9.645344	7.087856
H	-6.337131	-9.841946	9.884706
H	-5.545074	-9.068025	8.498031
H	-5.722614	-8.189598	10.023239
H	-8.644099	-9.095946	10.629193
H	-8.079907	-7.426615	10.788585
H	-9.482724	-7.785565	9.775099
H	-4.707889	1.933197	2.620584
H	-4.648693	0.623789	3.818113
H	-3.138548	1.336852	3.187694
H	-4.247369	1.563360	0.304473
H	-2.591082	1.076088	0.679259
H	-3.617605	0.046242	-0.340704
H	-6.224956	0.424312	1.255163
H	-5.623189	-1.123759	0.632123
H	-6.024378	-0.962232	2.353860
H	0.822883	-2.574564	-0.976247
H	-0.888983	-2.145992	-1.060389
H	0.204210	-1.236905	0.000467
H	1.821535	-3.655567	1.004186
H	1.212970	-2.368821	2.063525
H	0.847697	-4.061593	2.424153
H	0.232408	-4.934895	-0.506176
H	-0.774841	-5.372964	0.881454
H	-1.502042	-4.557864	-0.507446
H	-7.901414	1.555686	5.146595
H	-8.758894	-0.719541	7.006873
H	-9.031526	1.037921	7.249782
H	-8.497937	-1.384495	4.532289
H	-9.578404	-0.015022	4.200533
H	-8.025661	-0.148669	3.352985
H	-1.199669	-0.186312	6.117399

H	0.594400	-0.052477	7.875602
H	-0.044989	1.518870	8.392203
H	-1.025274	0.048593	8.585305
H	0.963301	0.915143	5.460765
H	-0.419413	1.638164	4.621446
H	0.321906	2.479266	6.000221
H	-4.922540	1.076822	8.685302
H	-5.031504	1.811976	5.937526
H	-3.976798	3.041309	6.686695
H	-4.263517	3.445158	9.211888
H	-5.663977	4.028787	8.289298
H	-5.911248	3.078349	9.766786

YBRSTS2SR.xyz

128

scf done: -2432.666409

C	-3.361310	-1.207916	2.167568
C	-3.697255	-1.988161	3.311978
C	-2.969887	-3.184427	3.541831
C	-1.916921	-3.556417	2.709431
C	-1.537795	-2.786362	1.608573
C	-2.290125	-1.630714	1.371092
O	-4.662048	-1.649296	4.156536
Y	-5.239158	-1.802182	6.241998
O	-3.382683	-0.201735	6.739630
C	-3.210419	1.019980	6.733621
O	-2.007866	1.575643	6.724263
C	-0.820386	0.729515	6.675568
C	-0.344109	0.485155	8.097813
C	-3.383438	-4.093924	4.662385
N	-3.259976	-3.515442	6.032142
C	-3.561007	-4.584071	7.001247
C	-3.717456	-4.060617	8.419317
N	-4.740800	-2.999935	8.519703
C	-4.345408	-2.026917	9.551753
C	-0.368536	-3.226669	0.718052
C	-0.681057	-4.603086	0.098000
C	-4.177521	0.035753	1.783490
C	-4.140588	1.078949	2.916258
O	-6.646710	-3.418000	6.163809
C	-6.950466	-4.563650	6.770578
C	-7.596455	-5.642735	6.105221
C	-7.768322	-6.840051	6.813167
C	-7.375668	-7.034629	8.140804
C	-6.803646	-5.936365	8.786664
C	-6.596859	-4.722159	8.135929
C	-8.154436	-5.492850	4.679842
C	-7.046909	-5.123899	3.675171
C	-6.075488	-3.547993	8.919064
C	-7.572273	-8.358543	8.891136

C	-8.503041	-8.134336	10.099502
O	-6.589265	0.241503	5.690955
C	-7.984207	0.537651	5.372103
C	-8.408099	0.376150	6.835479
C	-6.911798	0.395006	7.198946
O	-6.306984	-0.570994	7.835432
O	-6.587362	1.698805	7.606330
C	-5.240100	1.916516	7.993271
C	-4.314114	2.032985	6.745134
C	-5.222513	3.189010	8.823742
C	-8.196375	-9.445332	8.005327
C	-6.209553	-8.876755	9.391945
C	-8.820803	-6.779730	4.167672
C	-9.230688	-4.389695	4.695599
C	-1.900574	-3.005468	6.237150
C	-3.655943	0.719900	0.510899
C	-5.636029	-0.389538	1.520847
C	-0.101855	-2.239247	-0.426340
C	0.914862	-3.333030	1.565351
C	-8.575507	-0.373654	4.327402
C	0.186137	1.468483	5.814018
H	-2.764471	-5.349084	6.985318
H	-4.486106	-5.073485	6.688820
H	-3.959445	-4.901484	9.085394
H	-2.765346	-3.649754	8.769930
H	-6.016252	-3.843024	9.979817
H	-6.770423	-2.704045	8.848048
H	-2.778692	-5.015114	4.614209
H	-4.433250	-4.386895	4.549004
H	-2.033627	-1.025083	0.510954
H	-1.391591	-4.483593	2.935092
H	-8.241931	-7.664819	6.296650
H	-6.516319	-6.010303	9.834555
H	-1.159668	-3.822164	6.208336
H	-1.661433	-2.299212	5.441165
H	-1.823149	-2.491874	7.196957
H	-4.192315	-2.517760	10.526734
H	-3.415106	-1.532364	9.257504
H	-5.126239	-1.270935	9.643535
H	-9.618789	-4.213872	3.684874
H	-10.070442	-4.679001	5.337204
H	-8.814244	-3.456065	5.076552
H	-7.465779	-5.050351	2.664254
H	-6.586164	-4.167152	3.922744
H	-6.269819	-5.896958	3.655847
H	-9.213266	-6.602238	3.160566
H	-8.113442	-7.614032	4.101078
H	-9.662775	-7.090256	4.795711
H	-8.305893	-10.372114	8.578877
H	-9.191821	-9.158838	7.649991

