

Supporting Information

A Computational Mechanistic Study of an Unprecedented Heck-Type Relay Reaction: Insight into the Origins of Regio- and Enantioselectivities

Yanfeng Dang,[†] Shuanglin Qu,[†] Zhi-Xiang Wang,^{*,†,§} and Xiaotai Wang^{*,‡}

[†]School of Chemistry and Chemical Engineering, University of the Chinese Academy of Sciences, Beijing 100049, People's Republic of China

[‡]Department of Chemistry, University of Colorado Denver, Campus Box 194, P.O. Box 173364, Denver, Colorado 80217-3364, United States

[§]Collaborative Innovation Center of Chemical Science and Engineering, Tianjin, 300072, People's Republic of China

Table of Contents

■ Complete Gaussian 09 reference	S2
■ Schemes S1–S13 and Figures S1–S9	S3–S19
■ Cartesian Coordinates (Å), SCF Energies and Free Energies at 298.15 K and 1 atm for the Optimized Structures	S20–108

Gaussian 09, Revision **A.1**, 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, N. J.; 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.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

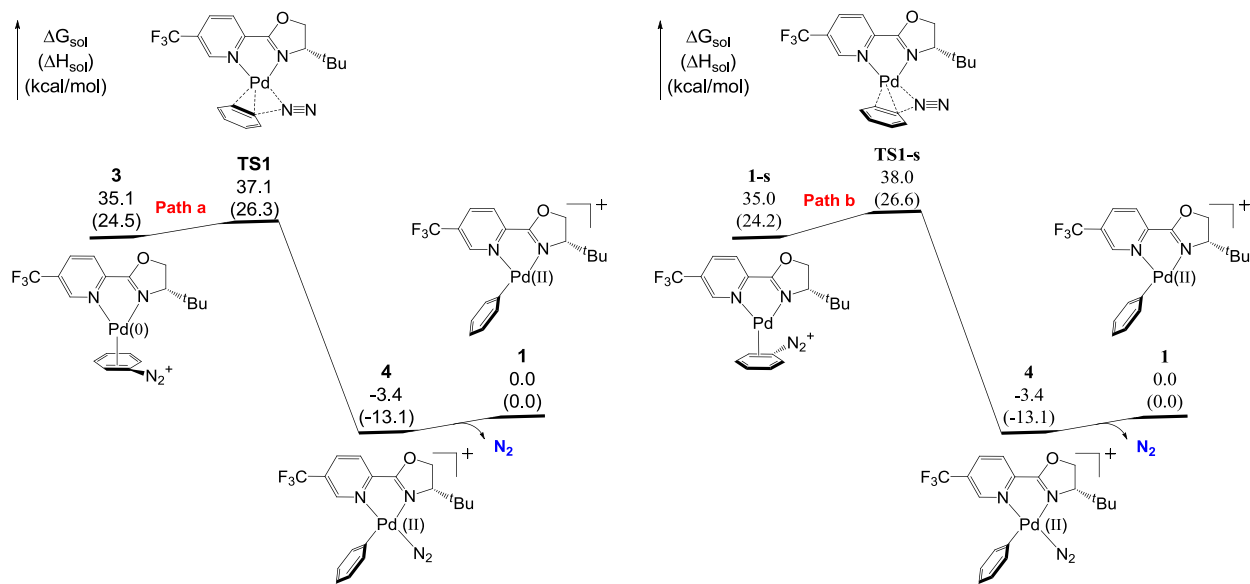


Figure S1. Free energy profiles for the oxidation of Pd(0) to Pd(II) by phenyldiazonium leading to Pd species **1**. Energies are relative to complex **1** and are mass-balanced (similarly hereinafter).

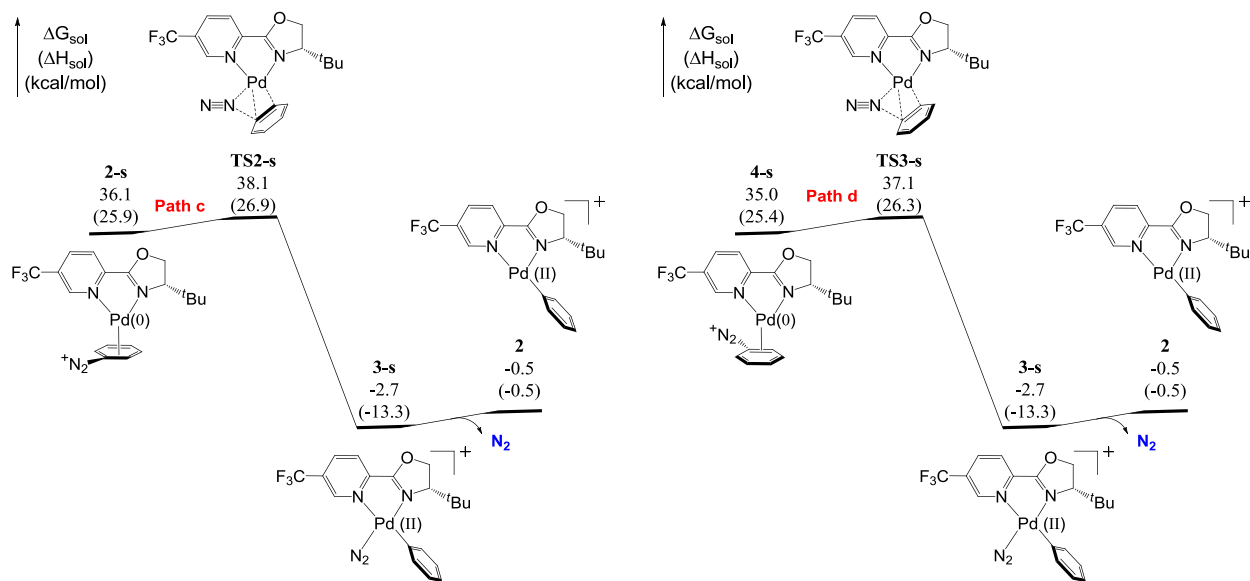
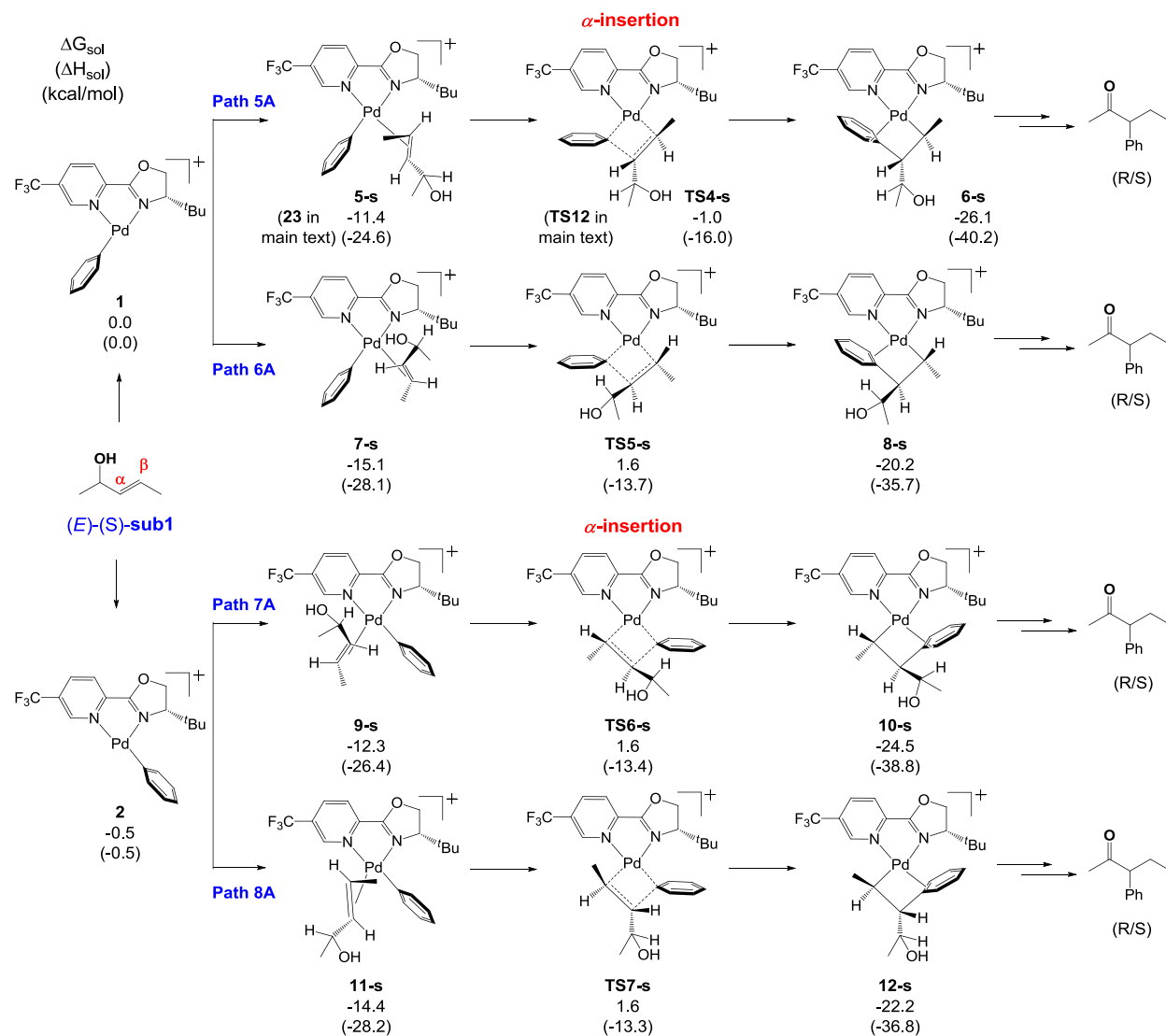
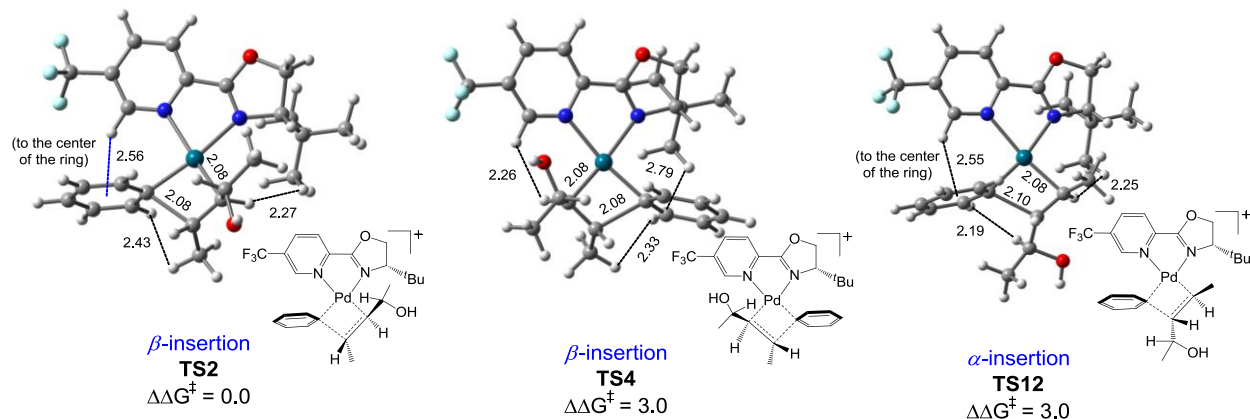


Figure S2. Free energy profiles for the oxidation of Pd(0) to Pd(II) by phenyldiazonium leading to Pd species **2**.

Scheme S1. Reactions of (*E*)-(*S*)-**sub1** with Pd catalyst **1** or **2** leading to α -substituted products



