Supplementary Information

# Investigating the photophysical properties of rhodamines using a spectroscopic single-molecule fluorescence method

Shangyuan Deng,<sup>‡ab</sup> Deqi Yi,<sup>‡ab</sup> Thitima Rujiralai,<sup>c</sup> Qinghua Ren,§<sup>d</sup> Chuang Tan§<sup>ab</sup> and Jie Ma§<sup>ab</sup>

<sup>a</sup> School of Physics, Sun Yat-sen University, Guangzhou 510275, China. E-mail: tanch26@mail.sysu.edu.cn; majie6@mail.sysu.edu.cn

<sup>b</sup> State Key Laboratory of Optoelectronic Materials and Technologies, Sun Yat-sen University, Guangzhou 510006, China

° Division of Physical Science, Faculty of Science, Prince of Songkla University, Songkhla, 90110, Thailand

<sup>d</sup> Department of Chemistry, Shanghai University, Shanghai 200444, China. E-mail: qinghua.ren@shu.edu.cn

‡ These authors contributed equally to this work.

§ Regarded as co-corresponding authors.



Fig. S1 The molecular structures of different kinds of rhodamine B in their "open" forms.

**Table S1** The reported peak wavelengths in the absorption spectra and emission spectra of five kinds of rhodamine B in 0.1% TFA – ethanol.<sup>1</sup>

	RhB-1	RhB-2	RhB-3a	RhB-3b	RhB-4	RhB-5
Absorption peak (nm)	554	540	531	528	519	509
Emission peak (nm)	578	564	556	554	543	531



Fig. S2 The blue shift of the emission peak of a single RhB molecule due to the transition to its dealkylated product. (a) Time profile of the blue shift process. (b) The variation of the peak wavelength with time. The peak wavelength shifts from  $\sim$  570 nm to  $\sim$  558 nm after transition at t = 13.5 s.



**Fig. S3** Single-molecule fluorescence signals and photobleaching lifetimes of three types of rhodamine B molecules in T50 buffer (pH 4.9). (a)-(c) Typical single-molecule fluorescence trajectories measured for RhB-1, RhB-2, and RhB-3 molecules, respectively. (d)-(f) Photobleaching time distributions of RhB-1, RhB-2, and RhB-3 molecules fitted with single exponential functions to generate characteristic photobleaching lifetimes. The photobleaching lifetime of RhB-1 molecules is  $32.5\pm2.1$  s, RhB-2 molecules is  $66.2\pm2.5$  s, and RhB-3 molecules is  $23.6\pm1.3$  s.



**Fig. S4** Single-molecule fluorescence signals and photobleaching lifetimes of three types of rhodamine B molecules in T50 buffer (pH 8.0 with PCA-PCD OSS). (a)-(c) Typical single-molecule fluorescence trajectories measured for RhB-1, RhB-2, and RhB-3 molecules. (d)-(f) Photobleaching time distributions of RhB-1, RhB-2, and RhB-3 molecules fitted with single exponential functions to generate characteristic photobleaching lifetimes. The photobleaching lifetime of RhB-1 molecules is 78.1±3.1 s, RhB-2 molecules is 113.3±4.1 s, and RhB-3 molecules is 62.9±3.3 s.



**Fig. S5** Single-molecule fluorescence signals and photobleaching lifetimes of three types of rhodamine B molecules in T50 buffer (pH 10.3). (a)-(c) Typical single-molecule fluorescence trajectories measured for RhB-1, RhB-2, and RhB-3 molecules in T50 buffer. (d)-(f) Photobleaching time distributions of RhB-1, RhB-2, and RhB-3 molecules in T50 buffer, fitted with single exponential functions to generate characteristic photobleaching lifetimes. The photobleaching lifetime of RhB-1 molecules is 23.8±1.6 s, RhB-2 molecules is 53.3±1.8 s, and RhB-3 molecules is 18.1±1.5 s.

**Table S2** The measured populations of RhB-1, RhB-2, and RhB-3 within the same sample under different T50buffer conditions (pH 4.9, pH 8.0, pH 10.3).

		T50 (pH 4.9)	T50 (pH 8.0)	T50 (pH 10.3)
	RhB-1	42%	43%	44%
Population	RhB-2	37%	38%	36%
	RhB-3	21%	19%	20%

### **Computational details**

Gaussian 16 program<sup>2</sup> is used for the density functional theory (DFT) calculations<sup>3</sup> in the gas phase geometry optimization where the B3LYP-D3 method<sup>4</sup> is selected using the Gaussian keyword "Empirical Dispersion = GD3" and the C, N, O and H atoms use 6-31G (d,p) basis set.<sup>5</sup> Frequency analysis is performed at the same level to ensure that the optimized geometry is at the minimum point on the potential energy surface without imaginary frequencies. Then the time-dependent DFT (TD-DFT) calculations<sup>6</sup> are preformed to calculate the fluorescent emission wavelengths using the M06 functionals<sup>7</sup> combined with the 6-31+G (d, p) basis set in water solvent with a SMD model.<sup>8</sup>

#### RhB-1\_open

RhB-2\_open



Fig. S6 Fully optimized structures of the "open"/fluorescent form of rhodamine molecules RhB-1, RhB-2, RhB-3a, and RhB-3b. (Color scheme: C, cyan; H, white; O, red; N, blue. Distances are given in Å.)