H	-7.572654	-9.667283	7.132734
H	-6.332661	-9.816248	9.944019
H	-5.530496	-9.061477	8.552657
H	-5.724930	-8.159726	10.062251
H	-8.648945	-9.069150	10.654163
H	-8.093003	-7.395648	10.795383
H	-9.484503	-7.774487	9.773632
H	-4.709491	1.971832	2.627545
H	-4.577714	0.667073	3.826057
H	-3.109280	1.390510	3.121000
H	-4.286452	1.586930	0.284749
H	-2.628528	1.083280	0.627362
H	-3.689505	0.055640	-0.359346
H	-6.255299	0.487225	1.292450
H	-5.689707	-1.073131	0.666333
H	-6.048349	-0.896365	2.395060
H	0.745643	-2.587083	-1.027167
H	-0.964683	-2.149819	-1.094730
H	0.145473	-1.239845	-0.052252
H	1.761203	-3.659971	0.949238
H	1.170747	-2.363908	2.007484
H	0.801079	-4.052762	2.382183
H	0.148014	-4.940657	-0.535771
H	-0.844860	-5.365245	0.866205
H	-1.584348	-4.554801	-0.519006
H	-8.043728	1.583660	5.045879
H	-8.849639	-0.600051	7.049280
H	-9.005625	1.176998	7.274017
H	-8.497102	-1.420292	4.631657
H	-9.635729	-0.134579	4.186522
H	-8.067731	-0.251378	3.367125
H	-1.112018	-0.212304	6.206142
H	0.555452	-0.137944	8.088477
H	-0.100679	1.430783	8.592060
H	-1.108924	-0.029513	8.685792
H	1.102893	0.877855	5.727225
H	-0.210165	1.635329	4.809222
H	0.440490	2.437194	6.254874
H	-4.920738	1.066112	8.606056
H	-4.932414	1.837646	5.863385
H	-3.883870	3.032794	6.658005
H	-4.207119	3.408025	9.170031
H	-5.578096	4.040226	8.234184
H	-5.873677	3.078867	9.694704

YBRSTS2SP.xyz

128

scf done: -2432.687708

C	-7.566914	-5.903904	5.858911
C	-6.981977	-4.804699	6.545826

C	-6.800833	-4.896782	7.949242
C	-7.101561	-6.074150	8.630727
C	-7.612168	-7.195011	7.971952
C	-7.844912	-7.060462	6.598098
O	-6.592473	-3.698269	5.932803
Y	-5.282965	-2.008093	6.083685
C	-6.625842	1.519038	8.333918
O	-5.707861	2.299194	7.710583
C	-4.522207	2.621895	8.454244
C	-3.943708	3.877334	7.829309
C	-6.400782	-3.671548	8.721715
N	-5.053462	-3.077716	8.443191
C	-4.817147	-2.049902	9.469276
C	-7.909231	-8.482288	8.752917
C	-8.474862	-9.592949	7.857487
C	-7.921735	-5.810683	4.366132
C	-8.600903	-7.087015	3.845325
O	-4.610178	-1.942041	4.050506
C	-3.567155	-2.237379	3.289364
C	-2.702899	-3.293453	3.680475
C	-1.551930	-3.573088	2.947004
C	-1.214851	-2.857143	1.795477
C	-2.120648	-1.871752	1.385123
C	-3.296610	-1.548662	2.073619
C	-3.109458	-4.206132	4.806630
N	-3.191034	-3.594559	6.162940
C	-1.888613	-3.035688	6.530617
C	-4.303189	-0.537300	1.498840
C	-3.854288	0.032063	0.144275
C	0.067534	-3.194292	1.022993
C	0.260715	-2.298742	-0.208805
O	-6.639019	-0.463656	6.331850
C	-7.441981	0.641947	6.115398
C	-8.696842	0.279345	5.321481
O	-6.461671	1.089661	9.458051
C	-5.657392	-1.243725	1.279234
C	-4.495447	0.654423	2.455578
C	1.290505	-3.008041	1.942525
C	0.013543	-4.658950	0.544778
C	-3.609285	-4.639575	7.115096
C	-3.975783	-4.092371	8.488259
C	-8.903734	-4.640224	4.151933
C	-6.657370	-5.580573	3.516295
C	-6.608661	-9.004150	9.395408
C	-8.940727	-8.192517	9.861430
C	-7.828741	1.279530	7.466977
C	-3.573368	1.409136	8.519324
C	-3.169481	0.802742	7.197225
O	-3.558363	-0.289062	6.789587
O	-2.304544	1.567539	6.550998

C	-1.734101	1.132262	5.274283
C	-1.648934	2.375915	4.410179
C	-0.377734	0.509640	5.557904
H	-2.808866	-5.391549	7.237944
H	-4.474620	-5.154721	6.691083
H	-4.266396	-4.934470	9.132075
H	-3.096447	-3.633709	8.951682
H	-6.449502	-3.909380	9.796850
H	-7.124745	-2.866470	8.536752
H	-2.407009	-5.056540	4.844735
H	-4.103514	-4.617914	4.597610
H	-1.907911	-1.333934	0.469544
H	-0.917948	-4.392266	3.284014
H	-8.272896	-7.902936	6.069915
H	-6.944446	-6.099032	9.708333
H	-1.127546	-3.827469	6.637820
H	-1.565353	-2.352085	5.744598
H	-1.953448	-2.480671	7.468940
H	-4.803865	-2.484709	10.481957
H	-3.854976	-1.565129	9.288495
H	-5.604212	-1.291882	9.432583
H	-9.154541	-4.546111	3.088289
H	-9.834227	-4.811628	4.704721
H	-8.467833	-3.698643	4.490834
H	-6.917714	-5.557453	2.451183
H	-6.182836	-4.631551	3.769438
H	-5.935344	-6.392247	3.665223
H	-8.855306	-6.951975	2.788517
H	-7.946525	-7.963455	3.914255
H	-9.530769	-7.308596	4.380575
H	-8.662771	-10.490662	8.456474
H	-9.423715	-9.300010	7.395771
H	-7.776608	-9.867943	7.059814
H	-6.799160	-9.918670	9.970003
H	-5.861011	-9.234266	8.628653
H	-6.171414	-8.267966	10.077592
H	-9.159405	-9.102123	10.433736
H	-8.578911	-7.437041	10.565913
H	-9.879233	-7.825214	9.433286
H	-5.244810	1.346720	2.052056
H	-4.829000	0.318317	3.438477
H	-3.558094	1.210290	2.567597
H	-4.615191	0.729207	-0.223319
H	-2.911809	0.586617	0.219689
H	-3.733315	-0.750290	-0.612659
H	-6.393448	-0.535090	0.879904
H	-5.551315	-2.062238	0.558812
H	-6.040432	-1.654756	2.214915
H	1.192298	-2.566139	-0.719472
H	-0.554905	-2.415289	-0.930272