B3LYP/BS1 geometries and M06/BS2//B3LYP/BS1 energies



M06/BS1 geometries and M06/BS2//M06/BS1 energies

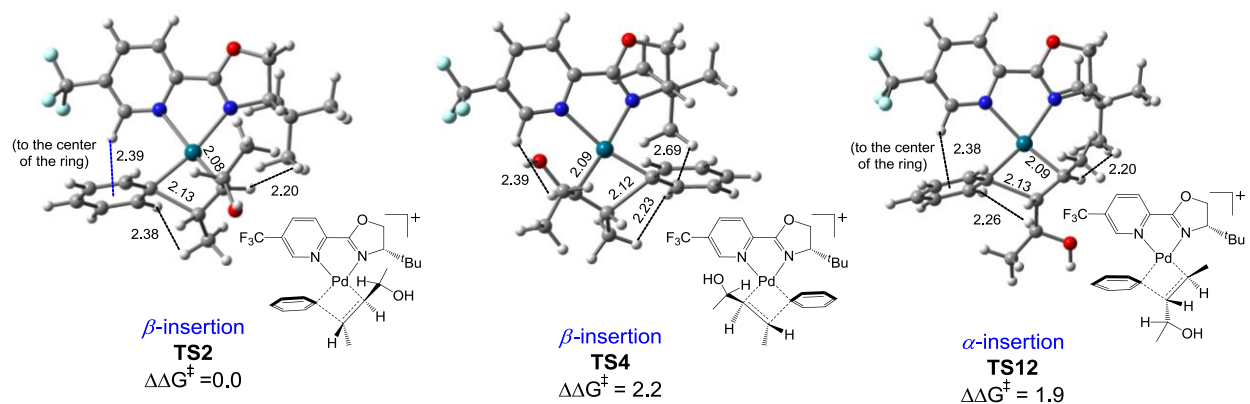
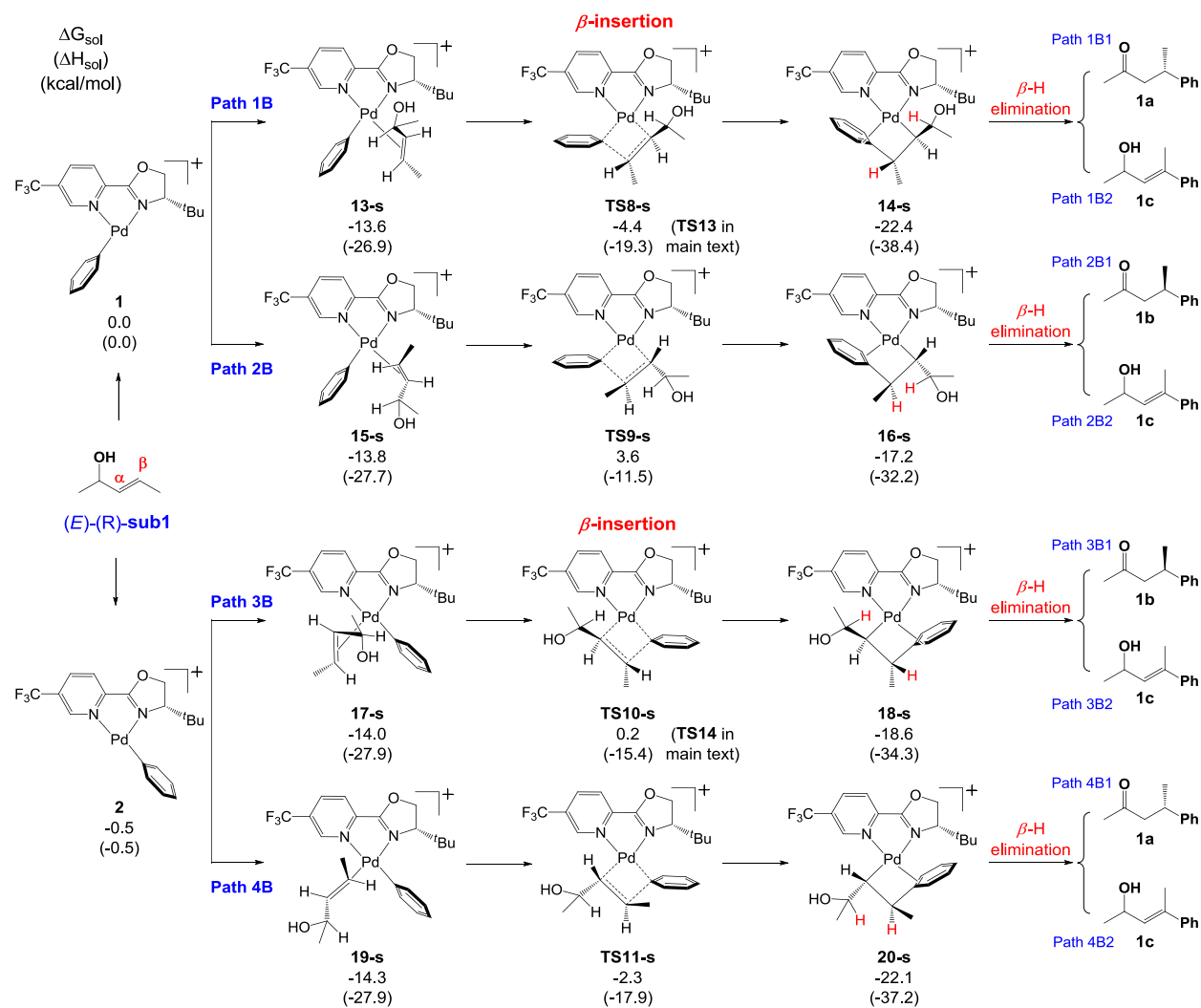
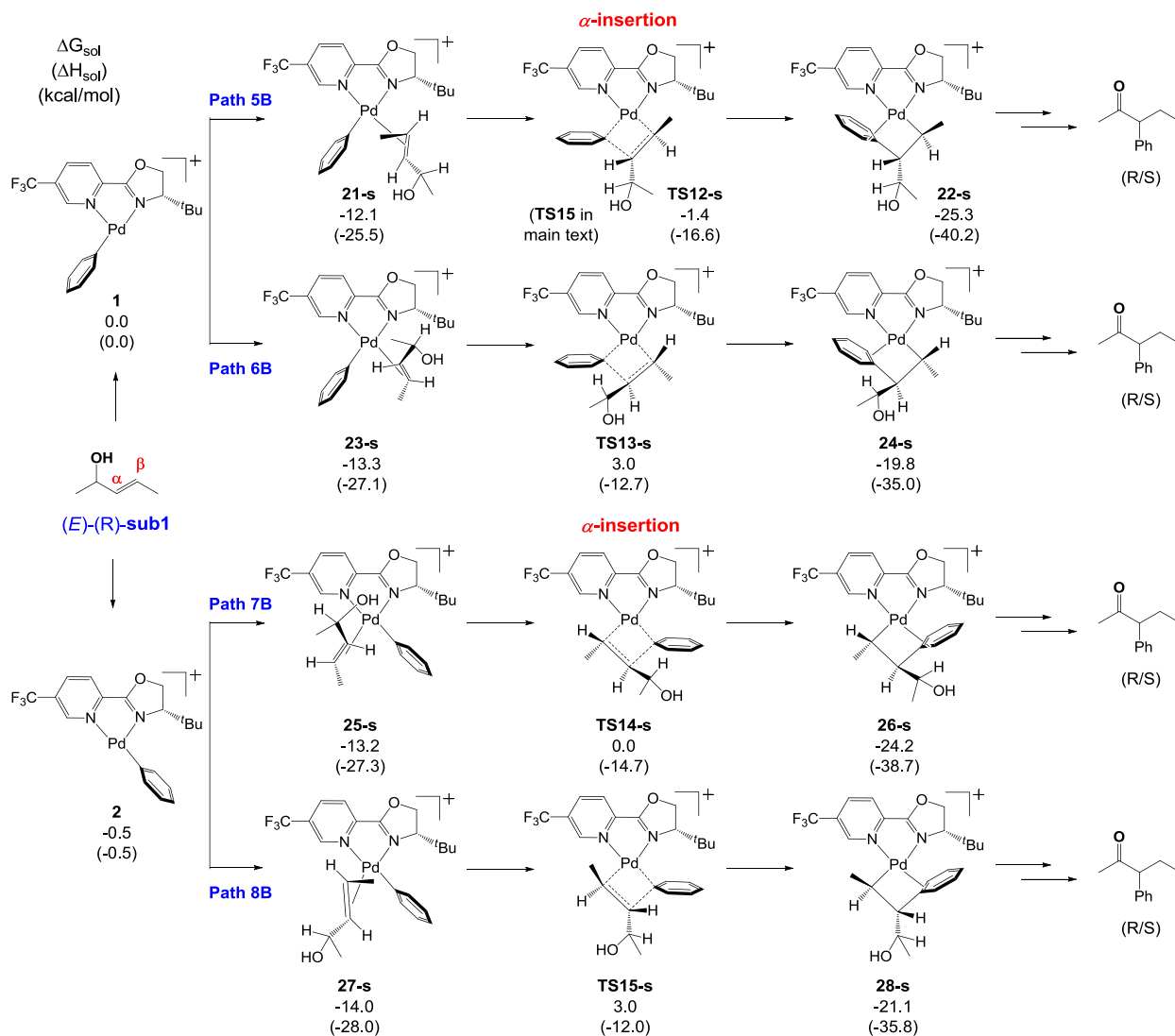


Figure S3. Comparing the key alkene insertion TSs for (*E*)-(*S*)-**sub1** obtained with different computational methods.

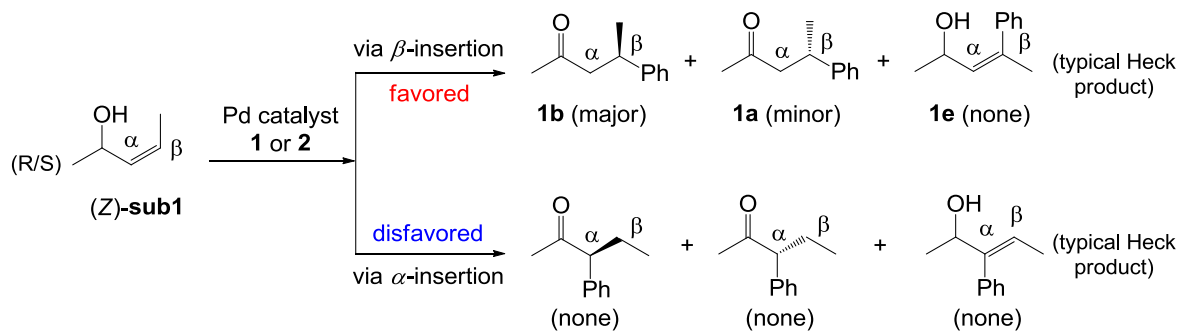
Scheme S2. Reactions of (*E*)-(*R*)-sub1 with Pd catalyst **1** or **2** leading to β -substituted products



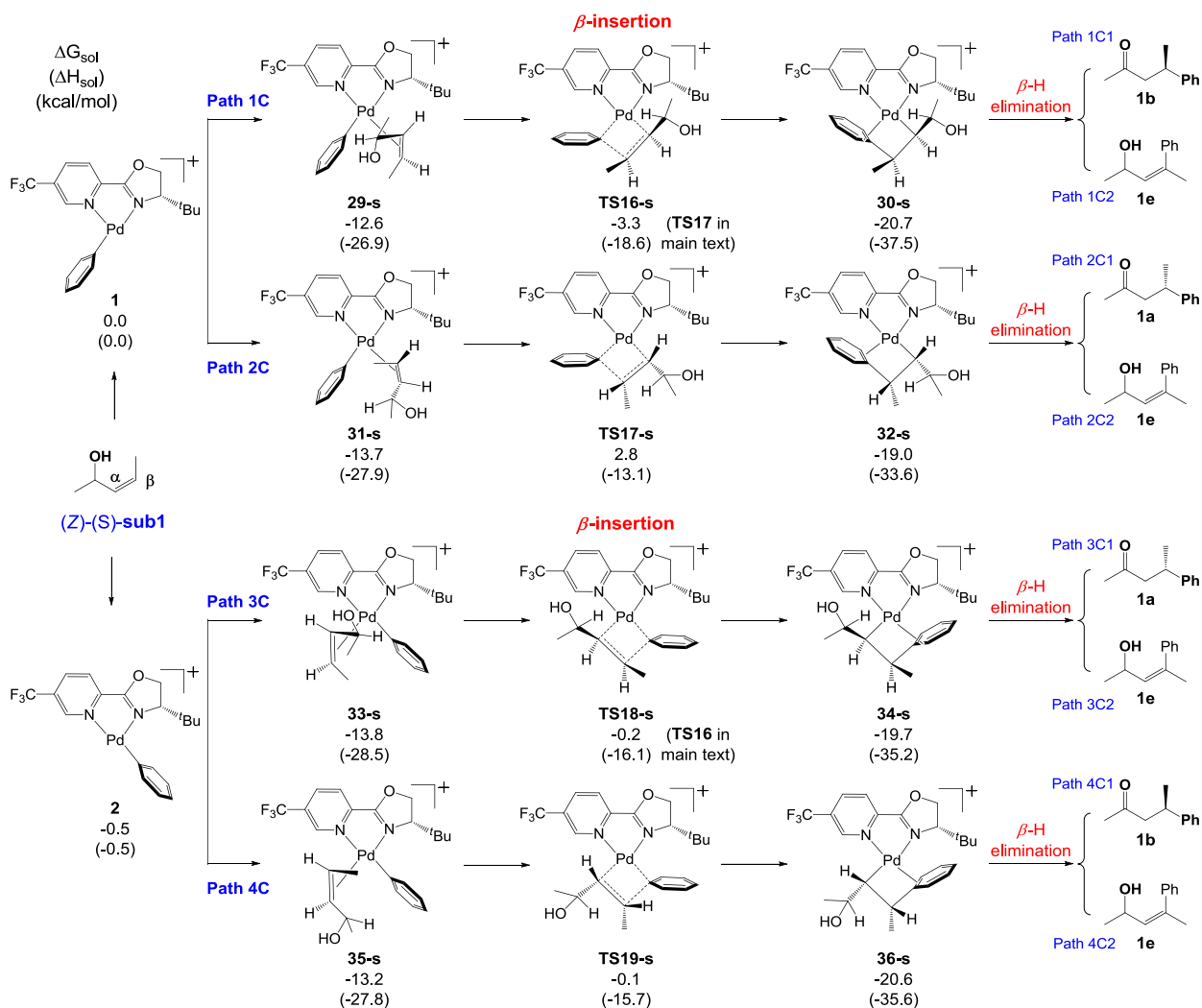
Scheme S3. Reactions of (*E*)-(*R*)-**sub1** with Pd catalyst **1** or **2** leading to α -substituted products



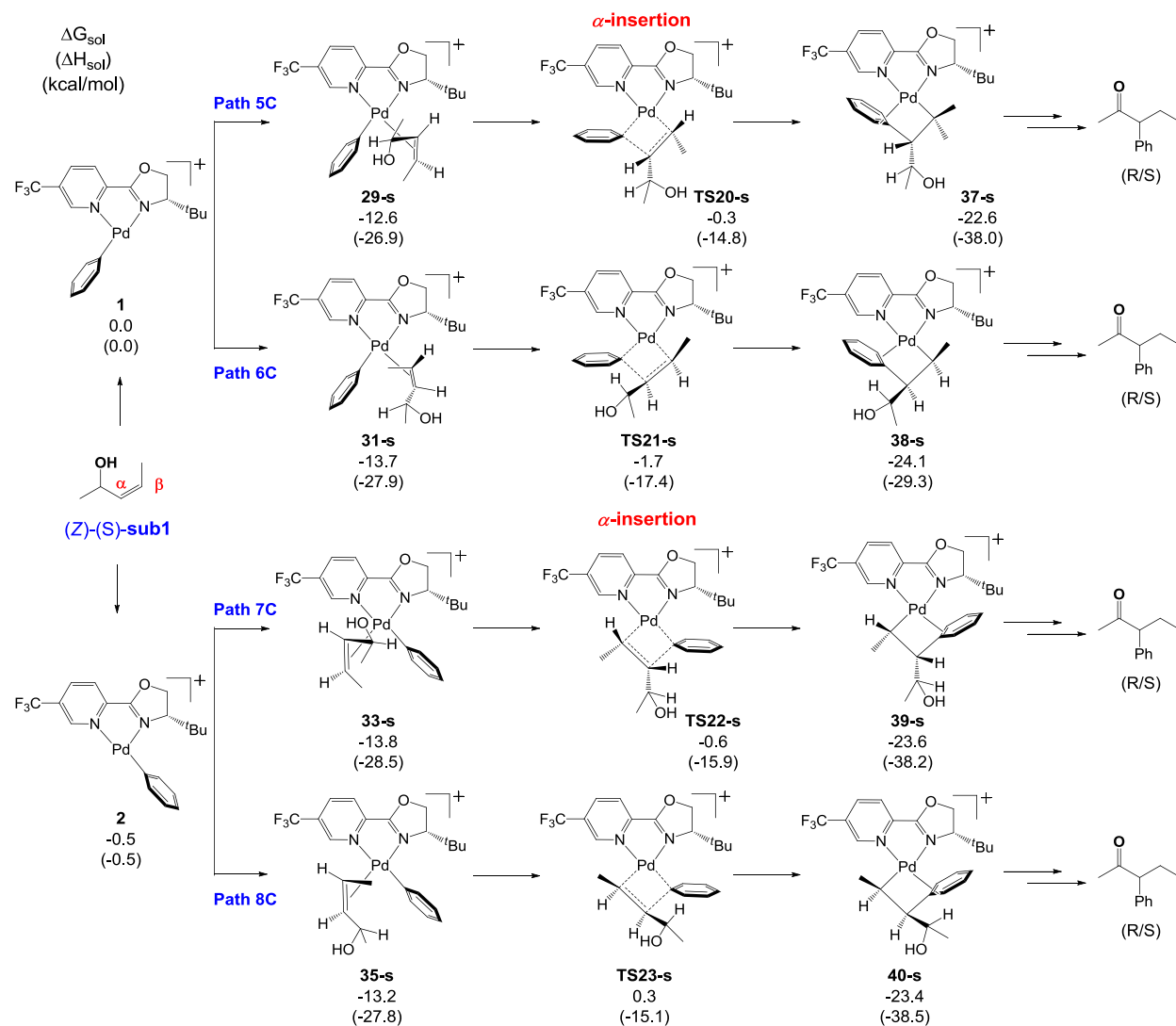
Scheme S4. The Heck Arylation of (Z)-Allylic Alcohol