## Cartesian coordinates (xyz file) of all molecules

1	1
h	Д
v	

RhB-1	_open (charge=1 m	ultiplicity=1 E	= -1263.519283 Hartree)
С	-0.02231200	5.29275000	-1.35492800
С	0.39828900	4.91798100	-0.08213000
С	0.34434200	3.57957200	0.32921200
С	-0.12252500	2.59467200	-0.56832800
С	-0.54657400	2.98621500	-1.84598800
С	-0.50078000	4.32399300	-2.23754900
Н	0.02051700	6.33454900	-1.65478600
Н	0.77092100	5.65266200	0.62307000
Н	-0.89720900	2.22873400	-2.53997000
Н	-0.83203400	4.60390500	-3.23248200
С	-0.12251000	1.13637000	-0.26293600
С	0.78291400	3.30719300	1.73253200
0	1.47516900	4.05949400	2.38287200
С	1.08991800	0.41877400	-0.21056600
С	1.06175300	-0.98326100	0.03773200
С	2.37966500	0.99069200	-0.39683200
С	2.19872900	-1.75921500	0.11546000
С	3.52224400	0.24256400	-0.31715500
Н	2.45381000	2.05047400	-0.61164900
С	3.48106100	-1.16959800	-0.03752200
Н	2.06461000	-2.81647900	0.28965100
Н	4.46845600	0.73856600	-0.47611500
С	-1.33382700	0.44229600	-0.08261400
С	-2.62310500	1.04810900	-0.08765000
С	-1.30636100	-0.96278300	0.15479100
С	-3.76463800	0.32084000	0.10353000
Н	-2.69174600	2.11803200	-0.24575300
С	-2.44471700	-1.71680300	0.34816300
С	-3.72234000	-1.09972600	0.33680800
Н	-4.71281200	0.83884500	0.08498200
Н	-2.31670200	-2.77778200	0.50501300
0	-0.12388900	-1.63507700	0.20156400
Ν	4.62526000	-1.89671600	0.07138300
Ν	-4.85901100	-1.81036700	0.55621400
С	5.92672000	-1.24622700	-0.21729800
Н	6.00695700	-0.35885300	0.41904400
Н	5.92468700	-0.89972200	-1.25925100
С	7.16236900	-2.10863700	0.01958800
Н	8.04202400	-1.50314100	-0.21524800
Н	7.25140700	-2.42463800	1.06247900
Н	7.19279400	-2.99164000	-0.62397600

U	-6.19027500	-1.18504200	0.45943400
Н	-6.88363100	-1.83137400	1.00154100
Н	-6.17966400	-0.23609300	1.00351500
С	-6.67808500	-0.98495600	-0.97896100
Н	-6.77940400	-1.94190500	-1.49654400
Н	-7.65620500	-0.49496900	-0.97528100
Н	-5.98590900	-0.36260500	-1.55270200
С	-4.81443000	-3.26644200	0.76964300
Н	-5.73068900	-3.54080400	1.29708700
Н	-3.99345000	-3.49653600	1.45545400
С	-4.69064400	-4.08105700	-0.52245700
Н	-4.62650600	-5.14708300	-0.28502100
Н	-5.55984200	-3.92952500	-1.16698300
Н	-3.79760400	-3.80177900	-1.08825100
0	0.30179000	2.14288500	2.23225500
Н	0.64072700	2.07655600	3.14135700
С	4.56221300	-3.35656600	0.23875600
Н	3.78205300	-3.58886200	0.96790800
Н	5.49237300	-3.68609400	0.69749500
С	4.32783800	-4.10207000	-1.07884900
Н	3.39448700	-3.78603900	-1.55302800
Н	5.14379000	-3.91312700	-1.78244900
Н	4.27587900	-5.17991800	-0.89912600
58			
RhE	B-2_open (charge=1 mu	ultiplicity=1 E	= -1263.519283 Hartree)
С	-1.20146700	4.93030200	1.25647900
С	-1.51051200	4.46385300	-0.01768600
С	-1.22814500		
		3.14229300	-0.38975900
С	-0.63852400	<ul><li>3.14229300</li><li>2.26805300</li></ul>	-0.38975900 0.54917900
C C	-0.63852400 -0.32904400	<ul><li>3.14229300</li><li>2.26805300</li><li>2.75124900</li></ul>	-0.38975900 0.54917900 1.82814900
C C C	-0.63852400 -0.32904400 -0.60506400	<ul><li>3.14229300</li><li>2.26805300</li><li>2.75124900</li><li>4.07208900</li></ul>	-0.38975900 0.54917900 1.82814900 2.18072900
C C C H	-0.63852400 -0.32904400 -0.60506400 -1.42236300	<ul><li>3.14229300</li><li>2.26805300</li><li>2.75124900</li><li>4.07208900</li><li>5.95786300</li></ul>	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800
C C C H H	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500
C C H H H	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000
C C H H H	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800
C C H H H H C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100
C C H H H C C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400
C C H H C C O	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100 -2.31611100	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600 3.41709800	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400 -2.50328800
C C H H C C C C C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100 -2.31611100 -1.43880800	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600 3.41709800 -0.10265900	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400 -2.50328800 0.27054100
C C H H C C C C C C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100 -2.31611100 -1.43880800 -1.15292800	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600 3.41709800 -0.10265900 -1.48383800	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400 -2.50328800 0.27054100 0.05657900
C C H H C C C C C C C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100 -2.31611100 -1.43880800 -1.15292800 -2.80790100	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600 3.41709800 -0.10265900 -1.48383800 0.24193600	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400 -2.50328800 0.27054100 0.05657900 0.45546200
C C H H C C C C C C C C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100 -2.31611100 -1.43880800 -1.15292800 -2.80790100 -2.13494600	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600 3.41709800 -0.10265900 -1.48383800 0.24193600 -2.44984000	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400 -2.50328800 0.27054100 0.05657900 0.45546200 0.01685700
C C H H C C C C C C C C C	-0.63852400 -0.32904400 -0.60506400 -1.42236300 -1.97101200 0.11692900 -0.35904200 -0.37621700 -1.57264100 -2.31611100 -1.43880800 -1.15292800 -2.80790100 -2.13494600 -3.80080300	3.14229300 2.26805300 2.75124900 4.07208900 5.95786300 5.11221700 2.07730900 4.42454600 0.82505200 2.77176600 3.41709800 -0.10265900 -1.48383800 0.24193600 -2.44984000 -0.70026500	-0.38975900 0.54917900 1.82814900 2.18072900 1.52557800 -0.75480500 2.55290000 3.17733800 0.28326100 -1.79702400 -2.50328800 0.27054100 0.05657900 0.45546200 0.01685700 0.41689500