H	0.325615	-1.239807	0.064113
H	2.216636	-3.263244	1.413595
H	1.369241	-1.968886	2.280588
H	1.229071	-3.643996	2.831349
H	0.924396	-4.920476	-0.007227
H	-0.078170	-5.355689	1.383871
H	-0.844688	-4.820473	-0.115660
H	-6.884909	1.407465	5.546859
H	-8.499690	0.617350	8.020572
H	-8.338943	2.236183	7.298243
H	-9.287248	-0.466625	5.864309
H	-9.325985	1.157595	5.134489
H	-8.411022	-0.151647	4.357729
H	-2.414261	0.397156	4.837812
H	0.064843	0.150668	4.624371
H	0.300269	1.244020	6.004088
H	-0.467808	-0.341177	6.237518
H	-1.222588	2.117614	3.436792
H	-2.638634	2.808420	4.243950
H	-1.007997	3.129942	4.877813
H	-4.819215	2.817357	9.490780
H	-2.661783	1.727217	9.037151
H	-4.063402	0.637205	9.110049
H	-3.041767	4.186297	8.365685
H	-3.682692	3.719474	6.781277
H	-4.675461	4.687259	7.887913

YBRSTS1M.xyz

128

scf done: -2432.658747

C	-3.784922	4.231658	-0.420256
C	-4.172962	3.064011	0.295298
C	-5.408850	2.450956	-0.031857
C	-6.183343	2.919150	-1.089636
C	-5.790450	4.017409	-1.858400
C	-4.601208	4.649938	-1.479466
O	-3.439066	2.523836	1.256206
Y	-2.883659	0.647868	2.189936
O	-3.047502	-1.694759	2.602052
C	-3.359042	-1.887437	3.794419
O	-4.509013	-2.560486	4.161022
C	-3.869394	-3.114795	5.358367
C	-3.912596	-4.624120	5.360592
C	-5.932981	1.354149	0.849291
N	-5.144403	0.091967	0.935104
C	-4.856330	-0.474190	-0.401063
C	-3.528298	-0.014819	-0.987647
N	-2.370050	-0.363092	-0.144191
C	-2.104910	-1.807703	-0.198077
C	-6.658226	4.493381	-3.030932

C	-6.805010	3.354187	-4.059290
C	-2.546766	5.047110	-0.011563
C	-2.717668	5.504483	1.450663
O	-0.750563	0.626138	2.125940
C	0.287295	0.227822	1.400869
C	0.126034	0.048444	0.004035
C	1.190958	-0.384649	-0.781313
C	2.452938	-0.645847	-0.242688
C	2.596316	-0.449888	1.134491
C	1.563764	-0.020936	1.976957
C	-1.185933	0.385062	-0.652284
C	1.807609	0.187818	3.479754
C	1.514092	1.654727	3.854856
C	3.597568	-1.115198	-1.150461
C	3.201431	-2.434190	-1.842942
O	-3.733895	-0.074991	4.202428
C	-3.985308	0.436608	5.475244
C	-5.262655	1.278365	5.488397
C	-2.769437	1.220879	6.014599
C	-2.408132	2.405931	5.162598
O	-2.056719	3.459081	5.888442
C	-1.635694	4.685034	5.210824
C	-0.398411	5.171620	5.942233
O	-2.417770	2.404404	3.936133
C	0.896130	-0.752137	4.293419
C	3.257271	-0.110178	3.891969
C	3.876940	-0.043968	-2.223192
C	4.898849	-1.359595	-0.373628
C	-5.956606	-0.867207	1.702980
C	-1.259925	4.210020	-0.131990
C	-2.359909	6.304454	-0.875173
C	-8.055017	4.891637	-2.514254
C	-6.054364	5.706830	-3.750894
C	-2.551666	-2.427107	4.974730
C	-2.797210	5.662467	5.254901
H	-4.138392	-0.398135	6.180781
H	-3.416203	-0.462285	-1.991692
H	-3.540589	1.069491	-1.119504
H	-5.659989	-0.220596	-1.109268
H	-4.854635	-1.563773	-0.305059
H	-6.954266	1.100481	0.518399
H	-6.016085	1.724814	1.880877
H	-1.090913	0.203361	-1.736361
H	-1.415183	1.449124	-0.524974
H	3.565075	-0.639680	1.578628
H	1.018816	-0.513169	-1.848863
H	-4.292122	5.525891	-2.035161
H	-7.123127	2.411164	-1.302249
H	-1.911734	-2.129774	-1.234870
H	-1.229782	-2.037588	0.409768

H	-2.947392	-2.366329	0.207904
H	-6.912448	-1.075929	1.194463
H	-5.403759	-1.795329	1.841260
H	-6.170018	-0.457099	2.692313
H	-1.838943	6.078273	1.772151
H	-3.598504	6.148339	1.554075
H	-2.835578	4.640070	2.107430
H	-0.386063	4.820865	0.126426
H	-1.283814	3.352357	0.541651
H	-1.121888	3.852749	-1.158897
H	-1.483780	6.857660	-0.519453
H	-2.185356	6.060153	-1.928946
H	-3.220687	6.979628	-0.816568
H	-6.701175	6.002820	-4.584055
H	-5.960350	6.570887	-3.084517
H	-5.064352	5.484613	-4.163386
H	-7.430209	3.671440	-4.902710
H	-5.827166	3.057563	-4.453545
H	-7.269184	2.467073	-3.616725
H	-8.691997	5.229504	-3.340628
H	-8.560835	4.052556	-2.026336
H	-7.983169	5.705476	-1.785051
H	1.045236	-0.589926	5.369264
H	-0.152748	-0.577864	4.047719
H	1.131530	-1.800013	4.075079
H	3.369441	0.062317	4.968276
H	3.538353	-1.150842	3.695997
H	3.972944	0.541395	3.379037
H	1.663700	1.806095	4.931995
H	2.194936	2.328797	3.323198
H	0.489446	1.925533	3.594379
H	5.682619	-1.694936	-1.061773
H	5.258014	-0.448024	0.115889
H	4.777895	-2.133734	0.391881
H	4.005208	-2.781726	-2.503294
H	3.004127	-3.218230	-1.104069
H	2.299128	-2.316538	-2.451250
H	4.687220	-0.364076	-2.889592
H	2.994424	0.149057	-2.841098
H	4.170641	0.903454	-1.759245
H	-4.349047	-2.702870	6.253135
H	-1.759154	-3.104574	4.647386
H	-2.147296	-1.697885	5.674515
H	-3.438434	-5.026206	4.460126
H	-3.384733	-5.015089	6.236912
H	-4.945814	-4.981980	5.396730
H	-1.399839	4.422734	4.177029
H	-0.031755	6.090954	5.475896
H	-0.622860	5.384463	6.992210
H	0.399291	4.425555	5.899042