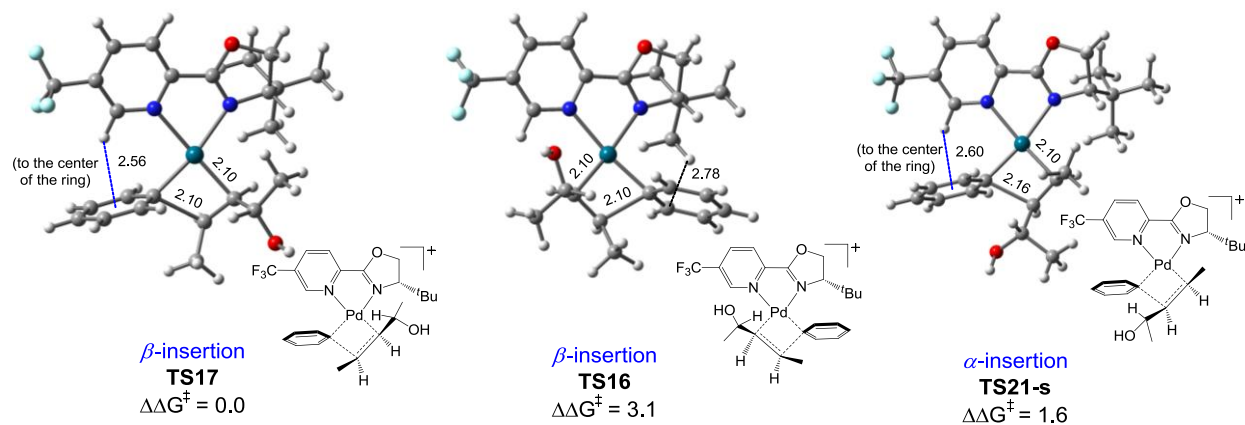
Scheme S5. Reactions of (Z)-(S)-sub1 with Pd catalyst 1 or 2 leading to β -substituted products



Scheme S6. Reactions of (Z)-(S)-sub1 with Pd catalyst **1** or **2** leading to α -substituted products



B3LYP/BS1 geometries and M06/BS2//B3LYP/BS1 energies



M06/BS1 geometries and M06/BS2//M06/BS1 energies

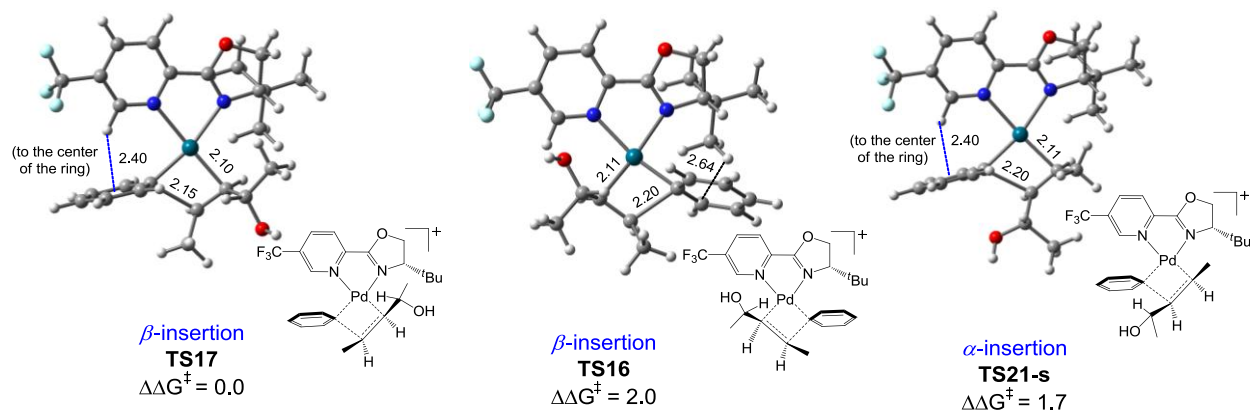
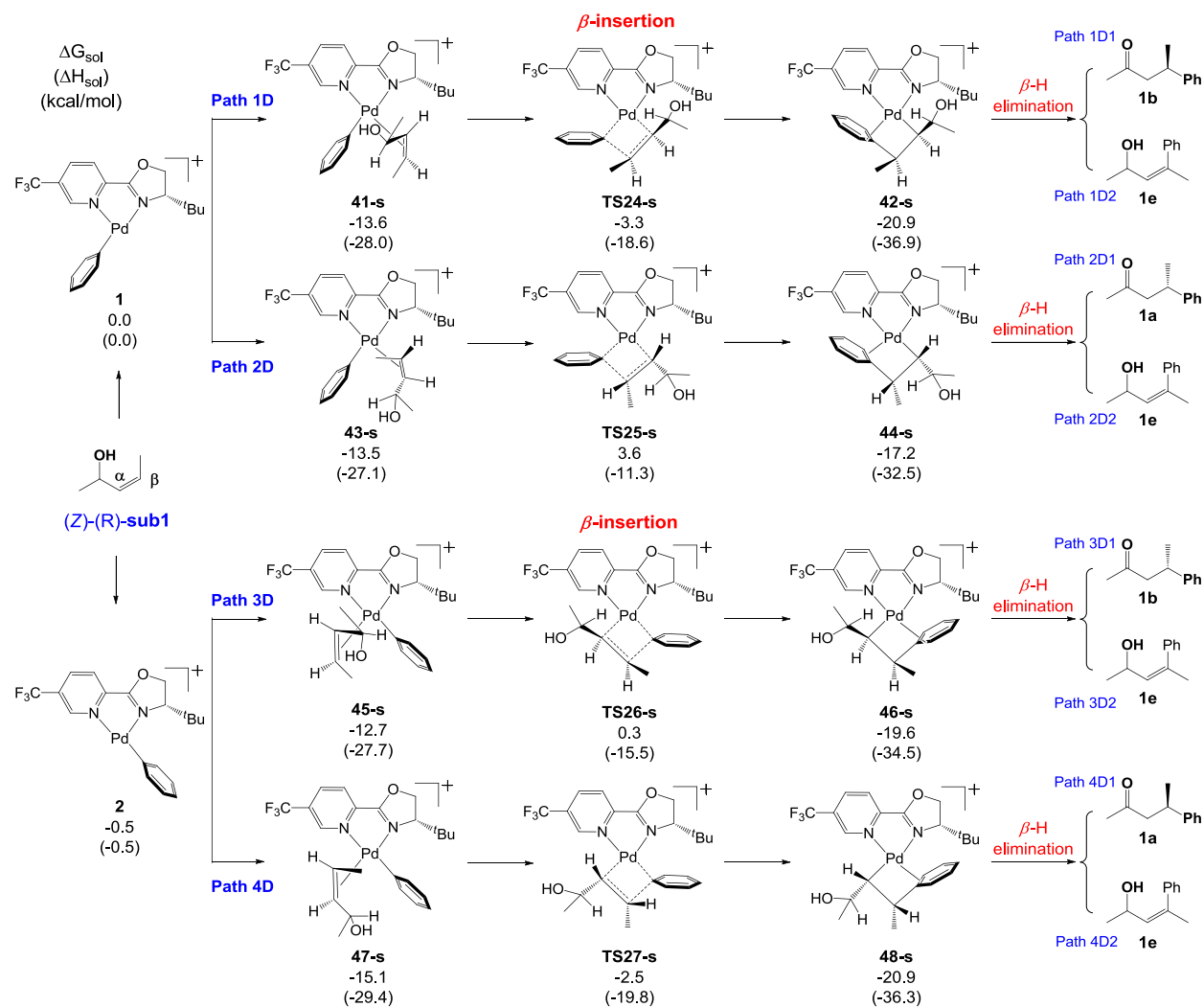
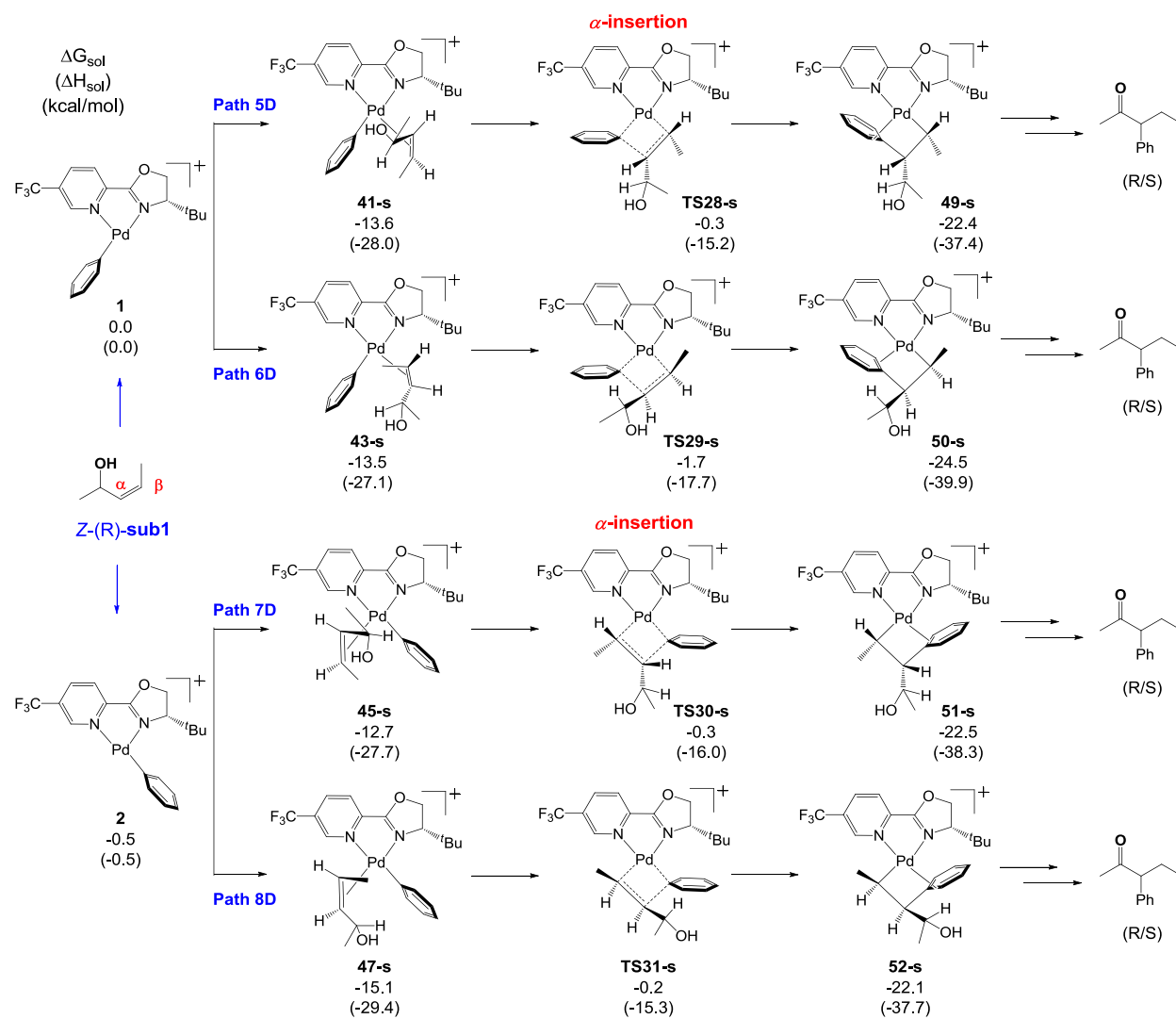


Figure S4. Comparing the key alkene insertion TSs for (Z)-(S)-**sub1** obtained with different computational methods.

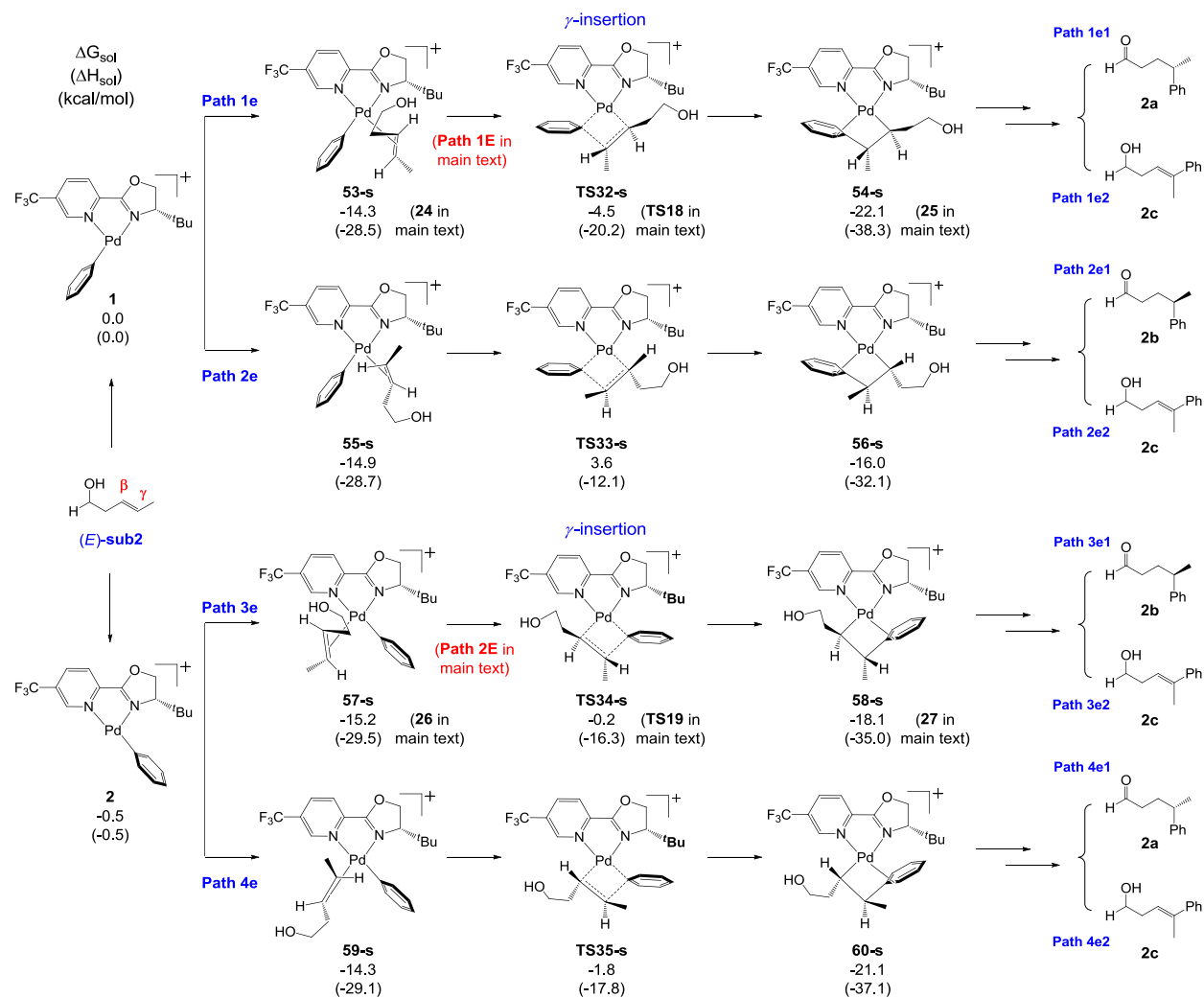
Scheme S7. Reactions of (Z)-(R)-sub1 with Pd catalyst **1** or **2** leading to β -substituted products