H-1.85180100-3.48350700-0.14937600H-4.830211000.360678000.10397000C0.939031001.038678000.07907400C1.16868300-1.031288000.07997400C3.348474000.68460300-0.11047900C2.42430400-1.567910000.28862000C2.42430400-1.567910000.28862000C3.56655100-0.725519000.30932700H4.185804001.367450000.11156600D0.12879500-1.90978900-0.11583900N-4.458047003.018934000.15297700N4.81227200-1.220468000.52402900C-5.891904002.777225000.31941900H-6.235264002.07593200-0.45175500H-6.66399500-2.037914001.2948200C-6.66399500-3.09269000.4520000H-6.73296000-3.012980001.2948200C-6.66399500-0.351860100.19932100C6.00298400-0.351860100.99932100C6.0599400-0.51783001.44824200C6.0599500-0.666704001.44824200C6.0599500-0.518642009.0199300C6.3598400-0.91735001.44824200C6.9579900-0.518642009.06670400C6.9579900-0.666704001.44824200C5.039207002.668769000.66670400C5.039207002.66876						
H-4.83021100-0.398145000.50662000C0.939031000.360678000.01937000C2.094645001.193897000.09957400C3.348474000.68460300-0.11047900C3.348474002.261315000.21560700C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.11156600H2.49275300-2.63768900-0.42080800O0.12879500-1.20468000.52402900C-5.89190400-2.777225000.31941900H-6.23526400-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-0.351869000.21978000H-6.3743800-4.59969000.34520000H-6.51743800-4.5996900-0.75738500H-6.35098400-3.5186900-0.49993800H-6.78642200-0.87282900-1.06766100C6.4957900-0.14890000.91091100H5.791234000.55864200-1.06766100C5.03920700-2.68676900-0.66670400H5.79123400-2.7932300-1.17762000H5.79123400-2.7932300-1.1762000H5.79123400-2.68676900-0.66670400H5.99612100-2.7932300-1.44824200H5.89291100-2.7932300-1.44821500H5.8642701 </td <td></td>						
C0.939031000.360678000.10397000C2.094645001.193897000.09957400C3.348474000.68460300-0.11047900H1.966063002.261315000.21560700C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.42080800O0.12879500-1.90978900-0.11156600H2.49275300-2.63768900-0.42080800O0.12879500-1.2046800-0.52402900C-5.89190400-2.777225000.31941900H-6.23526400-2.307194001.29482200C-5.89190400-2.307194001.29482200C-6.66399500-4.088560000.21978000H-6.51743800-4.55996900-0.45175500H-6.35098400-4.790514000.99932100C6.00298400-0.35186900-0.49993800H5.791234000.5584200-1.6676100C6.49579900-0.5145001.44824200H5.791234000.5584200-1.6667400H5.7962100-2.79392300-1.1776200H5.87291100-2.79392300-1.1776200H5.87291100-3.09259001.34215800C5.05284600-3.428802000.66404500H5.87291100-3.09216001.30201100H5.87291100-3.09259001.21353300H5.1864270-						
C2.094645001.193897000.07907400C1.16868300-1.03128800-0.09957400C3.348474000.68460300-0.11047900H1.966063002.261315000.21560700C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.42080800O0.12879500-1.90978900-0.11563900N-4.45804700-3.018934000.15297700N4.45804700-2.07593200-0.45175500C-5.89190400-2.777225000.31941900H-6.23526400-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-6.51743800-4.55996900-0.75738500H-6.51743800-4.790514000.99932100C6.00298400-0.5186900-0.49993800H5.791234000.5584200-1.6676100C6.49579900-0.5185900-1.6766100C6.39920700-2.68876900-0.66670400H5.79123400-2.79392300-1.17762000H5.7962100-2.79392300-1.1776200H5.87291100-3.09259001.34215800C5.05284600-3.428802000.66404500H5.18642700+4.49871000.47895100H5.18642700-4.49873001.21353300H5.18642700<						
C1.16868300-1.03128800-0.09957400C3.348474000.684603000.11047900H1.966063002.261315000.21560700C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.42080800O0.12879500-1.90978900-0.11156600N4.45804700-3.018934000.15297700N4.45804700-3.018934000.15297700N4.45804700-2.777225000.31941900C-5.89190400-2.777225000.31941900H-6.07093600-2.307194001.29482200C-6.66399500-3.902696000.34520000H-6.517438004.5596900-0.75738500H-6.517438004.5596900-0.75738500H-6.35098400-0.99321000.49993800C6.00298400-0.87282900-1.05435100H5.791234000.55864200-1.06766100C6.4957900-0.014890000.91091100H5.791234000.51454000.85329200H5.79123400-3.07925001.14824200H5.99612100-3.07925001.34215800C5.05284600-3.428802000.66670400H5.18642700-3.498701000.47895100H5.99612100-3.09216001.30201100H5.18642700-3.428802001.21353300H5.18642700 <td< td=""><td></td></td<>						
C3.348474000.684603000.11047900H1.966063002.261315000.21560700C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.42080800O0.12879500-1.90978900-0.11583900N-4.458047003.018934000.15297700N4.45804700-2.07593200-0.45175500R-6.23526400-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-3.902696000.34520000H-6.51743800-4.59596900-0.75738500H-6.51743800-4.59596900-0.75738500H-6.51743800-4.59596900-0.75738500H-6.51743800-0.99938100-0.49993800H-6.35098400-0.51864200-1.06766100C6.00298400-0.51864200-1.06766100C6.09298400-0.517353001.44824200H-7.73214000.51845000.91099100H5.79123400-0.517435001.4824200H-7.36149500-0.666704001.99100H5.99612100-2.79323001.17762000H5.99612100-3.428802000.666404500H5.99612100-3.428802000.66404500H5.99612100-3.90216001.3020100H5.186427004.49871000.47895100H-1.7515800						
H1.966063002.261315000.21560700C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.1156600H2.49275300-2.63768900-0.42080800O0.12879500-1.90978900-0.11583900N-4.45804700-3.018934000.15297700N4.81227200-1.22046800-0.52402900C-5.89190400-2.777225000.31941900H-6.23526400-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-6.51743800-4.5996900-0.75738500H-6.51743800-4.790514000.99932100C6.00298400-0.35186900-0.4593100H5.791234000.55864200-1.06766100C6.49579900-0.014890000.91099100H5.791234000.651454000.85329200H5.718727000.483319001.49739700C5.03920700-2.66876900-0.6667400H5.99612100-3.092216001.3020100H4.28218700-3.09225001.314215800C5.05284600-3.428802000.66404500H5.87291100-3.090216001.30200100H5.87291100-3.090216001.314215800C5.05284600-3.99593001.21353300H4.11784400						
C2.42430400-1.56791000-0.28862000C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.11156600H2.49275300-2.63768900-0.42080800O0.12879500-1.90978900-0.15297700N-4.45804700-3.018934000.15297700N4.81227200-1.22046800-0.52402900C-5.89190400-2.777225000.31941900H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-6.51743800-4.59969000.34520000H-6.51743800-4.790514000.99932100C6.00298400-0.35186900-0.45435100H-6.35098400-0.35186900-0.49993800H6.78642200-0.87282900-1.05435100G6.49579900-0.014890000.91099100H5.791234000.55864200-1.06766100C6.49579000-0.014890000.91099100H5.718727000.483319001.49739700C5.03920700-2.66876900-0.6667400H5.99612100-2.79392300-1.17762000H4.28218700-3.090216001.3020100H4.1784400-3.290590001.21353300H4.11784400-3.290590001.21353300H4.11784400-3.290590001.21353300H4.1178400-3.905950001.21353300H4.11784						
C3.56655100-0.72551900-0.30932700H4.185804001.36745000-0.11156600H2.49275300-2.63768900-0.42080800O0.12879500-1.90978900-0.11583900N-4.458047003.018934000.15297700N4.81227200-1.22046800-0.52402900C-5.89190400-2.777225000.31941900H-6.23526400-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-7.73296900-3.902696000.34520000H-6.51743800-4.790514000.99932100C6.00298400-0.35186900-0.4535100H-6.7502400-0.3788500-1.05435100H6.78642200-0.87282900-1.05435100G6.49579900-0.014890000.91099100H5.791234000.51454000.85329200H5.791234000.51454000.85329200H5.791727000.483319001.44824200H5.79123400-2.793923001.17762000H5.718727000.687450900.66670400H5.79123400-3.07925500-1.34215800C5.03920700-2.668769000.66670400H5.87291100-3.07925500-1.34215800H5.87291100-3.07925001.13200100H5.87291100-3.290590001.21353300H5.87291100<						