H	-2.510211	6.602321	4.774307
H	-3.663571	5.263877	4.720949
H	-3.084575	5.876424	6.289303
H	-2.929112	1.551890	7.044566
H	-1.893228	0.560459	6.012103
H	-5.479522	1.664973	6.490815
H	-5.176652	2.126953	4.801141
H	-6.108890	0.666009	5.165624

YBRSTS1MR.xyz

128

scf done: -2432.671311

C	-3.931099	4.309733	-0.437053
C	-4.242193	3.110997	0.265229
C	-5.468528	2.458565	-0.023483
C	-6.307396	2.927500	-1.031273
C	-5.994007	4.061538	-1.784098
C	-4.811477	4.726965	-1.443780
O	-3.439523	2.577042	1.173411
Y	-2.934471	0.731216	2.188084
O	-2.936608	-1.785688	2.551523
C	-3.076290	-2.488802	3.523977
O	-3.244672	-3.826134	3.512517
C	-3.352927	-3.862416	4.993851
C	-2.291429	-4.737836	5.605738
C	-5.917346	1.314281	0.841556
N	-5.088350	0.073128	0.829326
C	-4.791281	-0.382536	-0.545787
C	-3.435863	0.098668	-1.047254
N	-2.326283	-0.320514	-0.175896
C	-2.075981	-1.759367	-0.320231
C	-6.936498	4.538121	-2.896984
C	-7.099405	3.422664	-3.948628
C	-2.704837	5.159256	-0.064886
C	-2.842861	5.601229	1.405844
O	-0.789334	0.451582	2.248802
C	0.258100	0.062457	1.539691
C	0.161878	0.009861	0.124558
C	1.246687	-0.398493	-0.646635
C	2.469433	-0.762159	-0.077653
C	2.549519	-0.700689	1.317341
C	1.494224	-0.302852	2.146143
C	-1.106886	0.444238	-0.557830
C	1.671009	-0.241270	3.671242
C	1.437135	1.202888	4.158449
C	3.640760	-1.192431	-0.970583
C	3.235213	-2.427820	-1.798771
O	-4.185958	0.477300	3.928061
C	-4.504502	1.116286	5.106794
C	-5.537876	2.231216	4.908026

C	-3.237930	1.649649	5.829508
C	-2.482973	2.651600	5.005096
O	-2.164425	3.743471	5.693835
C	-1.406457	4.807310	5.040430
C	0.018102	4.751972	5.564507
O	-2.185248	2.488545	3.826028
C	0.664521	-1.189733	4.353242
C	3.076529	-0.661255	4.125972
C	4.009891	-0.041117	-1.926929
C	4.892563	-1.555451	-0.159821
C	-5.843951	-0.956715	1.559139
C	-1.398322	4.361797	-0.234929
C	-2.583662	6.426998	-0.924036
C	-8.316717	4.873965	-2.298270
C	-6.410603	5.790694	-3.611607
C	-3.161240	-2.337296	5.020451
C	-2.123619	6.105777	5.362416
H	-4.949205	0.398663	5.828993
H	-3.283899	-0.276864	-2.075627
H	-3.435679	1.189608	-1.099898
H	-5.567971	-0.041179	-1.245281
H	-4.820213	-1.476245	-0.554465
H	-6.945266	1.043386	0.546732
H	-5.956093	1.634164	1.890882
H	-0.962491	0.365894	-1.649037
H	-1.321329	1.497860	-0.340059
H	3.485826	-0.974090	1.787499
H	1.122122	-0.423356	-1.728373
H	-4.561061	5.628349	-1.988687
H	-7.236655	2.389622	-1.215034
H	-1.823464	-2.012033	-1.364004
H	-1.243624	-2.051864	0.319576
H	-2.951003	-2.334060	-0.016502
H	-6.824465	-1.145345	1.091195
H	-5.276521	-1.889195	1.575676
H	-5.987392	-0.623037	2.589715
H	-1.969271	6.192904	1.708087
H	-3.735080	6.223385	1.539821
H	-2.922657	4.729329	2.058677
H	-0.533550	5.000650	-0.017053
H	-1.371646	3.509814	0.445041
H	-1.293354	3.998539	-1.263604
H	-1.708763	7.000154	-0.598054
H	-2.444660	6.194241	-1.985687
H	-3.457944	7.079638	-0.825917
H	-7.107941	6.085584	-4.403394
H	-6.312483	6.639628	-2.926657
H	-5.435410	5.614067	-4.077926
H	-7.777622	3.741134	-4.749476
H	-6.134273	3.169553	-4.400272

H	-7.511196	2.508937	-3.508281
H	-9.008015	5.209438	-3.080919
H	-8.766764	4.005473	-1.807176
H	-8.233783	5.671135	-1.552043
H	0.761643	-1.127489	5.445325
H	-0.354624	-0.923480	4.067458
H	0.854077	-2.227440	4.054131
H	3.138137	-0.593834	5.218022
H	3.310290	-1.694435	3.845985
H	3.853796	-0.009313	3.713153
H	1.535117	1.256142	5.251069
H	2.182340	1.876442	3.720573
H	0.444158	1.551710	3.868776
H	5.698752	-1.855617	-0.838186
H	5.255686	-0.706540	0.429283
H	4.706856	-2.391484	0.523140
H	4.057606	-2.744181	-2.451950
H	2.977339	-3.267344	-1.144338
H	2.367584	-2.221595	-2.433234
H	4.839027	-0.332426	-2.583347
H	3.165552	0.242530	-2.562900
H	4.315354	0.847999	-1.365283
H	-4.363045	-4.193406	5.249757
H	-2.240123	-1.977664	5.484010
H	-4.005755	-1.722470	5.333843
H	-1.291557	-4.399415	5.318648
H	-2.369535	-4.704924	6.697273
H	-2.413424	-5.776459	5.286201
H	-1.424601	4.611179	3.966371
H	0.613398	5.547801	5.106177
H	0.038218	4.889025	6.650506
H	0.486730	3.795455	5.320612
H	-1.594816	6.945301	4.901418
H	-3.146064	6.094030	4.975884
H	-2.159815	6.273492	6.443552
H	-3.480887	2.086049	6.802140
H	-2.562148	0.802040	5.996745
H	-5.808258	2.712494	5.855403
H	-5.157872	2.996507	4.222038
H	-6.447904	1.812459	4.467677