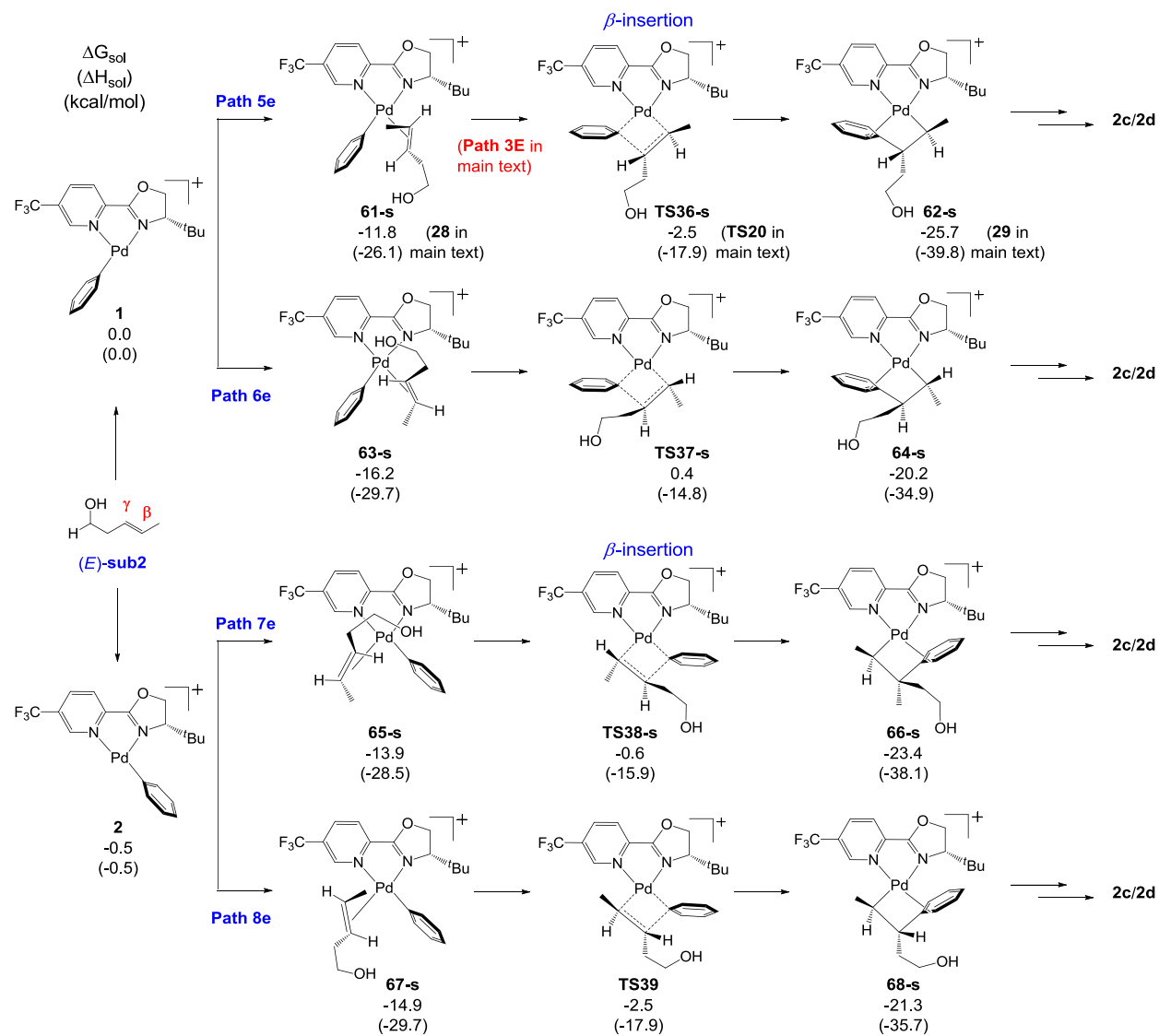
Scheme S8. Reactions of (Z)-(R)-sub1 with Pd catalyst **1** or **2** leading to α -substituted products



Scheme S9. Reactions of (*E*)-sub2 with Pd catalyst 1 or 2 leading to γ -substituted products



Scheme S10. Reactions of (*E*)-sub2 with Pd catalyst **1** or **2** leading to β -substituted products^a



^aPath 5e is the most favorable pathway leading to **2c** and **2d**. More details about the **29** to **2c/2d** transformation are shown in Scheme S11 and Figure S7 on p. S16.

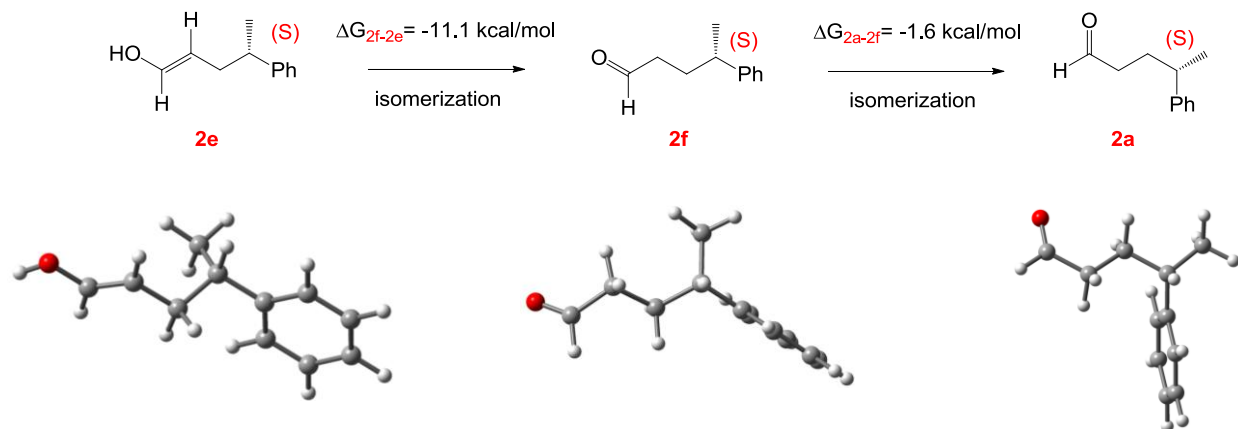


Figure S5. Conversion from the (S)-enol product **2e** to the (S)- γ -phenyl ketone product **2a**.

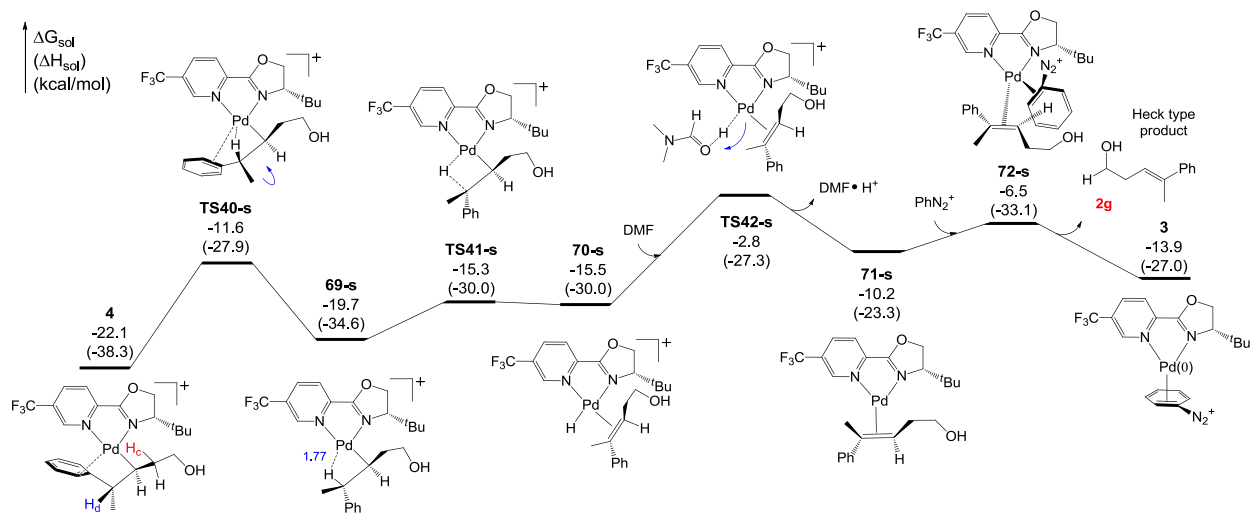


Figure S6. Free energy profile for the reaction with (E)-sub2 leading to the typical Heck product **2g**.

Scheme S11. Mechanistic analysis of the C=C bond migration in path 5e leading to **2c/2d**

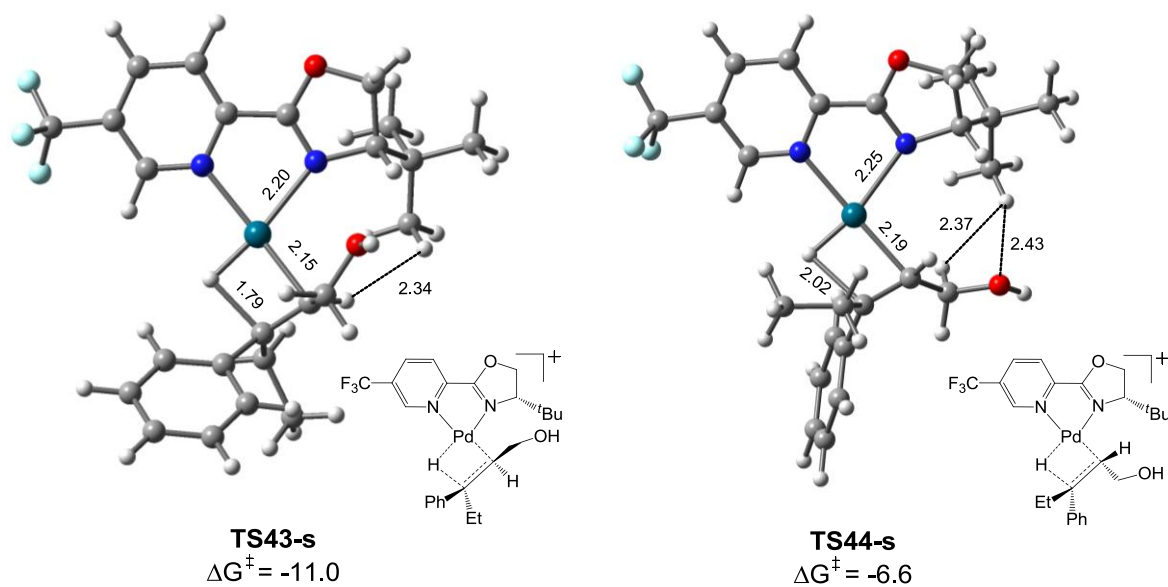
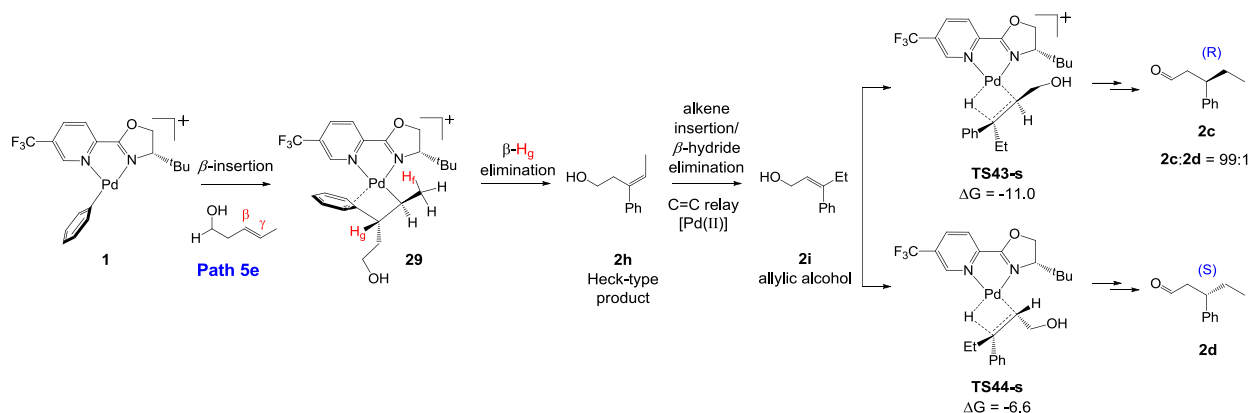
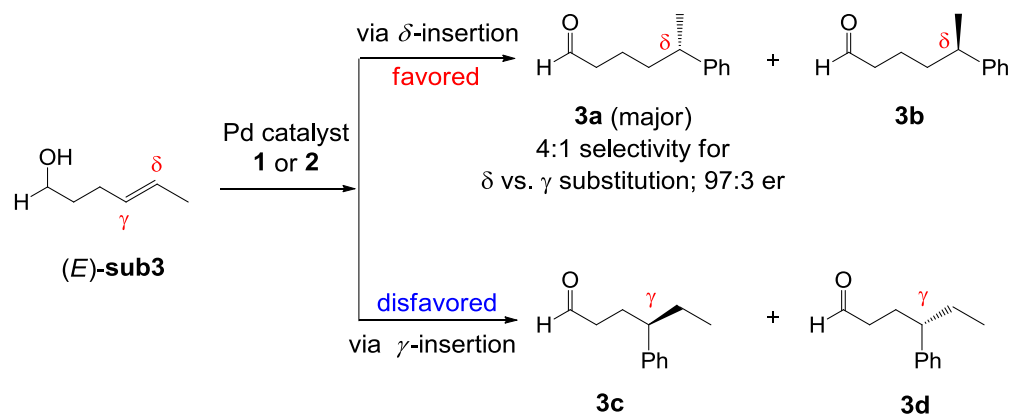


Figure S7. Optimized structures of **TS43-s** (leading to **2c**) and **TS44-s** (leading to **2d**) with selected distances given in Å. **TS43-s** is 4.4 kcal/mol lower than **TS44-s**, giving a calculated enantioselectivity (> 99%) in favor of **2c** which agrees with the experimental values as shown in Scheme S11.