H4.185804001.367450000.11156600H2.49275300-2.63768900-0.42080800O0.12879500-1.909789000.11583900N-4.45804700-3.018934000.15297700N4.81227200-1.22046800-0.52402900C-5.89190400-2.077925000.31941900H-6.07093600-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-7.73296900-3.902696000.34520000H-6.51743800-4.790514000.99932100C6.00298400-0.35186900-0.45993800H6.78642200-0.87282900-1.05435100H5.791234000.55864200-1.06766100C6.49579000-0.014890000.91099100H5.791234000.51454000.85329200H5.791234000.51454000.85329200H5.7918727000.651454000.85329200H5.7918727000.651454000.85329200H5.7918727000.66670400H5.7921700-1.34215800C5.03920700-2.66876900-0.66670400H5.99612100-3.07925500-1.34215800C5.05284600-3.290590001.30200100H4.18642700-3.97538400-0.00769900H5.87291100-3.97538400-0.00769900H-1.239502001.51521000-3.1492						
H2.49275300-2.63768900-0.42080800O0.12879500-1.90978900-0.11583900N-4.45804700-3.018934000.15297700N4.8122700-1.22046800-0.52402900C-5.89190400-2.777255000.31941900H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-6.51743800-4.55996900-0.75738500H-6.51743800-4.790514000.99932100C6.00298400-0.35186900-0.49993800H6.78642200-0.87282900-1.06766100C6.49579000-0.917353001.44824200H5.791234000.55864200-1.06766100C6.49579000-0.917353001.44824200H5.718727000.483319001.49739700C5.03920700-2.66876900-0.66670400H5.99612100-3.79255001.17762000H4.28218700-3.079255001.34215800C5.05284600-3.428802000.66404500H5.867291100-3.090216001.30200100H4.17515800-3.97538400-2.23139000H-1.239502001.51521000-2.23139000H-1.239502001.51521000-3.14928800C3.23805800-3.784726001.8961400C3.23805800-3.784726001.8961400						
O0.12879500-1.909789000.11583900N-4.45804700-3.018934000.15297700N4.81227200-1.220468000.52402900C-5.89190400-2.777225000.31941900H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-7.73296900-3.902696000.34520000H-6.51743800-4.790514000.99932100C6.00298400-0.35186900-0.75738500H6.78642200-0.87282900-1.06766100C6.49579900-0.014890000.91099100H5.791234000.55864200-1.06766100C6.49579900-0.014890000.91099100H5.718727000.483319001.44824200H5.99612100-2.79392300-1.17762000H5.8642700-3.07925500-1.34215800C5.05284600-3.428802000.66670400H5.18642700-3.090216001.30200100H4.11784400-3.290590001.21353300H-4.17515800-3.97538400-0.00769900G-0.947784001.64982300-2.23139000H-1.239502001.5152100-3.14928800C3.23805800-3.784726001.18961400C3.23805800-3.784726001.18961400						
N         -4.45804700         -3.01893400         0.15297700           N         4.81227200         -1.22046800         -0.52402900           C         -5.89190400         -2.77722500         0.31941900           H         -6.23526400         -2.07593200         -0.45175500           H         -6.07093600         -2.30719400         1.29482200           C         -6.66399500         -4.08856000         0.21978000           H         -7.73296900         -3.90269600         0.34520000           H         -6.51743800         -4.55996900         -0.75738500           H         -6.35098400         -4.79051400         0.99932100           C         6.00298400         -0.35186900         -0.49993800           H         5.79123400         0.55864200         -1.06766100           C         6.49579900         -0.01489000         0.91099100           H         5.71872700         0.48331900         1.44824200           K         5.99612100         -2.66876900         -0.66670400           H         5.99612100         -2.7939230         -1.17762000           H         5.87291100         -3.09021600         1.34215800           C         5.05284600						
N4.81227200-1.22046800-0.52402900C-5.89190400-2.777225000.31941900H-6.23526400-2.07593200-0.45175500H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-7.73296900-3.902696000.34520000H-6.51743800-4.55996900-0.75738500H-6.35098400-4.790514000.99932100C6.00298400-0.35186900-0.49993800H6.78642200-0.87282900-1.06766100C6.49579000-0.014890000.91099100H5.791234000.55864200-1.06766100C6.49579000-0.014890000.91099100H5.718727000.483319001.44824200H5.30920700-2.66876900-0.66670400H5.99612100-2.79392300-1.17762000H5.95284600-3.428802000.66404500H5.18642700-3.428802000.66404500H5.18642700-3.428802001.3020100H4.11784400-3.290590001.21353300H4.11784400-3.290590001.21353300H-1.239502001.51521000-2.21319000H-1.239502001.51521000-2.21319000H-1.239502001.51521000-3.14928800S2S2S2S2TS38195100-3.784726001.18961400C3.23805800-3.784726						
C       -5.89190400       -2.77722500       0.31941900         H       -6.23526400       -2.07593200       -0.45175500         H       -6.07093600       -2.30719400       1.29482200         C       -6.66399500       -4.08856000       0.21978000         H       -7.73296900       -3.90269600       0.34520000         H       -6.51743800       -4.55996900       -0.75738500         H       -6.35098400       -4.79051400       0.99932100         C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       7.36149500       0.65145400       0.85329200         H       7.36149500       0.66876900       -0.66670400         H       5.71872700       0.48331900       1.49739700         C       5.05284600       -3.42880200       0.66404500         H       5.87291100       -3.09021600       1.30200100         H       5.18642700       4.49870100       0.47895100         H       5.1852100       -3.1923830						
H       -6.23526400       -2.07593200       -0.45175500         H       -6.07093600       -2.30719400       1.29482200         C       -6.66399500       -4.08856000       0.21978000         H       -7.73296900       -3.90269600       0.34520000         H       -6.51743800       -4.55996900       -0.75738500         H       -6.35098400       -4.79051400       0.99932100         C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       5.71872700       0.48331900       1.44824200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.87291100       -3.09021600       1.30200100         H       5.18642700       -4.49870100       0.47895100         H       5.18642700       1.5152						
H-6.07093600-2.307194001.29482200C-6.66399500-4.088560000.21978000H-7.73296900-3.902696000.34520000H-6.51743800-4.55996900-0.75738500H-6.35098400-4.790514000.99932100C6.00298400-0.35186900-0.49993800H5.791234000.55864200-1.05435100H5.791234000.55864200-1.06766100C6.49579900-0.014890000.91099100H5.718727000.651454000.85329200H5.718727000.483319001.44824200H5.99612100-2.79392300-1.17762000H5.99612100-2.79392300-1.34215800C5.05284600-3.07925500-1.34215800H5.18642700-4.498701000.47895100H4.11784400-3.290590001.21353300H-1.239502001.51521000-3.14928800C3.23805800-3.784726001.18961400C3.23805800-3.784726001.18961400						