YBRSTS1MP.xyz

128

scf done: -2432.665938

C	-3.524964	4.176042	-0.459061
C	-4.032172	3.089126	0.307379
C	-5.294405	2.546251	-0.044391
C	-5.973995	2.987186	-1.176316
C	-5.458185	3.993861	-1.997071
C	-4.249128	4.570192	-1.592014

O	-3.387800	2.564496	1.338354
Y	-2.933144	0.666956	2.305518
O	-3.370708	-1.524338	2.781150
C	-3.425839	-1.638646	4.077995
O	-4.631861	-2.204107	4.646452
C	-3.887832	-3.232141	5.351890
C	-4.285893	-4.625022	4.914974
C	-5.955379	1.581363	0.898824
N	-5.279678	0.286069	1.188029
C	-5.054050	-0.515295	-0.033079
C	-3.767419	-0.165186	-0.770147
N	-2.550543	-0.424592	0.023655
C	-2.257643	-1.865293	0.063945
C	-6.220669	4.435355	-3.253595
C	-6.362833	3.238544	-4.215002
C	-2.262400	4.940412	-0.024560
C	-2.487486	5.489942	1.398855
O	-0.818726	0.634889	2.148599
C	0.188631	0.268219	1.362293
C	-0.056059	0.045931	-0.016027
C	0.977786	-0.357230	-0.857135
C	2.283169	-0.542558	-0.396412
C	2.505052	-0.307504	0.963958
C	1.507234	0.090668	1.861775
C	-1.417565	0.309989	-0.605488
C	1.830612	0.335923	3.344354
C	1.493359	1.793624	3.719092
C	3.389911	-0.975508	-1.367428
C	3.017208	-2.326636	-2.009205
O	-3.290609	-0.239186	4.549094
C	-3.415963	0.120619	5.919089
C	-4.825960	0.607090	6.228928
C	-2.327591	1.156192	6.219995
C	-2.418292	2.388722	5.354758
O	-2.172122	3.495514	6.036941
C	-2.152671	4.772269	5.318223
C	-1.158101	5.645418	6.058534
O	-2.666311	2.382066	4.152784
C	1.016505	-0.635054	4.223172
C	3.315281	0.111167	3.671277
C	3.546808	0.085093	-2.475269
C	4.747943	-1.139922	-0.671626
C	-6.167879	-0.464229	2.094148
C	-1.022103	4.027694	-0.025481
C	-1.955269	6.136119	-0.940056
C	-7.624229	4.938666	-2.861647
C	-5.504785	5.565203	-4.005859
C	-2.557839	-2.675273	4.830111
C	-3.562158	5.336707	5.287190
H	-3.203270	-0.762005	6.535074

H	-3.734228	-0.740108	-1.712237
H	-3.780080	0.892856	-1.039690
H	-5.901759	-0.399602	-0.728437
H	-5.030465	-1.566643	0.267655
H	-6.971101	1.365427	0.525578
H	-6.073981	2.073193	1.874724
H	-1.385656	0.058624	-1.678940
H	-1.664121	1.375636	-0.534027
H	3.507919	-0.440628	1.348941
H	0.746048	-0.521292	-1.908186
H	-3.847077	5.380260	-2.186538
H	-6.936713	2.533379	-1.407682
H	-2.117470	-2.259813	-0.955840
H	-1.342599	-2.032386	0.632697
H	-3.062064	-2.400035	0.566942
H	-7.140416	-0.670715	1.617474
H	-5.689179	-1.396062	2.393126
H	-6.354446	0.127815	2.995263
H	-1.591701	6.020991	1.745819
H	-3.326133	6.195543	1.411896
H	-2.706999	4.672341	2.088726
H	-0.134235	4.598100	0.274494
H	-1.139818	3.195607	0.669883
H	-0.832903	3.627805	-1.028151
H	-1.071392	6.660724	-0.560986
H	-1.734177	5.824904	-1.967128
H	-2.779706	6.856949	-0.968628
H	-6.081824	5.841983	-4.894972
H	-5.400408	6.463389	-3.387841
H	-4.506919	5.262459	-4.340659
H	-6.916278	3.528335	-5.116550
H	-5.379057	2.869052	-4.523840
H	-6.899652	2.406719	-3.747893
H	-8.184068	5.253025	-3.750702
H	-8.209146	4.161575	-2.359580
H	-7.555438	5.794240	-2.181630
H	1.223622	-0.450116	5.285783
H	-0.053513	-0.519872	4.041769
H	1.290372	-1.673381	4.005056
H	3.484394	0.307535	4.735959
H	3.631262	-0.919167	3.474263
H	3.968040	0.784860	3.105727
H	1.693699	1.967019	4.784524
H	2.114044	2.489604	3.144003
H	0.445730	2.017907	3.510876
H	5.502164	-1.451774	-1.402454
H	5.092054	-0.201993	-0.222763
H	4.713342	-1.902888	0.113544
H	3.792621	-2.645675	-2.716174
H	2.911076	-3.104783	-1.245878

H	2.071978	-2.267454	-2.557825
H	4.329440	-0.209501	-3.184924
H	2.618971	0.220477	-3.039629
H	3.820772	1.055653	-2.048451
H	-4.025888	-3.119214	6.436949
H	-2.017343	-3.325091	4.139800
H	-1.866499	-2.283057	5.579597
H	-4.138415	-4.743393	3.837218
H	-3.684033	-5.377926	5.436100
H	-5.340003	-4.813932	5.141255
H	-1.810133	4.565044	4.301428
H	-1.072161	6.612106	5.553950
H	-1.482263	5.822629	7.088758
H	-0.168709	5.180886	6.078687
H	-3.560730	6.301626	4.771919
H	-4.237352	4.669841	4.745741
H	-3.942098	5.487980	6.302669
H	-2.351938	1.452610	7.271629
H	-1.346369	0.707459	6.021927
H	-4.924425	0.864129	7.289186
H	-5.074299	1.493113	5.635137
H	-5.538188	-0.184455	5.988471