Scheme S12. The Heck Arylation of Alkenyl Alcohol (*E*)-sub3



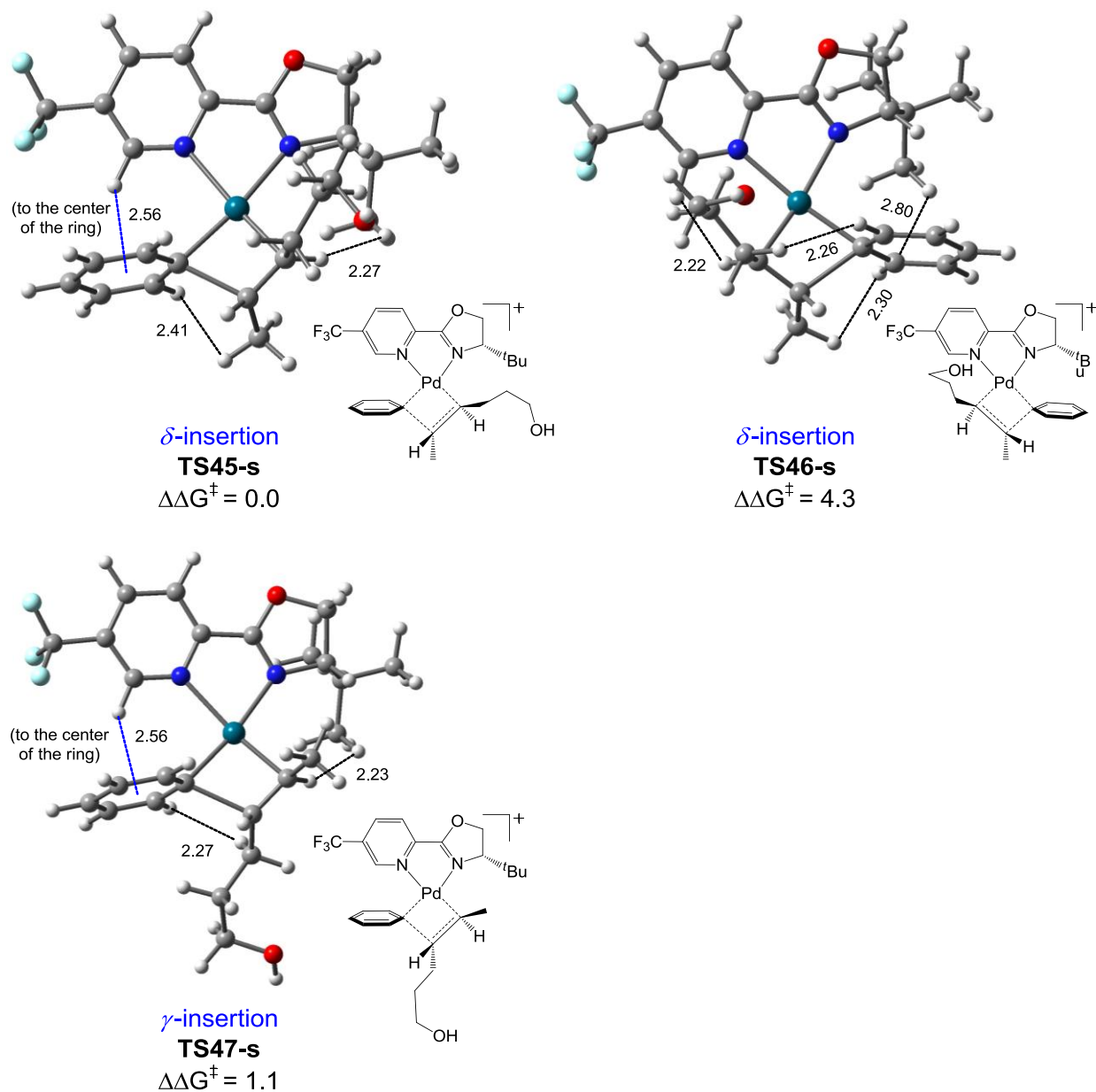


Figure S8. Selectivity-determining alkene insertion TSs of **TS45-s** (leading to **3a**), **TS46-s** (leading to **3b**), and **TS47-s** for the (*E*)-**sub3** system. Geomtries are optimized with B3LYP/BS1 and energies calculated with M06/BS2//B3LYP/BS1. **TS45-s** is 4.3 kcal/mol lower than **TS46-s**, giving a calculated enantioselectivity (> 99%) in favor of **3a**. **TS45-s** of δ -insertion is 1.1 kcal/mol lower than **TS47-s** of γ -insertion, giving a calculated regioselectivity of $\delta:\gamma = 6.4:1$. These calculated selectivities agree with the experimental values as shown in Scheme S12.

Scheme S13. Dissociation of Enol **1d** from Species **14** and **16**

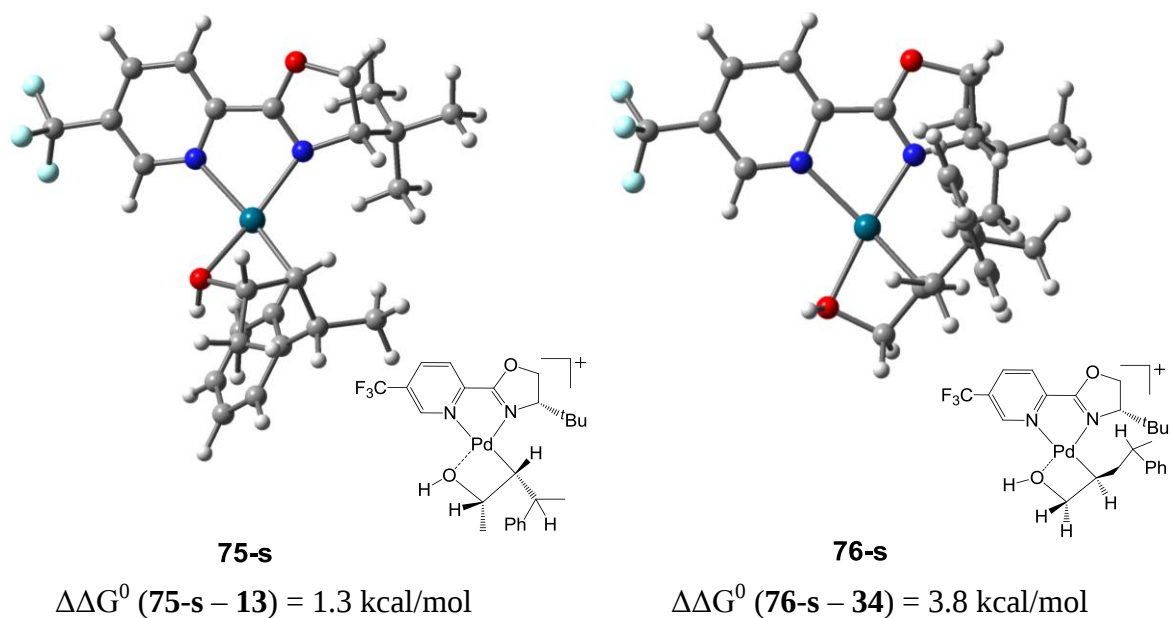
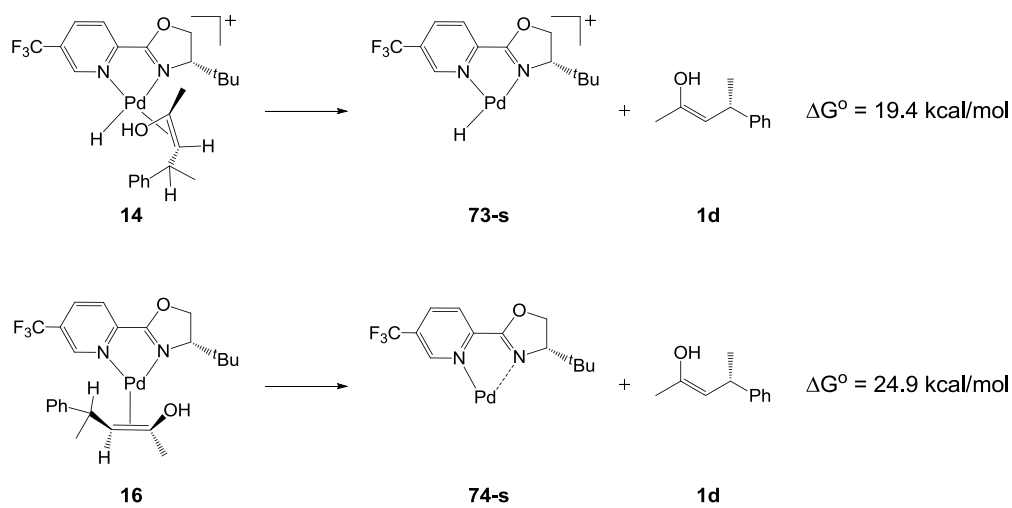


Figure S9. Optimized structures of **75-s** (isomer of **13**) and **76-s** (isomer of **34**) with the OH group coordinated with the metal center. They are in higher energies than **13** and **34** and would not affect the energy profiles shown in Figures 3 and 10.

Cartesian Coordinates (Å), SCF Energies and Free Energies at 298.15 K and 1 atm for the Optimized Structures

1				N	-0.89459100	1.00081800	-0.34469200
B3LYP SCF energy in DMF: -1348.150874 a.u.				C	-1.45243400	3.03954300	-1.34093400
M06 SCF energy in DMF: -1347.667094 a.u.				C	-2.07528000	1.89588900	-0.50701600
M06 Free energy in DMF: -1347.363076 a.u.				H	-1.61067900	2.91269500	-2.41470400
C	-2.00320100	-0.68389100	0.05452900	H	-2.83552600	1.37014200	-1.08766100
C	-0.02206400	-1.87732700	-0.17824900	O	-0.00219400	2.90957800	-1.10703200
C	-0.68374200	-3.09294300	-0.07617900	H	-1.73761100	4.04469100	-1.03878300
C	-2.06805700	-3.09425000	0.09551500	N	1.54585400	-0.11766200	0.03322100
C	-2.72976500	-1.87363100	0.16037100	C	-2.71305700	2.34316100	0.84948100
H	-2.49231800	0.27979200	0.10505600	C	-3.19278200	1.11592600	1.64515800
H	-0.12445400	-4.01915100	-0.12787300	H	-2.35954200	0.47577700	1.94921300
H	-2.61087500	-4.02851800	0.18032600	H	-3.70867500	1.44628100	2.55347900
C	1.43440700	-1.77227900	-0.35398500	H	-3.89481700	0.51081600	1.06238100
N	2.02095300	-0.63177600	-0.43144300	C	-3.94193000	3.21243000	0.51263100
C	3.56924800	-2.41508100	-0.54128800	H	-4.44548900	3.51658400	1.43620300
C	3.46965200	-0.86496100	-0.61806900	H	-3.67539800	4.12623200	-0.02879900
H	3.99131700	-2.86778700	-1.43828600	H	-4.66477800	2.65746400	-0.09628200
H	3.73051100	-0.52150100	-1.62568300	C	-1.72396500	3.14903700	1.71174900
O	2.17368700	-2.87553300	-0.43386500	H	-1.38597200	4.06530100	1.21648700
H	4.09244700	-2.78535700	0.34160900	H	-2.21143400	3.44885800	2.64560400
N	-0.67772100	-0.68446500	-0.11592500	H	-0.84206000	2.55748100	1.98205800
C	4.35386400	-0.07115600	0.38558200	C	5.23500900	-0.76737600	0.22471500
C	4.16561000	1.43561700	0.12434700	F	5.13561700	-1.70535800	1.18894000
H	3.13794300	1.76012500	0.33293500	F	5.64007500	-1.39589800	-0.90143800
H	4.82923200	2.01957100	0.77154200	F	6.21891600	0.08304600	0.57963300
H	4.39912500	1.69270300	-0.91529400	Pd	-0.49293000	-0.98551300	0.05851300
C	5.82546700	-0.44246500	0.11784800	C	-2.27963500	-1.76034500	-0.14706200
H	6.48475500	0.14503400	0.76569700	C	-3.10997500	-1.56415300	-1.25602500
H	6.02547600	-1.50079500	0.31880300	C	-2.59225900	-2.73325100	0.81203200
H	6.10577600	-0.23548100	-0.92148100	C	-4.23868300	-2.37598700	-1.42274900
C	3.98682600	-0.39069700	1.84476400	H	-2.88174800	-0.79835800	-1.99224300
H	4.12830400	-1.44992500	2.08635000	C	-3.72234400	-3.54238800	0.63465100
H	4.62491900	0.18568100	2.52313900	H	-1.96493400	-2.86808400	1.69238600
H	2.94583100	-0.12919800	2.06416300	C	-4.54486200	-3.36211200	-0.48034800
C	-4.22848000	-1.79682200	0.30747700	H	-4.87715500	-2.23384300	-2.29094000
F	-4.73982100	-2.93877100	0.80481900	H	-3.96121000	-4.30098100	1.37547300
F	-4.59109300	-0.78992100	1.12975600	H	-5.42638200	-3.98341700	-0.61115600
F	-4.82887600	-1.57096800	-0.88183100	3			
Pd	0.57851000	0.98679500	-0.27628900	B3LYP SCF energy in DMF: -1457.611994 a.u.			
C	-0.78067000	2.39762700	-0.11770000	M06 SCF energy in DMF: -1457.114284 a.u.			
C	-1.79643900	2.60346100	-1.05903100	M06 Free energy in DMF: -1456.804587 a.u.			
C	-0.56188000	3.33088600	0.90492300	C	-2.56548000	0.03761600	-0.07609500
C	-2.57190600	3.76817500	-0.99435200	C	-1.12140800	-1.76791900	-0.13548700
H	-1.98288600	1.87516200	-1.84465600	C	-2.16370600	-2.67900500	0.00345300
C	-1.34317900	4.49243700	0.96118800	C	-3.46571800	-2.19065800	0.10302900
H	0.21055400	3.16440800	1.65390500	C	-3.66644800	-0.81374100	0.06449800
C	-2.34644100	4.71002000	0.01312700	H	-2.68740800	1.11469200	-0.10578300
H	-3.35120800	3.93498300	-1.73351300	H	-1.96160700	-3.74264000	0.03601100
H	-1.17053200	5.21763200	1.75215900	H	-4.30161700	-2.87242200	0.21332700
H	-2.95485500	5.60862500	0.06326800	C	0.28853100	-2.18507000	-0.24154800
2				N	1.26659800	-1.35140100	-0.27196700
B3LYP SCF energy in DMF: -1348.14835 a.u.				C	2.01511200	-3.60322600	-0.37993500
M06 SCF energy in DMF: -1347.667675 a.u.				C	2.51943100	-2.13317100	-0.42116700
M06 Free energy in DMF: -1347.363845 a.u.				H	2.26408100	-4.17219100	-1.27633600
C	2.72091700	-0.70703300	0.25431600	H	2.92807400	-1.90576000	-1.41282600
C	1.52571900	1.14885600	-0.44431000	O	0.55440100	-3.49161300	-0.31970800
C	2.68095100	1.87138000	-0.71595300	H	2.32781700	-4.16040400	0.50492000
C	3.91120800	1.25663500	-0.48220700	N	-1.31967300	-0.42978100	-0.17744700
C	3.92969700	-0.04623300	0.00861100	C	3.61917200	-1.77783500	0.62155400
H	2.69513200	-1.72236100	0.63432200	C	4.09148600	-0.33315500	0.37849800
H	2.62425500	2.88316900	-1.09870900	H	3.28006000	0.38168200	0.54058000
H	4.83528200	1.78853700	-0.68025900	H	4.90645200	-0.08024800	1.06590900
C	0.16883400	1.68299000	-0.63462900	H	4.46483500	-0.20513900	-0.64447100
				C	4.81208400	-2.72916700	0.39945800

H	5.63385800	-2.46293600	1.07298300
H	4.55443700	-3.77527500	0.59774300
H	5.18756300	-2.66245700	-0.62841700
C	3.09750500	-1.91070200	2.06282400
H	2.76028200	-2.92769300	2.29190300
H	3.89522500	-1.66552000	2.77237900
H	2.26251500	-1.22691000	2.25064400
C	-5.05094200	-0.22478700	0.12019700
F	-5.91797600	-1.03854000	0.75462900
F	-5.05995400	0.96337600	0.76178800
F	-5.54446500	-0.00559500	-1.12027800
Pd	0.53808000	0.76442500	-0.38858600
C	0.17146300	2.79437800	-0.70101800
C	-0.60998500	3.49026100	0.29120900
C	1.60148500	2.66383200	-0.40099400
C	-0.06369900	3.91621900	1.47213900
H	-1.65359300	3.68632900	0.06286000
C	2.17008000	3.16087100	0.83842600
C	1.33374400	3.74600600	1.74308200
H	-0.68176600	4.42721300	2.20378600
H	3.23737800	3.06611100	1.00428300
H	1.74372500	4.11600500	2.67771900
H	-0.14434500	2.85598600	-1.74150700
N	2.46933400	2.46467800	-1.43865100
N	3.21552100	2.30840100	-2.26494800

TS1

B3LYP SCF energy in DMF: -1457.610091 a.u.