C       -6.66399500       -4.08856000       0.21978000         H       -7.73296900       -3.90269600       0.34520000         H       -6.51743800       -4.55996900       -0.75738500         H       -6.35098400       -4.79051400       0.99932100         C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       5.79187200       0.48331900       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       5.99612100       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.18642700       -4.49870100       1.30200100         H       4.1178400       -3.29059000       1.21353300         H       -1.23950200       1.5152100						
H       -7.73296900       -3.90269600       0.34520000         H       -6.51743800       -4.55996900       -0.75738500         H       -6.35098400       -4.79051400       0.99932100         C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       6.79748500       -0.91735300       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.18642700       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -1.23950200       1.51521000						
H       -6.51743800       -4.55996900       -0.75738500         H       -6.35098400       -4.79051400       0.99932100         C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       6.79748500       -0.91735300       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       -1.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521						
H       -6.35098400       -4.79051400       0.99932100         C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       6.79748500       -0.91735300       1.44824200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.87291100       -3.09021600       1.30200100         H       4.17515800       -3.97538400       -0.00769900         G       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800						
C       6.00298400       -0.35186900       -0.49993800         H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       6.79748500       -0.91735300       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.18642700       -3.09021600       1.30200100         H       4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52       S2       S2       S2       S2         RhB-3a_op=r (charge=1 mJtriplicity=1 E= -1263.519283 Ha						
H       6.78642200       -0.87282900       -1.05435100         H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       6.79748500       -0.91735300       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         S2       S2       S2       S2       S2         RhB-3a_open (charge=1 mJtriplicity=1 E= -1263.519283 Ha						
H       5.79123400       0.55864200       -1.06766100         C       6.49579900       -0.01489000       0.91099100         H       6.79748500       -0.91735300       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.18642700       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         S2       I       I       -3.23805800       -3.78472600       1.18961400         C       3.23805800       -3.78472600       1.18961400       I						
C 6.49579900 -0.01489000 0.91099100 H 6.79748500 -0.91735300 1.44824200 H 7.36149500 0.65145400 0.85329200 H 5.71872700 0.48331900 1.49739700 C 5.03920700 -2.66876900 -0.66670400 H 5.99612100 -2.79392300 -1.17762000 H 4.28218700 -3.07925500 -1.34215800 C 5.05284600 -3.42880200 0.66404500 H 5.18642700 -4.49870100 0.47895100 H 5.87291100 -3.09021600 1.30200100 H 4.11784400 -3.29059000 1.21353300 H -4.17515800 -3.97538400 -0.00769900 O -0.94778400 1.64982300 -2.23139000 H -1.23950200 1.51521000 -3.14928800 52 RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha C 3.23805800 -3.78472600 1.18961400 C 3.38195100 -3.19241800 -0.06154400						
H       6.79748500       -0.91735300       1.44824200         H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52       S2       S2       S2       S2         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha       C       3.23805800       -3.78472600       1.18961400         C       3.23805800       -3.19241800       -0.06154400       S2						
H       7.36149500       0.65145400       0.85329200         H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         S2       S2       S2       S2       S2         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha       C       3.23805800       -3.78472600       1.18961400         C       3.23805800       -3.19241800       -0.06154400       S2						
H       5.71872700       0.48331900       1.49739700         C       5.03920700       -2.66876900       -0.66670400         H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         S2       S2       S2       S2       S2         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Hat       S2       S2       S2         C       3.23805800       -3.78472600       1.18961400       S2         C       3.23805800       -3.19241800       -0.06154400						
C 5.03920700 -2.66876900 -0.66670400 H 5.99612100 -2.79392300 -1.17762000 H 4.28218700 -3.07925500 -1.34215800 C 5.05284600 -3.42880200 0.66404500 H 5.18642700 -4.49870100 0.47895100 H 5.87291100 -3.09021600 1.30200100 H 4.11784400 -3.29059000 1.21353300 H -4.17515800 -3.97538400 -0.00769900 O -0.94778400 1.64982300 -2.23139000 H -1.23950200 1.51521000 -3.14928800 52 RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha C 3.23805800 -3.78472600 1.18961400 C 3.38195100 -3.19241800 -0.06154400						
H       5.99612100       -2.79392300       -1.17762000         H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         S2       S2       S2       S2       S2         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha       S2       S2         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
H       4.28218700       -3.07925500       -1.34215800         C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha       C       3.23805800       -3.78472600       1.18961400         C       3.23805800       -3.19241800       -0.06154400       -0.06154400						
C       5.05284600       -3.42880200       0.66404500         H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
H       5.18642700       -4.49870100       0.47895100         H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
H       5.87291100       -3.09021600       1.30200100         H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
H       4.11784400       -3.29059000       1.21353300         H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
H       -4.17515800       -3.97538400       -0.00769900         O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
O       -0.94778400       1.64982300       -2.23139000         H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
H       -1.23950200       1.51521000       -3.14928800         52         RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400						
52 RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha C 3.23805800 -3.78472600 1.18961400 C 3.38195100 -3.19241800 -0.06154400						
RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Ha         C       3.23805800 -3.78472600 1.18961400         C       3.38195100 -3.19241800 -0.06154400						
C       3.23805800       -3.78472600       1.18961400         C       3.38195100       -3.19241800       -0.06154400	RhB-3a_open (charge=1 multiplicity=1 E= -1263.519283 Hartree)					
C 3.38195100 -3.19241800 -0.06154400						
C 2.64950600 -2.04833700 -0.40625700						