YBRSTS2M.xyz

128

scf done: -2432.651665

C	-6.774463	-4.869978	8.019600
C	-6.982763	-4.668516	6.627908
C	-7.426896	-5.770426	5.842088
C	-7.551273	-7.016795	6.471058
C	-7.292685	-7.246822	7.825678
C	-6.918102	-6.135258	8.584075
O	-6.742697	-3.469550	6.112939
Y	-5.509801	-1.706613	6.351592
O	-7.604214	-1.080770	7.645295
C	-8.432970	-0.178301	7.718847
C	-8.257986	1.047971	8.565280
C	-7.358395	2.083834	7.857501
C	-7.442245	3.434702	8.555568
C	-7.806133	-5.604769	4.358914
C	-8.927923	-4.554902	4.237515
C	-7.432509	-8.624063	8.487291
C	-6.090185	-9.030004	9.127368
C	-6.523029	-3.694736	8.929155
N	-5.306614	-2.857269	8.705939
C	-5.285646	-1.829174	9.761444
O	-4.833535	-1.748584	4.333997
C	-3.858275	-2.135555	3.519557
C	-3.620222	-1.516040	2.261248
C	-2.512346	-1.945533	1.519574

C	-1.643136	-2.965756	1.921150
C	-1.944749	-3.601020	3.127423
C	-3.030221	-3.216868	3.910706
C	-4.571658	-0.443963	1.705481
C	-5.989840	-1.039029	1.584944
C	-3.390214	-4.029241	5.122609
N	-3.417359	-3.301935	6.422831
C	-2.119942	-2.658488	6.652104
C	-0.430640	-3.413123	1.094357
C	0.851746	-3.264910	1.936718
O	-6.200452	0.531384	5.912175
C	-5.438034	1.144977	6.723306
C	-4.209985	1.960376	6.305755
C	-3.317160	1.128445	7.218092
C	-1.949582	0.772556	6.679377
O	-4.253360	0.034247	7.349146
C	-3.680957	-4.296631	7.478374
C	-4.071668	-3.660904	8.799735
C	-0.600096	-4.889940	0.685771
C	-0.256226	-2.582205	-0.184484
C	-4.608260	0.784577	2.633091
C	-4.156371	0.044062	0.309164
C	-6.597525	-5.147783	3.521163
C	-8.329166	-6.909422	3.737433
C	-8.517192	-8.564251	9.581042
C	-7.828258	-9.717152	7.484833
O	-5.995696	1.672796	7.894940
O	-9.569270	-0.153558	7.044196
C	-9.852764	-1.208111	6.067731
C	-9.681963	-0.599326	4.687084
C	-11.259885	-1.695972	6.356755
H	-2.790494	-4.930964	7.633282
H	-4.487260	-4.949763	7.139436
H	-4.183974	-4.449810	9.560727
H	-3.269072	-3.003257	9.148754
H	-6.488579	-4.066530	9.967288
H	-7.367944	-3.003248	8.859206
H	-2.677992	-4.867563	5.207528
H	-4.388314	-4.461554	4.998365
H	-2.321676	-1.459442	0.571145
H	-1.333836	-4.433426	3.474193
H	-7.871339	-7.855060	5.866039
H	-6.743386	-6.241491	9.653886
H	-1.315526	-3.408824	6.731369
H	-1.890091	-1.999606	5.815277
H	-2.143579	-2.065907	7.567485
H	-5.166135	-2.282589	10.759068
H	-4.474421	-1.123757	9.572344
H	-6.224857	-1.274829	9.737532
H	-9.211736	-4.422527	3.186284

H	-9.817879	-4.871718	4.793374
H	-8.589005	-3.594600	4.629014
H	-6.882209	-5.061980	2.465442
H	-6.229189	-4.175423	3.851107
H	-5.782515	-5.877900	3.584278
H	-8.607840	-6.722689	2.694716
H	-7.570628	-7.699959	3.735193
H	-9.218882	-7.286490	4.253537
H	-7.901577	-10.681618	7.999195
H	-8.801302	-9.515838	7.024290
H	-7.087253	-9.824386	6.685402
H	-6.174432	-10.008857	9.614595
H	-5.300932	-9.093444	8.370625
H	-5.768048	-8.308856	9.885340
H	-8.626435	-9.538850	10.071976
H	-8.273465	-7.827888	10.353559
H	-9.486326	-8.287935	9.152489
H	-5.260610	1.558324	2.208515
H	-4.989944	0.518971	3.619475
H	-3.605017	1.215419	2.738388
H	-4.882574	0.785173	-0.042353
H	-3.172881	0.527428	0.315048
H	-4.136034	-0.769248	-0.424486
H	-6.689355	-0.279435	1.214162
H	-5.996939	-1.878075	0.880398
H	-6.344215	-1.397289	2.553095
H	0.626362	-2.928058	-0.733696
H	-1.118196	-2.677505	-0.853365
H	-0.112514	-1.519451	0.038218
H	1.729905	-3.591613	1.366633
H	1.005928	-2.221316	2.231389
H	0.807268	-3.865348	2.850942
H	0.263396	-5.232632	0.102752
H	-0.692822	-5.543395	1.558988
H	-1.499105	-5.023466	0.074945
H	-3.210778	1.603546	8.203641
H	-3.990063	1.793891	5.249426
H	-4.283257	3.029994	6.517654
H	-2.023842	0.295594	5.697829
H	-1.360701	1.690220	6.566474
H	-1.402372	0.111894	7.357507
H	-9.124885	-2.007089	6.228970
H	-9.873889	-1.357536	3.922601
H	-10.384855	0.227072	4.539302
H	-8.664980	-0.222607	4.550110
H	-11.524383	-2.488411	5.650931
H	-11.334735	-2.103088	7.369026
H	-11.985691	-0.883406	6.251599
H	-7.680828	2.177317	6.814186
H	-7.785348	0.772875	9.512096