M06 SCF energy in DMF: -1457.111695 a.u.

M06 Free energy in DMF: -1456.801299 a.u.

C	-2.52570500	-0.02528900	-0.01921200
C	-1.02719200	-1.78079800	-0.16445900
C	-2.03793900	-2.72946700	-0.04859200
C	-3.35357300	-2.28615500	0.08385400
C	-3.59838700	-0.91591300	0.09946900
H	-2.67957900	1.04813900	-0.00567000
H	-1.80302600	-3.78684000	-0.06205000
H	-4.16664900	-2.99772300	0.17586700
C	0.39502500	-2.14349000	-0.30712800
N	1.33815800	-1.26941500	-0.33108800
C	2.16678900	-3.46090300	-0.66289800
C	2.62753100	-1.99231400	-0.44877300
H	2.31642100	-3.80771200	-1.68738300
H	3.14099400	-1.62255000	-1.34211000
O	0.71876800	-3.43286400	-0.42225400
H	2.59409200	-4.18225300	0.03281600
N	-1.26844900	-0.44938500	-0.15117100
C	3.57733000	-1.75905300	0.76675200
C	3.92719300	-0.26272500	0.85608300
H	3.03897900	0.34759700	1.04568200
H	4.63536200	-0.08894200	1.67403200
H	4.39575600	0.09021100	-0.06998400
C	4.87472200	-2.55245900	0.51425800
H	5.59063900	-2.36589900	1.32201700
H	4.70249300	-3.63336500	0.47415600
H	5.34680400	-2.25007000	-0.42771500
C	2.92999600	-2.21331100	2.08715200
H	2.68461800	-3.28118200	2.08465600
H	3.62077700	-2.04325300	2.92014600
H	2.01290300	-1.65318900	2.30076300
C	-5.00104300	-0.37528000	0.18524300
F	-5.83723900	-1.24267500	0.78925800
F	-5.04673400	0.78509600	0.87412400
F	-5.50770800	-0.12342000	-1.04370800
Pd	0.56962700	0.80011800	-0.43580100
C	0.07779200	2.85977600	-0.79105200
C	-0.77552200	3.55034400	0.13068100
C	1.48250500	2.83318600	-0.44764700
C	-0.28278600	4.09086000	1.29336200
H	-1.82458900	3.65708900	-0.12781900
C	1.99667700	3.40390200	0.76335400

C	1.10893800	4.02526900	1.60191500
H	-0.95005700	4.60571800	1.97738100
H	3.06009200	3.35395000	0.96843800
H	1.47767400	4.49320900	2.50931900
H	-0.22360900	2.77776300	-1.83427100
N	2.34046300	2.23445800	-1.33023300
N	3.19381700	2.00272900	-2.04960000

4

B3LYP SCF energy in DMF: -1457.684937 a.u.

M06 SCF energy in DMF: -1457.174635 a.u.

M06 Free energy in DMF: -1456.8659 a.u.

C	-1.97033400	-0.81760400	0.11573400
C	0.03769500	-1.87474300	-0.37693100
C	-0.56918100	-3.12108900	-0.42583300
C	-1.94151400	-3.20896600	-0.18795200
C	-2.64358700	-2.04299100	0.09130700
H	-2.49097000	0.10819100	0.32393400
H	0.01952000	-4.00460300	-0.64081000
H	-2.44327500	-4.16920900	-0.21602400
C	1.48249000	-1.67987600	-0.56909400
N	2.03807600	-0.52788800	-0.42107400
C	3.58932000	-2.15449200	-1.12480800
C	3.50415000	-0.70596600	-0.57519000
H	3.76143700	-2.18924400	-2.20259500
H	3.86218400	0.00638200	-1.32368200
O	2.24910400	-2.71717500	-0.88676900
H	4.30403000	-2.79970200	-0.61667000
N	-0.65765100	-0.73391300	-0.11612000
C	4.29172900	-0.45085700	0.74865000
C	4.06197200	0.99885000	1.21235100
H	3.01872300	1.17405700	1.49380100
H	4.68230100	1.21337300	2.08938500
H	4.33345900	1.71576800	0.42920600
C	5.79121600	-0.63953900	0.44557400
H	6.38319400	-0.41858900	1.34011200
H	6.02988200	-1.66445700	0.14212700
H	6.12376400	0.03548100	-0.35150300
C	3.85467500	-1.41668200	1.86469300
H	4.03541700	-2.46518100	1.60436700
H	4.42247600	-1.20971400	2.77817100
H	2.79215000	-1.30185600	2.10596100
C	-4.13325400	-2.05233500	0.32498300
F	-4.59307900	-3.29220600	0.57447400
F	-4.47134800	-1.26836900	1.37025400
F	-4.79914700	-1.58221300	-0.75270200
Pd	0.50382600	1.01968800	-0.22827700
C	-1.09600700	2.22476100	-0.06819600
C	-1.82905500	2.57444800	-1.20731400
C	-1.48382500	2.68946800	1.19330300
C	-2.97014900	3.37657900	-1.07651700
H	-1.52677200	2.22564800	-2.19138600
C	-2.62724000	3.49009200	1.31420900
H	-0.91193300	2.43201100	2.08112400
C	-3.37068400	3.83225900	0.18194900
H	-3.54184900	3.64269200	-1.96195300
H	-2.93083500	3.84541800	2.29562500
H	-4.25636900	4.45374400	0.27960300
N	2.18148100	3.61508300	-0.67208100
N	1.59042300	2.69796500	-0.48753200

5

B3LYP SCF energy in DMF: -1619.944794 a.u.

M06 SCF energy in DMF: -1619.354096 a.u.

M06 Free energy in DMF: -1618.917284 a.u.

C	-2.34570200	-0.80939500	0.17098700
C	-0.50037200	-1.99107300	-0.57356200
C	-1.27619000	-3.08551900	-0.93399000
C	-2.65216400	-3.03163900	-0.71212200
C	-3.18639900	-1.88307400	-0.14017300

H	-2.73544600	0.10515900	0.60099300
H	-0.81195700	-3.96280500	-1.36737300
H	-3.28579400	-3.87126600	-0.97345700
C	0.96509800	-1.98843400	-0.69155100
N	1.70570400	-1.06778100	-0.17553700
C	2.96973500	-2.61299200	-1.42902900
C	3.12078600	-1.49874600	-0.36899700
H	3.14055000	-2.25549600	-2.44774500
H	3.69098000	-0.65863600	-0.77301900
O	1.55274700	-2.99350800	-1.33949400
H	3.55938600	-3.50986100	-1.24962900
N	-1.02907600	-0.85971100	-0.04361500
C	3.80618100	-1.95685500	0.95946900
C	3.77907700	-0.80744900	1.97903400
H	2.75679000	-0.56970700	2.28511900
H	4.33909700	-1.08896300	2.87779900
H	4.23940000	0.09897500	1.57062500
C	5.27521900	-2.29361500	0.63634100
H	5.79824300	-2.59570800	1.55009700
H	5.36794700	-3.11725700	-0.07961000
H	5.79964400	-1.42466800	0.22222400
C	3.10993600	-3.18668700	1.57114000
H	3.15392700	-4.06289000	0.91594600
H	3.60453600	-3.46086000	2.50911600
H	2.05902600	-2.98354600	1.80535900
C	-4.66285200	-1.74206700	0.12521900
F	-5.31305300	-2.91241000	-0.01430200
F	-4.89501500	-1.29024300	1.37679500
F	-5.23296700	-0.85734600	-0.72296800
Pd	0.41065600	0.74957800	0.18477800
C	-1.09521900	2.07352400	0.21973900
C	-1.58970800	2.57954200	-0.98918200
C	-1.75144800	2.38237700	1.41910900
C	-2.74130900	3.37781700	-0.99680800
H	-1.09459400	2.35369100	-1.92965700
C	-2.90256400	3.18081000	1.40390200
H	-1.37696600	2.00767600	2.36844900
C	-3.40007200	3.67949800	0.19722300
H	-3.11999800	3.76020600	-1.94152400
H	-3.40562900	3.41201200	2.33963700
H	-4.29221700	4.29943300	0.18809900
C	2.15828000	2.10433800	-0.13805400
C	1.51992000	2.64756000	0.95942800
H	2.99975900	1.43244100	0.02345200
H	0.85096400	3.48326300	0.77223200
C	1.89396800	2.44800500	2.39762500
C	2.09802200	2.75028500	-1.50971300
H	1.15082500	3.29989700	-1.60092900
H	1.00883900	2.32204800	3.02947900
H	2.56940600	1.60570500	2.54871000
C	2.22697600	1.75599300	-2.66185300
H	1.39313200	1.04695900	-2.67068900
H	3.16422500	1.19422900	-2.58352600
H	2.39930100	3.36027100	2.74461100
H	2.22551200	2.28745600	-3.62074400
O	3.19790300	3.67648800	-1.50934400
H	3.27344800	4.02701300	-2.40988600

TS2

B3LYP SCF energy in DMF: -1619.92703 a.u.

M06 SCF energy in DMF: -1619.339756 a.u.

M06 Free energy in DMF: -1618.900915 a.u.

C	-2.38463400	-0.66221700	0.09024700
C	-0.64128800	-2.05728100	-0.50283100
C	-1.50240800	-3.10524900	-0.80862100
C	-2.87307000	-2.90613900	-0.64385700
C	-3.31585200	-1.67003300	-0.18389400
H	-2.69761900	0.31187200	0.44793100
H	-1.11263500	-4.05261000	-1.16086600
H	-3.57484700	-3.70187900	-0.86650000
C	0.82246100	-2.17264700	-0.59095700

N	1.61851100	-1.20955100	-0.26645400
C	2.80202900	-3.06600000	-1.08132800
C	3.00200300	-1.76525500	-0.27142700
H	3.03216900	-2.94128300	-2.14268500
H	3.65796000	-1.07684100	-0.80724300
O	1.35825500	-3.32698900	-0.98220000
H	3.31620400	-3.94298700	-0.69311200
N	-1.07392300	-0.85246900	-0.06177400
C	3.58476300	-1.97140900	1.16629600
C	3.65304000	-0.62249200	1.90365000
H	2.65836500	-0.19223900	2.05457900
H	4.11128900	-0.75895800	2.88955400
H	4.26265200	0.10257000	1.35309000
C	5.01954200	-2.51613300	1.01467800
H	5.48351800	-2.62429800	2.00086600
H	5.04616700	-3.49907200	0.53302500
H	5.64303400	-1.83454200	0.42452000
C	2.73774500	-2.95520000	1.99490300
H	2.68562500	-3.95024800	1.54069300
H	3.18111300	-3.07797800	2.98891300
H	1.71508300	-2.58894700	2.13801100
C	-4.78375900	-1.37577400	-0.02158100
F	-5.50740700	-2.50200800	0.13335500
F	-5.01666200	-0.58821800	1.05015600
F	-5.27922400	-0.72797000	-1.10060300
Pd	0.57100000	0.66449100	0.00260600
C	-0.69578100	2.29933500	0.33495900
C	-1.35426700	2.77865000	-0.81380400
C	-1.36511900	2.33184900	1.57056300
C	-2.67078700	3.23643700	-0.73277000
H	-0.83494800	2.80308400	-1.76780800
C	-2.67981700	2.80207700	1.64824200
H	-0.86644300	1.99061500	2.47269800
C	-3.33534300	3.25203500	0.49844200
H	-3.17238200	3.59434200	-1.62792100
H	-3.18813800	2.81863500	2.60854300
H	-4.35433500	3.62290900	0.56241100
C	2.10210100	2.05054500	-0.24206500
C	1.26486900	2.97596300	0.46095100
H	2.93753900	1.63736700	0.32386300
H	0.92077000	3.82574800	-0.11976600
C	1.53448900	3.28709600	1.91108300
C	2.41494400	2.36654800	-1.69973400
H	1.47477900	2.61827300	-2.21481400
H	0.71473700	3.83513400	2.37893100
H	1.75017900	2.39051400	2.49792400
C	3.11245300	1.24216900	-2.45786800
H	2.47189200	0.35878600	-2.53597800
H	4.04673500	0.96017700	-1.96093700
H	2.42480800	3.92914700	1.94260700
H	3.35497200	1.56900800	-3.47608300
O	3.25364200	3.53689200	-1.64887400
H	3.47822500	3.76452700	-2.56395800

6

B3LYP SCF energy in DMF: -1619.958331 a.u.

M06 SCF energy in DMF: -1619.372185 a.u.

M06 Free energy in DMF: -1618.928953 a.u.