С	1.76657900	-1.47971300	0.53770000
С	1.62701400	-2.08861900	1.79266100
С	2.35415500	-3.23355600	2.11767300
Н	3.80977600	-4.67286800	1.43739100
Н	4.05866600	-3.60491300	-0.80161600
Н	0.95409100	-1.64751700	2.52133500
Н	2.23239400	-3.68724900	3.09607300
С	1.00955600	-0.21725100	0.30450600
С	2.86182600	-1.52902800	-1.79246900
0	3.79796000	-1.84094300	-2.49521800
С	1.67281500	1.02976100	0.34214000
С	0.91566500	2.22251500	0.16012800
С	3.07277000	1.18776400	0.55277300
С	1.48726700	3.48065500	0.17173300
С	3.65871700	2.42419200	0.56566200
Н	3.68002400	0.30345600	0.70672800
С	2.87545700	3.60507000	0.37173000
Н	0.85643500	4.35043700	0.02725400
Н	4.72769900	2.51985500	0.72752400
С	-0.38125600	-0.24505700	0.10914600
С	-1.16554100	-1.43370200	0.03788200
С	-1.08984300	0.98059500	-0.06200600
С	-2.51599300	-1.39615300	-0.16384400
Н	-0.66724700	-2.38968000	0.14852100
С	-2.45162500	1.04308000	-0.26377400
С	-3.21963900	-0.14899300	-0.33038300
Н	-3.05642500	-2.33105900	-0.20157900
Н	-2.89480500	2.02254200	-0.36729800
0	-0.42945500	2.17060600	-0.03169200
Ν	3.47101200	4.81912300	0.38721700
Ν	-4.55661100	-0.12224800	-0.55834500
С	-5.36413800	-1.35606400	-0.56675300
Н	-6.28044800	-1.13069200	-1.11607100
Н	-4.84384200	-2.11830900	-1.15375200
С	-5.70727100	-1.88114200	0.83096700
Н	-6.30989700	-1.15829500	1.38618800
Н	-6.28057500	-2.80914900	0.74854000
Н	-4.80509100	-2.08690900	1.41366500
С	-5.27950900	1.15527700	-0.68571500
Н	-6.20513100	0.94631300	-1.22594400
Н	-4.70046400	1.82444900	-1.32937900
С	-5.59475000	1.82496500	0.65609200
Н	-6.09243400	2.78386800	0.48437100
Н	-6.25883600	1.20198000	1.26012200