H	-9.237358	1.491101	8.762014
H	-7.123065	3.350901	9.599303
H	-6.788735	4.154466	8.056234
H	-8.465581	3.822033	8.534045

YBRSTS2MR.xyz

128

scf done: -2432.654782

C	-6.799670	-4.940291	8.055256
C	-7.031173	-4.783154	6.662249
C	-7.459800	-5.913620	5.911558
C	-7.541727	-7.146739	6.572135
C	-7.256061	-7.334717	7.928229
C	-6.901860	-6.194456	8.653194
O	-6.828020	-3.594002	6.109379
Y	-5.621964	-1.828242	6.320321
O	-7.817180	-1.194400	7.546311
C	-8.476735	-0.158407	7.549010
C	-8.302877	0.945317	8.554382
C	-7.177734	1.930199	8.163037
C	-7.144718	3.106197	9.131308
C	-7.865560	-5.787264	4.432235
C	-9.012559	-4.764221	4.308401
C	-7.346058	-8.697806	8.626929
C	-5.980374	-9.050859	9.248854
C	-6.575260	-3.733048	8.928685
N	-5.369681	-2.881416	8.685469
C	-5.372516	-1.822515	9.711255
O	-4.941028	-1.846669	4.306442
C	-3.933476	-2.185549	3.510421
C	-3.687603	-1.537020	2.268905
C	-2.560282	-1.931304	1.537264
C	-1.672704	-2.936028	1.938510
C	-1.968315	-3.586040	3.138586
C	-3.074328	-3.238598	3.910125
C	-4.646916	-0.465592	1.726443
C	-6.054880	-1.075669	1.569484
C	-3.417232	-4.052183	5.125642
N	-3.479061	-3.309571	6.418417
C	-2.218086	-2.594829	6.645089
C	-0.443158	-3.348672	1.118762
C	0.828956	-3.174694	1.971629
O	-6.150883	0.383042	6.098820
C	-5.343773	0.976289	6.933583
C	-4.368862	2.081574	6.470239
C	-3.253779	1.221534	7.068115
C	-2.068338	0.906051	6.188530
O	-4.173430	0.098864	7.288511
C	-3.708739	-4.300406	7.485785
C	-4.120730	-3.661712	8.799622

C	-0.574588	-4.826660	0.700378
C	-0.279334	-2.506324	-0.153932
C	-4.707794	0.739254	2.685113
C	-4.218861	0.063512	0.349053
C	-6.676910	-5.325567	3.567908
C	-8.370143	-7.115853	3.847496
C	-8.409455	-8.638857	9.741370
C	-7.732077	-9.825957	7.660218
O	-5.918112	1.277610	8.211071
O	-9.433197	0.120066	6.677634
C	-9.707200	-0.806878	5.581271
C	-9.350030	-0.093610	4.289474
C	-11.171909	-1.191839	5.687529
H	-2.798663	-4.904361	7.646423
H	-4.495621	-4.981156	7.153839
H	-4.226554	-4.446451	9.565027
H	-3.333163	-2.987147	9.150610
H	-6.537113	-4.071090	9.977805
H	-7.431228	-3.058229	8.832501
H	-2.679216	-4.865531	5.226402
H	-4.400814	-4.517676	4.999571
H	-2.367784	-1.428312	0.598037
H	-1.335330	-4.399936	3.489570
H	-7.849521	-8.007555	5.992661
H	-6.712229	-6.268595	9.723190
H	-1.377272	-3.299244	6.757567
H	-2.013543	-1.951160	5.789816
H	-2.284345	-1.974529	7.540879
H	-5.262951	-2.247024	10.722396
H	-4.564437	-1.114545	9.518587
H	-6.314636	-1.276480	9.656580
H	-9.308084	-4.651181	3.258159
H	-9.890080	-5.095068	4.875274
H	-8.697065	-3.791206	4.688415
H	-6.977582	-5.267099	2.514697
H	-6.320852	-4.340532	3.872727
H	-5.847800	-6.039571	3.634988
H	-8.670930	-6.958264	2.806102
H	-7.594504	-7.889708	3.849052
H	-9.242352	-7.500395	4.387342
H	-7.770336	-10.778614	8.199751
H	-8.718550	-9.661089	7.214040
H	-7.003880	-9.934374	6.849253
H	-6.027153	-10.018742	9.762339
H	-5.204964	-9.111940	8.477721
H	-5.663663	-8.301629	9.981470
H	-8.483644	-9.603831	10.257234
H	-8.168733	-7.878414	10.491154
H	-9.393867	-8.397145	9.327076
H	-5.384786	1.504586	2.284440

H	-5.067776	0.445288	3.672300
H	-3.715507	1.195284	2.788079
H	-4.947211	0.807432	0.008025
H	-3.239907	0.554919	0.380357
H	-4.182433	-0.729845	-0.405550
H	-6.758496	-0.316477	1.205923
H	-6.039190	-1.896653	0.844059
H	-6.419421	-1.463707	2.522053
H	0.614236	-2.828876	-0.699507
H	-1.134711	-2.616863	-0.828893
H	-0.160635	-1.441975	0.075789
H	1.718933	-3.476294	1.406174
H	0.955553	-2.129454	2.273621
H	0.792675	-3.781803	2.881794
H	0.300610	-5.145068	0.121132
H	-0.657447	-5.487463	1.569042
H	-1.466093	-4.977807	0.082715
H	-2.921970	1.583590	8.048935
H	-4.324362	2.146844	5.381591
H	-4.517619	3.068608	6.911428
H	-2.390537	0.481129	5.233444
H	-1.521843	1.833652	5.983406
H	-1.373403	0.213647	6.671657
H	-9.073103	-1.684486	5.729039
H	-9.520840	-0.761103	3.439566
H	-9.970729	0.798699	4.157436
H	-8.299482	0.206863	4.289275
H	-11.429006	-1.887592	4.883535
H	-11.380458	-1.683291	6.642036
H	-11.814382	-0.309938	5.599313
H	-7.372862	2.289442	7.144795
H	-8.048454	0.500647	9.520886
H	-9.244262	1.493378	8.648782
H	-6.944730	2.758849	10.150161
H	-6.350030	3.801992	8.849546
H	-8.095907	3.647976	9.128652

YBRSTS2MP.xyz

128

scf done: -2432.697352

C	-6.980539	-5.130156	7.097301
C	-7.087254	-4.758279	5.731584
C	-7.564253	-5.721087	4.798914
C	-7.818799	-7.015853	5.268253
C	-7.663338	-7.417220	6.600583
C	-7.256672	-6.433081	7.505174
O	-6.739396	-3.529459	5.382370
Y	-5.154099	-2.104781	5.810595
O	-8.528223	-0.380921	8.975645
C	-9.399715	0.463394	8.939691