C	2.71233400	0.04341400	-0.01989900
C	1.29143800	1.80556600	-0.44944800
C	2.34661800	2.67863000	-0.69510200
C	3.64827400	2.19206800	-0.58426300
C	3.83028600	0.85741100	-0.23437100
H	2.82385000	-1.00224800	0.23792200
H	2.15544300	3.71067000	-0.96299800
H	4.49643500	2.84237700	-0.76788600
C	-0.11317300	2.23943800	-0.47929400
N	-1.09917100	1.45035100	-0.20677600
C	-1.85991300	3.57609100	-0.83026700
C	-2.32509400	2.29324700	-0.10779000
H	-2.12486000	3.58388300	-1.89062800

H	-3.13259700	1.81072200	-0.66032900	C	-3.74427900	-1.97375300	-0.88411700
O	-0.39203400	3.51133500	-0.75350900	C	-3.89066300	-0.60768900	-1.57481200
H	-2.16645300	4.50963800	-0.36349600	H	-2.92308400	-0.15121200	-1.79922500
N	1.46573500	0.50351300	-0.12468200	H	-4.43086200	-0.72623900	-2.52089000
C	-2.80430200	2.51750800	1.36637900	H	-4.46529200	0.09052700	-0.95604600
C	-3.12611500	1.16937900	2.03549500	C	-5.15581700	-2.52188900	-0.59026800
H	-2.24212800	0.52858900	2.10356900	H	-5.72444800	-2.60494800	-1.52267700
H	-3.49460600	1.34047500	3.05309800	H	-5.13391800	-3.51675600	-0.13309700
H	-3.90518500	0.62744400	1.48943100	H	-5.70924600	-1.85403400	0.08021000
C	-4.10001900	3.35258600	1.31001200	C	-2.99668700	-2.93684800	-1.82482900
H	-4.49858400	3.48793700	2.32109300	H	-2.90079700	-3.94367700	-1.40484000
H	-3.94024000	4.35023200	0.88733100	H	-3.54627200	-3.03185600	-2.76742400
H	-4.86962100	2.85142400	0.71155600	H	-1.99388400	-2.56904100	-2.06850800
C	-1.74652000	3.25480900	2.20878300	C	4.73369100	-1.49343900	-0.48622300
H	-1.51273700	4.24801800	1.81133600	F	5.53258200	-2.52976400	-0.16987200
H	-2.12134200	3.39570200	3.22826000	F	4.88346800	-1.25604900	-1.80846400
H	-0.81391300	2.68414000	2.28207000	F	5.19896200	-0.40342600	0.16217500
C	5.21074400	0.28956900	-0.03420000	Pd	-0.43913000	0.66373800	0.30020300
F	6.12100800	0.90141700	-0.81832300	C	0.94718100	2.10238900	0.19797100
F	5.62439600	0.43811800	1.24485400	C	1.73644200	2.42216600	1.31172700
F	5.25354700	-1.03126800	-0.31187700	C	1.22983500	2.69284600	-1.04134900
Pd	-0.56641300	-0.61417000	-0.21426300	C	2.80687100	3.31611900	1.18143700
C	-0.80256000	-2.82589000	0.52324900	H	1.53195100	1.97683200	2.28206100
C	0.13393800	-2.92495600	-0.54151100	C	2.30407500	3.58394100	-1.16488600
C	-0.31176300	-2.92386000	1.85241800	H	0.60771800	2.47723300	-1.90503500
C	1.49660500	-3.18938600	-0.27724400	C	3.09457200	3.89667100	-0.05633300
H	-0.21845100	-2.99105000	-1.56657400	H	3.41389400	3.55467000	2.05137900
C	1.02968900	-3.17721900	2.09548700	H	2.51611800	4.03495000	-2.13132000
H	-1.00221800	-2.84792000	2.68508300	H	3.92587900	4.58919900	-0.15527700
C	1.93862600	-3.32384200	1.02939000	C	-2.19696700	2.03991500	0.32415900
H	2.18517000	-3.31167400	-1.10812900	C	-1.63026200	2.09653900	1.58757200
H	1.37876200	-3.28370700	3.11866100	H	-0.96954200	2.93298300	1.80635500
H	2.98138200	-3.54818100	1.23427100	C	-2.12141700	1.33681500	2.78716600
C	-2.43162100	-1.38560700	-0.54589800	H	-1.29408300	0.99170400	3.41515100
C	-2.29916800	-2.73748200	0.17392400	H	-2.72463000	2.01873600	3.40323400
H	-3.12406300	-0.70640500	-0.04353800	H	-2.74746800	0.48406700	2.51524000
H	-2.51589000	-3.54607000	-0.53406500	H	-3.01804400	1.34532300	0.15852800
C	-3.24665400	-2.89109000	1.36313800	C	-2.11985000	3.16820000	-0.67741900
C	-2.77866800	-1.50995300	-2.03174000	H	-1.24777200	3.79651600	-0.45469400
H	-2.05391000	-2.18321600	-2.51382400	C	-3.38598400	4.02844700	-0.59527200
H	-3.09615300	-3.84753500	1.87624100	H	-4.28156800	3.42520900	-0.77801500
H	-3.12378800	-2.08783800	2.09773200	H	-3.47594800	4.50227600	0.38756100
C	-2.82089000	-0.20120200	-2.81618000	H	-3.34586400	4.82405100	-1.34868900
H	-1.84231000	0.28886000	-2.83260800	O	-1.98885000	2.58128300	-1.97870600
H	-3.55446500	0.48877400	-2.38670600	H	-2.01956800	3.30385300	-2.62363800
H	-4.28094900	-2.86082000	1.00725200				
H	-3.11204800	-0.39904600	-3.85474300				
O	-4.07650300	-2.13902900	-2.04829900				
H	-4.26029000	-2.38664600	-2.96687800				

7

B3LYP SCF energy in DMF: -1619.951833 a.u.

M06 SCF energy in DMF: -1619.355967 a.u.

M06 Free energy in DMF: -1618.917496 a.u.

C	2.38560200	-0.70130300	-0.16215900
C	0.64230200	-2.12363400	0.38523700
C	1.48798600	-3.22408300	0.45109500
C	2.84459500	-3.04190200	0.18078600
C	3.29287800	-1.76550400	-0.13879100
H	2.70634800	0.30844800	-0.38634300
H	1.09470900	-4.20179000	0.70103200
H	3.53033200	-3.88059600	0.21730600
C	-0.81285800	-2.23187500	0.58056900
N	-1.62688100	-1.25900000	0.35031900
C	-2.73912500	-3.14033300	1.22710900
C	-3.00603600	-1.81023300	0.48591000
H	-2.87096700	-3.05729900	2.30899500
H	-3.59588300	-1.13491800	1.11040300
O	-1.31279900	-3.39893000	0.98574700
H	-3.29211800	-3.99976900	0.85347700
N	1.08771600	-0.87548900	0.09523600

TS3

B3LYP SCF energy in DMF: -1619.922355 a.u.

M06 SCF energy in DMF: -1619.330665 a.u.

M06 Free energy in DMF: -1618.891978 a.u.

C	-2.50310700	-0.49128200	0.08295800
C	-0.88475000	-1.97989000	-0.61805300
C	-1.82654800	-2.95607100	-0.92385100
C	-3.17301600	-2.67239300	-0.69658500
C	-3.51160400	-1.42685200	-0.17717600
H	-2.73946500	0.49510800	0.46401900
H	-1.51536700	-3.91378400	-1.32321900
H	-3.93586400	-3.40928800	-0.92072300
C	0.56377900	-2.20784400	-0.72359400
N	1.42818900	-1.32523000	-0.34957500
C	2.48229500	-3.21454600	-1.22579200
C	2.74837100	-2.01144400	-0.30151700
H	2.72506400	-3.00400800	-2.27127800
H	3.50804700	-1.34498000	-0.70963000
O	1.01902200	-3.38524200	-1.15155800
H	2.93617700	-4.15534600	-0.92076400
N	-1.21568000	-0.75805700	-0.13391800
C	3.16321300	-2.39782300	1.16249900
C	3.12711300	-1.15890100	2.07628500
H	2.10921900	-0.77234300	2.19183900
H	3.49718800	-1.42481300	3.07296000

H	3.75105900	-0.35661700	1.67674400
C	4.60887900	-2.92994100	1.09836600
H	4.95012100	-3.21643300	2.09904500
H	4.69578600	-3.81432800	0.45755900
H	5.29706900	-2.16838500	0.71446100
C	2.24601800	-3.47933900	1.76723100
H	2.27475600	-4.41972300	1.20780900
H	2.57221000	-3.70209900	2.78897200
H	1.20385400	-3.14662100	1.82937900
C	-4.94018500	-1.07743200	0.14724000
F	-5.81155500	-1.81188800	-0.57222200
F	-5.21908900	-1.29256500	1.45283000
F	-5.20018000	0.22502000	-0.09971600
Pd	0.57578900	0.65077800	-0.22296000
C	-0.46028300	2.41559500	0.17385500
C	-1.69642000	2.67514700	-0.43932700
C	-0.24083100	2.85831600	1.49317300
C	-2.70905500	3.32909300	0.26987900
H	-1.87844200	2.36324900	-1.46303700
C	-1.26266100	3.49370700	2.20185000
H	0.72985200	2.71687300	1.96141600
C	-2.49764800	3.73401600	1.59048000
H	-3.66399800	3.51787300	-0.21325900
H	-1.08676100	3.81700600	3.22433200
H	-3.28539200	4.24534300	2.13630500
C	2.16320800	1.83547200	-0.92168600
C	1.15395000	2.83986300	-1.07256700
H	1.27338500	3.72022400	-0.44961800
C	0.59182000	3.13089200	-2.44357100
H	-0.28569600	3.77845200	-2.40441000
H	1.37118800	3.66121200	-3.00605400
H	0.34423100	2.21930800	-2.99379900
H	2.42755800	1.29845200	-1.83642200
C	3.37285500	2.08354800	-0.03211600
H	3.06336400	2.14901400	1.02180000
C	4.10849100	3.37694000	-0.40853100
H	4.40367700	3.36245800	-1.46316000
H	3.48531000	4.25808300	-0.22868100
H	5.01282300	3.48006700	0.20288200
O	4.24150900	0.96075200	-0.22576300
H	5.03504800	1.11109400	0.30896600

8

B3LYP SCF energy in DMF: -1619.953984 a.u.

M06 SCF energy in DMF: -1619.364727 a.u.

M06 Free energy in DMF: -1618.922849 a.u.

C	-2.64057100	-0.31041800	0.21273500
C	-1.12591300	-1.78357100	-0.70126900
C	-2.13077800	-2.60182200	-1.20659800
C	-3.45876300	-2.23843700	-0.98055800
C	-3.71342000	-1.07935000	-0.25676900
H	-2.81143300	0.59939200	0.77554700
H	-1.88310700	-3.49830700	-1.76211800
H	-4.26953400	-2.84857500	-1.36200500
C	0.30079400	-2.11740100	-0.82313800
N	1.24518100	-1.36018900	-0.37031500
C	2.11652300	-3.26496300	-1.41012500
C	2.49624200	-2.17039400	-0.39619400
H	2.39566100	-3.00736100	-2.43580400
H	3.30577900	-1.54208900	-0.76123900
O	0.64464400	-3.28783200	-1.35867700
H	2.46466800	-4.26784700	-1.17143400
N	-1.37143800	-0.64758900	-0.00626100
C	2.88835500	-2.70860400	1.02484300
C	3.01922800	-1.54526400	2.02644800
H	2.05817300	-1.04854700	2.19505500
H	3.37180900	-1.92685100	2.99155000
H	3.72970100	-0.79533800	1.67111300
C	4.26137600	-3.39760800	0.88641700
H	4.58282900	-3.79422800	1.85554100
H	4.23835300	-4.23487800	0.18018500

H	5.02590600	-2.69093000	0.54368300
C	1.85872400	-3.71590200	1.57271300
H	1.76540000	-4.60818000	0.94524800
H	2.17024200	-4.05323500	2.56737800
H	0.86548000	-3.26638200	1.68300900
C	-5.11462700	-0.62477600	0.05274900
F	-6.03848900	-1.32191200	-0.63563700
F	-5.40146200	-0.76074200	1.36702700
F	-5.28183500	0.68340600	-0.24851200
Pd	0.60923800	0.64862400	0.02546600
C	0.15569500	2.89783800	0.07204100
C	-1.11564800	3.18847900	-0.49337400
C	0.21466000	2.55019700	1.44970100
C	-2.25535500	3.18406300	0.29494200
H	-1.18758800	3.45908600	-1.54108700
C	-0.95785800	2.52593400	2.23381500
H	1.17946000	2.46501900	1.94293900
C	-2.17815300	2.85876900	1.66368900
H	-3.21614200	3.43608700	-0.14436300
H	-0.88919800	2.28862100	3.29125700
H	-3.07788900	2.87371200	2.27215500
C	2.18670900	1.77801100	-0.70129100
C	1.48926600	3.14403300	-0.66085900
H	2.05504800	3.83607600	-0.02672200
C	1.34577200	3.77891500	-2.04524300
H	0.82373000	4.74058900	-1.99133400
H	2.33596400	3.95793700	-2.47455200
H	0.79705800	3.12771200	-2.73462500
H	2.23814000	1.37300400	-1.71989600
C	3.56381900	1.72139900	-0.05378200
H	3.46634700	1.82590400	1.03842100
C	4.50244900	2.82930900	-0.56205700
H	4.61441700	2.77478800	-1.64980800
H	4.15455700	3.82949100	-0.29072100
H	5.49260000	2.69778200	-0.10889700
O	4.14084600	0.44985000	-0.37571300
H	5.02343600	0.42176900	0.02234200

9

B3LYP SCF energy in DMF: -1619.952557 a.u.

M06 SCF energy in DMF: -1619.356212 a.u.

M06 Free energy in DMF: -1618.917653 a.u.

C	2.80012900	0.06666000	0.29531300
C	1.40575400	1.64318500	-0.64539500
C	2.47397000	2.41810000	-1.08186300
C	3.76831800	1.98300300	-0.79878000
C	3.93018700	0.79411400	-0.09617300
H	2.90513100	-0.86397100	0.84020300
H	2.29912100	3.34032900	-1.62256600
H	4.62632500	2.56443100	-1.11687200
C	0.00621200	2.05359400	-0.83716800
N	-0.98983200	1.40792300	-0.32492700
C	-1.72634500	3.19234700	-1.65245200
C	-2.21130600	2.23251000	-0.54506800
H	-1.97037200	2.83938000	-2.65752200
H	-3.01086600	1.58668400	-0.91316400
O	-0.25794300	3.15454400	-1.53174900
H	-2.03324900	4.22992100	-1.53863300
N	1.56018800	0.47895300	0.02979500
C	-2.70570300	2.94684200	0.75762100
C	-3.02608400	1.90818600	1.84612000
H	-2.13484900	1.34942300	2.14808700
H	-3.41799500	2.41423300	2.73551700
H	-3.78063000	1.19195700	1.50799900
C	-4.00259300	3.70297200	0.40451900
H	-4.40682800	4.18842200	1.29916600
H	-3.84142900	4.48489900	-0.34545200
H	-4.76754300	3.01923000	0.01903800
C	-1.65802200	3.93533800	1.30359000
H	-1.42810400	4.73753600	0.59493800
H	-2.04094300	4.40965700	2.21352400

H	-0.72251300	3.43148200	1.57115300
C	5.30086500	0.24718300	0.20713500
F	5.33552100	-0.37250600	1.40597100
F	5.68281100	-0.66203700	-0.71786600
F	6.23486200	1.21800900	0.22081700
Pd	-0.46240300	-0.58998400	0.22894400
C	-2.34053300	-1.24371300	-0.02674200
C	-2.79391900	-1.35558400	-1.34918200
C	-3.22249500	-1.51965300	1.02581000
C	-4.11489800	-1.73954300	-1.61222200
H	-2.12181800	-1.15813400	-2.17912300
C	-4.54397000	-1.90092000	0.75674400
H	-2.89938500	-1.43547600	2.05945600
C	-4.99359400	-2.01230500	-0.56066000
H	-4.45193500	-1.82455700	-2.64253200
H	-5.21796000	-2.10936400	1.58404800
H	-6.01813600	-2.30965600	-0.76654800
C	0.46712800	-2.61959000	0.27072100
C	-0.10072300	-2.41067500	1.51683700
H	1.52261700	-2.38870700	0.13184100
H	-1.07835000	-2.85096100	1.69879200
C	0.63634300	-1.96882300	2.74974900
H	0.01865900	-1.31359200	3.37205700
H	0.86517600	-2.85776800	3.35447100
H	1.57793700	-1.46406100	2.52423800
C	-0.08398400	-3.57339300	-0.76177500
H	-1.16418700	-3.69346900	-0.61127600
C	0.59494400	-4.94198600	-0.62694200
H	0.21594900	-5.62487400	-1.39655000
H	1.67995800	-4.85371800	-0.74784000
H	0.38491600	-5.38916300	0.35004100
O	0.18103800	-3.00033700	-2.04793300
H	-0.13220900	-3.63091600	-2.71325000

TS4

B3LYP SCF energy in DMF: -1619.926297 a.u.