Н	-4.68553500	2.00949800	1.23455100	
Н	2.94124400	5.66578900	0.25581700	
Н	4.46385800	4.91122300	0.52989700	
0	1.88428000	-0.68844500	-2.21219100	
Н	2.12283400	-0.42532300	-3.11758900	
52				
RhB-3b_o	pen (charge=1 n	nultiplicity=1 I	E= -1263.5192	83 Hartree)
С	0.24270900	4.85858900	-1.14520100	
С	0.57344500	4.38772800	0.12214000	
С	0.44980700	3.02869100	0.44071500	
С	0.00266100	2.12242800	-0.54530400	
С	-0.33141100	2.60996800	-1.81656300	
С	-0.21558200	3.96725200	-2.11573600	
Н	0.33923500	5.91495000	-1.37285900	
Н	0.92826700	5.06096500	0.89458100	
Н	-0.66739100	1.91278800	-2.57775700	
Н	-0.47717800	4.32265700	-3.10729000	
С	-0.06926000	0.64836900	-0.33769000	
С	0.79761700	2.65140100	1.84529400	
0	1.45496300	3.34615100	2.58888100	
С	1.11033700	-0.12289300	-0.29910800	
С	1.01233000	-1.53801600	-0.14222500	
С	2.42546800	0.41467300	-0.40397800	
С	2.11704100	-2.35896000	-0.08118900	
С	3.53753900	-0.38105600	-0.34264200	
Н	2.54074800	1.48426400	-0.53563200	
С	3.41205900	-1.79909900	-0.17561600	
Н	1.97417800	-3.42742400	0.03817600	
Н	4.51970300	0.06630700	-0.42555700	
С	-1.31572800	0.00022200	-0.24174500	
С	-2.57208200	0.67276300	-0.24674500	
С	-1.35383600	-1.41997500	-0.09548400	
С	-3.75484800	-0.00752900	-0.14041500	
Н	-2.57916700	1.75282100	-0.33489400	
С	-2.53205700	-2.12531000	0.01175200	
С	-3.76625200	-1.43531700	-0.01175700	
Н	-4.68905100	0.53922500	-0.14721600	
Н	-2.49351000	-3.20389400	0.11845800	
0	-0.20300400	-2.14439200	-0.05059500	
Ν	4.50072800	-2.59369800	-0.11351500	
Ν	-4.92556500	-2.11736700	0.09179400	
С	-6.26802100	-1.53350800	0.08988400	
Н	-6.35261000	-0.81422400	0.91433200	
Н	-6.42352100	-0.98184100	-0.84592600	