C	-10.011405	1.019356	7.669750
C	-9.213280	0.661692	6.429076
C	-9.876335	1.094352	5.133823
C	-7.823479	-5.342612	3.331426
C	-8.829733	-4.174360	3.274676
C	-7.948720	-8.844520	7.087292
C	-6.686027	-9.426326	7.753314
C	-6.699644	-4.065127	8.119524
N	-5.371915	-3.382511	8.076981
C	-5.345463	-2.417293	9.191174
O	-4.206798	-1.904242	3.913192
C	-3.113221	-2.251975	3.245807
C	-2.580424	-1.463034	2.189875
C	-1.409932	-1.907324	1.564206
C	-0.731509	-3.081260	1.909675
C	-1.285041	-3.840803	2.942377
C	-2.450811	-3.454206	3.599436
C	-3.271562	-0.163757	1.746480
C	-4.716172	-0.465273	1.298687
C	-3.053523	-4.366199	4.633483
N	-3.256656	-3.776973	5.991516
C	-2.013955	-3.164456	6.482679
C	0.550799	-3.550304	1.208798
C	1.692299	-3.664215	2.238451
O	-6.862268	-0.398581	5.703975
C	-6.835040	0.731041	6.198733
C	-5.583607	1.503677	6.461225
C	-4.639136	0.742211	7.446849
C	-3.368446	1.568862	7.653627
O	-4.356565	-0.518351	6.981017
C	-3.723253	-4.850324	6.890222
C	-4.249772	-4.332944	8.221980
C	0.311548	-4.930030	0.564106
C	1.002548	-2.582343	0.106687
C	-3.281569	0.841869	2.915186
C	-2.557379	0.512441	0.566107
C	-6.512569	-4.926716	2.636173
C	-8.421762	-6.505192	2.524354
C	-9.097568	-8.820389	8.115203
C	-8.355243	-9.782800	5.942969
O	-7.943183	1.364016	6.561685
O	-9.973470	1.012781	10.017217
C	-9.529789	0.550871	11.324134
C	-10.723693	0.699909	12.248824
C	-8.319951	1.363959	11.755388
H	-2.905672	-5.566642	7.084845
H	-4.518510	-5.398087	6.376971
H	-4.546851	-5.193497	8.841259
H	-3.445926	-3.822647	8.761870
H	-6.828933	-4.498275	9.125944

H	-7.444015	-3.265246	8.015842
H	-2.413303	-5.258333	4.731358
H	-4.040807	-4.712673	4.301968
H	-1.007269	-1.301953	0.762309
H	-0.809307	-4.771428	3.248077
H	-8.164741	-7.750807	4.552272
H	-7.165088	-6.669579	8.564658
H	-1.222793	-3.919726	6.618555
H	-1.667621	-2.425617	5.758261
H	-2.188795	-2.652347	7.430721
H	-5.392326	-2.933019	10.164654
H	-4.439294	-1.812663	9.132357
H	-6.207000	-1.749064	9.118428
H	-9.008808	-3.880521	2.233006
H	-9.789901	-4.471906	3.711713
H	-8.450706	-3.309355	3.821959
H	-6.705619	-4.671711	1.586931
H	-6.062014	-4.057072	3.116944
H	-5.789837	-5.751105	2.648404
H	-8.612634	-6.170301	1.498971
H	-7.741720	-7.362383	2.465551
H	-9.374838	-6.849233	2.941130
H	-8.535326	-10.789245	6.336183
H	-9.276579	-9.451084	5.452748
H	-7.571406	-9.858803	5.181837
H	-6.873190	-10.443651	8.117875
H	-5.854895	-9.467793	7.041166
H	-6.363514	-8.822434	8.607470
H	-9.310008	-9.831199	8.484257
H	-8.854123	-8.194781	8.979787
H	-10.013248	-8.422794	7.665006
H	-3.804463	1.761380	2.621880
H	-3.778101	0.414795	3.788028
H	-2.258401	1.111845	3.200125
H	-3.098710	1.425189	0.293669
H	-1.530246	0.802514	0.813811
H	-2.529435	-0.129865	-0.320920
H	-5.222213	0.462045	1.001577
H	-4.716424	-1.139946	0.435435
H	-5.286293	-0.935840	2.100935
H	1.918409	-2.957954	-0.362574
H	0.247375	-2.478579	-0.679701
H	1.220344	-1.585754	0.505474
H	2.615478	-4.007725	1.756051
H	1.892742	-2.694695	2.706764
H	1.449953	-4.374824	3.035064
H	1.220102	-5.286386	0.063652
H	0.025787	-5.680476	1.307962
H	-0.490260	-4.878609	-0.179940
H	-5.170959	0.695201	8.419809

H	-5.047848	1.606087	5.510432
H	-5.836270	2.497074	6.839744
H	-2.830939	1.675854	6.705439
H	-3.586167	2.566052	8.053624
H	-2.710436	1.049775	8.356758
H	-9.249468	-0.501850	11.218884
H	-10.465320	0.346487	13.251470
H	-11.030453	1.747890	12.322459
H	-11.573744	0.115214	11.886876
H	-7.983658	1.040433	12.745469
H	-7.492726	1.228007	11.054469
H	-8.569388	2.428430	11.808070
H	-8.998495	-0.408556	6.415299
H	-10.124387	2.103937	7.769279
H	-11.025104	0.609733	7.580588
H	-10.049670	2.174855	5.120745
H	-9.249190	0.827539	4.279595
H	-10.838625	0.586752	5.016262

References

-
- (1) Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *J. Appl. Cryst.* **1999**, *32*, 115-119.
 - (2) Sheldrick, G. M. *Acta Cryst. A64* **2008**, 112-122.
 - (3) Farrugia, L. J. *J. Appl. Cryst.* **1999**, *32*, 837-838.
 - (4) Sluis, P. V.D.; Spek, A.L. *Acta Cryst. A990* **A46**, 194-201.
 - (5) Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7-13.
 - (6) Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.
 - (7) Becke, A. D. *J. Chem. Phys.* 1993, **98**, 5648-5642.
 - (8) Perdew, J. P.; Wang, Y. *Phys. Rev. B* 1992, **45**, 13244-13249.
 - (9) Andrae, D.; Haeussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. *Theor. Chim. Acta* 1990, **77**, 123-141.
 - (10) (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* 1971, **54**, 724-728. (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* 1972, **56**, 2257-2261. (c) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta*. 1973, **28**, 213-222.
 - (11) Schlegel, H. B. *J. Comput. Chem.* 1982, **3**, 214-218.
 - (12) (a) Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys.* 1989, **90**, 2154-2161. (b) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* 1990, **94**, 5523-5527.