С	-7.32010900	-2.62764900	0.23737400
Н	-7.19330200	-3.17165800	1.17878100
Н	-8.31941400	-2.18684600	0.23647500
Н	-7.26662900	-3.34096100	-0.59133100
Н	4.34793300	-3.58630700	-0.00279600
Н	-4.86891100	-3.12220500	0.18157900
С	5.89308600	-2.14965500	-0.19970600
Н	6.09448300	-1.42787600	0.60186700
Н	6.05232800	-1.63384500	-1.15518700
С	6.83586500	-3.34256900	-0.08203700
Н	7.87302100	-3.00624900	-0.14621500
Н	6.70687800	-3.85384500	0.87728600
Н	6.66509600	-4.06161300	-0.88969200
0	0.27794100	1.45987800	2.23011900
Н	0.55881000	1.32589400	3.15151900

#### References

1. Butkevich, A. N.; Bossi, M. L.; Lukinavičius, G.; Hell, S. W., J Am Chem Soc 2019, 141 (2), 981-989.

 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.; MontgomeryJr., J. A.; Peralta, J. E.; Ogliaro, F.; M. Bearpark, Heyd, J. J.; Brothers, E. K.; 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, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. *Gaussian 16, Revision A03;* Gaussian, Inc., Wallingford, CT, **2016**. 3. Hohenberg, P.; Kohn, W., *Phys. Rev.* **1964**, *136*, B864–B871.

4. (a) Becke, A. D., *Phys. Rev. A* 1988, *38*, 3098–3100. (b) Becke, A. D., *J. Chem. Phys.* 1993, *98*, 5648–5652.
(c) Lee, C.; Yang, W.; Parr, R. G., *Phys. Rev. B* 1988, *37*, 785–789. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J., *J. Phys. Chem.* 1994, *98*, 11623–11627. (e) Hertwig, R. H.; Koch, W., *Chem. Phys. Lett.* 1997, *268*, 345–351. (f) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* 2010, *132*, 154104/1-20.
5. (a) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A., *J. Chem. Phys.* 1980, *72*, 650–654. (b) Frisch, M. J.; Pople, J. A.; Binkley, J. S., *J. Chem. Phys.* 1984, *80*, 3265-3269. (c) Lin, X.; Phillips, D. L. *J. Org. Chem.* 2008, *73*, 3680–3688.

6. Perdew, J. P.; Burke, K.; Ernzerhof, M. Phys. Rev. Lett. 1996, 18, 3865-3868.

7. (a) Zhao, Y.; Chen, F. J. Mult. Analy. 2008, 99, 215–231. (b) Zhao, Y.; Truhlar, D. G. J. Phys. Chem. C

**2008**, *112*, 6860–6868.

8. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., J. Phys. Chem. B 2009, 113, 6378-6396.