M06 SCF energy in DMF: -1619.335604 a.u.

M06 Free energy in DMF: -1618.896209 a.u.

C	-2.65000600	-0.29223800	0.34447400
C	-1.13529000	-1.77072500	-0.58664000
C	-2.13818500	-2.66256200	-0.94962600
C	-3.45697900	-2.34537000	-0.62794400
C	-3.71019400	-1.15245800	0.04225700
H	-2.82298500	0.65330100	0.83959500
H	-1.89171300	-3.58691200	-1.45771700
H	-4.26372000	-3.02245800	-0.88507700
C	0.29468300	-2.05766100	-0.78156000
N	1.22190100	-1.33902700	-0.24712500
C	2.11316900	-3.03327800	-1.61182300
C	2.50674200	-2.05422000	-0.48353800
H	2.33382600	-2.64024000	-2.60788100
H	3.25377300	-1.33781400	-0.83361300
O	0.64952300	-3.12457100	-1.50001400
H	2.51070300	-4.04193500	-1.51740800
N	-1.38759300	-0.59235400	0.03339200
C	3.05559200	-2.74735500	0.80959300
C	3.26259700	-1.70542200	1.92174300
H	2.32013600	-1.23281200	2.21470300
H	3.68351600	-2.18900600	2.81044200
H	3.95691700	-0.92121100	1.60746800
C	4.42228500	-3.36971300	0.46118500
H	4.85506500	-3.84360300	1.34889500
H	4.34684900	-4.13927900	-0.31455600
H	5.12796800	-2.60730200	0.11146200
C	2.10147600	-3.84226100	1.32371900
H	1.94744600	-4.64408100	0.59415400
H	2.52229900	-4.30295300	2.22402500
H	1.12238300	-3.43340100	1.59720700
C	-5.11453700	-0.74098700	0.39749000
F	-5.14939500	-0.03498100	1.54803600
F	-5.66012400	0.04209200	-0.56121100

F	-5.92597700	-1.80718200	0.54724900
Pd	0.35526100	0.70063500	0.15727500
C	2.10353300	1.83898400	-0.03966100
C	2.34898900	2.15319800	-1.39201700
C	3.19136100	1.64357800	0.82438400
C	3.65697700	2.21444800	-1.87613500
H	1.52017900	2.35908200	-2.06328400
C	4.49999200	1.72401100	0.33803700
H	3.02588500	1.42670600	1.87412200
C	4.73578900	2.00389600	-1.01069300
H	3.83338000	2.44536200	-2.92328900
H	5.33439600	1.56877800	1.01668400
H	5.75403600	2.07124500	-1.38311500
C	-0.62645400	2.51669900	0.42938900
C	0.64463300	3.05252800	0.81314400
H	-1.31054000	2.28231700	1.25015200
H	1.03967400	3.83011800	0.16570300
C	0.97689300	3.24298200	2.27135700
H	2.03482000	3.45859600	2.43137500
H	0.40629800	4.11354500	2.62104600
H	0.68806100	2.38451700	2.88324600
C	-1.29917200	3.09489600	-0.80477200
H	-0.52638000	3.30659900	-1.55909700
C	-2.01893900	4.40575200	-0.46349100
H	-2.50730300	4.81293700	-1.35708600
H	-2.78305100	4.24125300	0.30400900
H	-1.31247900	5.15816000	-0.09822200
O	-2.22586100	2.13116900	-1.31537800
H	-2.74113600	2.56847100	-2.00921500

10

B3LYP SCF energy in DMF: -1619.958496 a.u.

M06 SCF energy in DMF: -1619.369854 a.u.

M06 Free energy in DMF: -1618.927452 a.u.

C	-2.47204600	-0.49921900	0.35978600
C	-0.85960500	-1.92870500	-0.48170500
C	-1.78364800	-2.95157800	-0.66797000
C	-3.10931400	-2.72739800	-0.30263100
C	-3.45010700	-1.48843000	0.23232100
H	-2.71953600	0.47686400	0.75192200
H	-1.46697300	-3.90488900	-1.07284000
H	-3.85288700	-3.50745900	-0.42249200
C	0.57901100	-2.11108300	-0.73083200
N	1.46698100	-1.26904700	-0.32892300
C	2.42695400	-3.03018300	-1.55967000
C	2.79096100	-1.91050600	-0.56035300
H	2.56817500	-2.72957300	-2.60157500
H	3.46303600	-1.18081600	-1.01800200
O	0.98364100	-3.21936800	-1.35732600
H	2.90974400	-3.99009800	-1.38582400
N	-1.20216900	-0.71181200	0.00707400
C	3.44906700	-2.41854100	0.76720500
C	3.60303600	-1.25170700	1.75733000
H	2.63358100	-0.82745200	2.03666300
H	4.09197500	-1.60260700	2.67315900
H	4.21862400	-0.45170400	1.33717700
C	4.85060800	-2.95805000	0.41763600
H	5.36174000	-3.29191700	1.32709700
H	4.81077900	-3.81188200	-0.26716500
H	5.46907200	-2.18242500	-0.04879100
C	2.61740000	-3.53015600	1.43497800
H	2.50358000	-4.41174600	0.79603400
H	3.11629400	-3.85858400	2.35314300
H	1.61905000	-3.17846600	1.71808300
C	-4.87085400	-1.17525300	0.61930700
F	-4.92802300	-0.27470900	1.62361800
F	-5.56315800	-0.65213300	-0.41850700
F	-5.53362100	-2.27871700	1.02018900
Pd	0.37645700	0.74623200	-0.09791000
C	1.58833100	2.75102300	0.20073000
C	1.85373900	2.33981400	-1.13466400

C	2.63399800	2.63606300	1.15220100
C	3.13431800	1.87048300	-1.50191500
H	1.13648400	2.55385100	-1.92134700
C	3.89293600	2.19884300	0.77020900
H	2.46250100	2.94078200	2.17852500
C	4.14903000	1.81461900	-0.55985200
H	3.32216200	1.59263800	-2.53482900
H	4.69191500	2.15984600	1.50486400
H	5.14317200	1.48343000	-0.84509900
C	-0.81142700	2.40359700	0.09664800
C	0.24473500	3.44235000	0.50276500
H	-1.46867500	2.13881000	0.93357700
H	0.18257700	4.32114100	-0.15303600
C	0.08463000	3.92252500	1.94558100
H	0.85964300	4.64645200	2.21845900
H	-0.88593300	4.41484300	2.06162000
H	0.12454300	3.09107900	2.65839900
C	-1.61871200	2.78669100	-1.14023600
H	-0.93037700	3.15470400	-1.91681200
C	-2.61754500	3.90640200	-0.81566700
H	-3.18178400	4.18032900	-1.71573700
H	-3.32713800	3.57895600	-0.04813400
H	-2.10987000	4.80886400	-0.46115000
O	-2.31041200	1.63135600	-1.62861300
H	-2.91178600	1.93089100	-2.32649200

11

B3LYP SCF energy in DMF: -1619.947335 a.u.

M06 SCF energy in DMF: -1619.354438 a.u.

M06 Free energy in DMF: -1618.915775 a.u.

C	2.81553700	-0.04555600	0.15012400
C	1.45764600	1.73004300	-0.41189600
C	2.54322400	2.56724400	-0.64378600
C	3.82729000	2.05419200	-0.46325900
C	3.96109500	0.73230500	-0.05222400
H	2.90182800	-1.07819100	0.46563100
H	2.38902300	3.59357300	-0.95412500
H	4.69789800	2.67767700	-0.63286100
C	0.06717600	2.19842400	-0.51721100
N	-0.94694000	1.46605200	-0.18888600
C	-1.63354100	3.52687400	-1.06576800
C	-2.15275600	2.34270400	-0.22363300
H	-1.85908600	3.42168700	-2.13017000
H	-2.95524300	1.81743000	-0.74514600
O	-0.16884800	3.43822800	-0.92976000
H	-1.93075700	4.51431500	-0.71951200
N	1.58557100	0.43659200	-0.03051200
C	-2.65989500	2.73711200	1.20467700
C	-2.99646200	1.47544600	2.01730000
H	-2.10884800	0.86130700	2.19634400
H	-3.40544100	1.76303300	2.99232800
H	-3.74372600	0.85914600	1.50916300
C	-3.95014500	3.56228200	1.02564800
H	-4.35586800	3.83643600	2.00536000
H	-3.77982900	4.49136100	0.47157100
H	-4.71798300	2.98831000	0.49411400
C	-1.61559400	3.56458200	1.97828800
H	-1.38091500	4.51378100	1.48587800
H	-2.00330400	3.80562800	2.97381000
H	-0.68122700	3.01015300	2.12107200
C	5.31837000	0.10262000	0.12111500
F	6.25969800	1.01716600	0.42547900
F	5.31455000	-0.82548200	1.10102800
F	5.71798600	-0.51964800	-1.01099400
Pd	-0.44824200	-0.61967200	-0.18424800
C	-2.33918100	-1.15151400	-0.58865700
C	-2.78295800	-0.95115400	-1.90423000
C	-3.23599600	-1.63227400	0.37161800
C	-4.11112300	-1.22802200	-2.25175500
H	-2.10217100	-0.58055100	-2.66657900
C	-4.56448400	-1.90774900	0.01826600

H	-2.92194100	-1.78631100	1.39864400
C	-5.00509800	-1.70817400	-1.29140200
H	-4.44049000	-1.06904900	-3.27567300
H	-5.25149800	-2.27769500	0.77545900
H	-6.03479500	-1.92524100	-1.56161400
C	0.36786700	-2.64167800	0.30150100
C	0.09681300	-2.64984600	-1.05612000
H	1.38008700	-2.40754700	0.62795800
H	-0.83805500	-3.10761800	-1.37254200
C	1.10197800	-2.43166300	-2.15203000
H	1.36799300	-3.41325400	-2.56867700
H	0.68426600	-1.84294200	-2.97500400
H	2.01893500	-1.95604800	-1.79758000
C	-0.42542600	-3.43063100	1.32300900
C	-0.43089900	-2.78245100	2.70501400
H	0.59399900	-2.64304500	3.06702700
H	-0.92686100	-1.80728100	2.68428400
H	-0.96558800	-3.41626700	3.42214900
H	-1.45443700	-3.56030100	0.96502700
O	0.23875700	-4.70626600	1.36004800
H	-0.13726000	-5.19878800	2.10538100

TS5

B3LYP SCF energy in DMF: -1619.923575 a.u.

M06 SCF energy in DMF: -1619.335355 a.u.

M06 Free energy in DMF: -1618.895459 a.u.

C	2.74977700	0.12935400	0.04066400
C	1.28009000	1.83916200	-0.45635600
C	2.31636600	2.72552100	-0.72967800
C	3.63020300	2.27850400	-0.60200900
C	3.84490600	0.96126000	-0.20958700
H	2.89755900	-0.89896900	0.34161900
H	2.09780400	3.74133900	-1.03520900
H	4.46151100	2.94443300	-0.80435700
C	-0.13437100	2.23261900	-0.54155800
N	-1.09845300	1.44045600	-0.22188400
C	-1.89903200	3.47586700	-1.08097800
C	-2.35052700	2.24548300	-0.26320900
H	-2.12447800	3.38067300	-2.14668200
H	-3.11549300	1.68111700	-0.80209100
O	-0.43467300	3.46727200	-0.94857400
H	-2.25336300	4.43703400	-0.71401400
N	1.48870000	0.55488800	-0.07253600
C	-2.90115100	2.57878000	1.16402600
C	-3.17439100	1.27739100	1.93700200
H	-2.25562500	0.70836300	2.10910100
H	-3.61193900	1.51051500	2.91429100
H	-3.87824800	0.63415100	1.40056100
C	-4.23351500	3.33411400	0.98691900
H	-4.67325900	3.55100200	1.96643900
H	-4.10730600	4.28977300	0.46686500
H	-4.95646900	2.73533400	0.42082400
C	-1.91552400	3.44354600	1.97237900
H	-1.73359700	4.41829300	1.50830400
H	-2.32567100	3.63323200	2.97019000
H	-0.95130800	2.94120000	2.10853900
C	5.23660900	0.39578000	-0.10220700
F	6.14586700	1.35217600	0.17056700
F	5.32088500	-0.53960900	0.86771300
F	5.61701700	-0.19768800	-1.25643200
Pd	-0.34870300	-0.65608700	-0.08131700
C	-2.13647800	-1.66444300	-0.54877600
C	-2.68828900	-1.30040800	-1.79125800
C	-3.00050400	-2.01567500	0.50484600
C	-4.07373900	-1.25156900	-1.96187600
H	-2.03829600	-1.05805700	-2.62687500
C	-4.38500800	-1.97125800	0.32819700
H	-2.59453200	-2.34091500	1.45834300
C	-4.92435300	-1.58876900	-0.90401600
H	-4.48723200	-0.96228800	-2.92430100
H	-5.04117500	-2.24467700	1.15006700

H	-6.00135900	-1.56638900	-1.04391300
C	0.48301000	-2.54949400	0.09372900
C	-0.59453100	-3.03431600	-0.71876100
H	1.44897500	-2.45669300	-0.40858100
H	-1.25937700	-3.74352600	-0.23647500
C	-0.37658100	-3.29722600	-2.18664000
H	0.19470900	-4.23195900	-2.26444900
H	-1.31440200	-3.43585000	-2.72764300
H	0.20562200	-2.50839600	-2.66975800
C	0.55573600	-3.05890500	1.52749800
C	1.51125000	-2.28991500	2.43472600
H	2.53413500	-2.32378000	2.04506300
H	1.20520900	-1.24385500	2.53778000
H	1.51715100	-2.73507200	3.43668400
H	-0.45562800	-3.01629600	1.95939600
O	0.96361500	-4.43508700	1.41170800
H	1.01951100	-4.79094900	2.31164300

12

B3LYP SCF energy in DMF: -1619.957103 a.u.

M06 SCF energy in DMF: -1619.369507 a.u.

M06 Free energy in DMF: -1618.928728 a.u.

C	2.49022300	0.54680700	0.04223500
C	0.75623400	1.94259500	-0.58088800
C	1.63464700	2.94330500	-0.98152100
C	3.00498200	2.72363500	-0.85404800
C	3.43359400	1.50963800	-0.32813000
H	2.80546300	-0.40567700	0.44827000
H	1.25119300	3.87429200	-1.38073500
H	3.71580100	3.48535100	-1.15366300
C	-0.70362700	2.11427900	-0.63272000
N	-1.52485800	1.21481100	-0.21779200
C	-2.65550300	3.05931400	-1.13483000
C	-2.88008400	1.82468800	-0.23202600
H	-2.92270100	2.87157400	-2.17817200
H	-3.57737100	1.12586400	-0.69960000
O	-1.20007500	3.26513900	-1.09333800
H	-3.12523700	3.98010100	-0.79339400
N	1.17675000	0.75263900	-0.07954600
C	-3.40161600	2.14741100	1.20859100
C	-3.43659500	0.86221000	2.05530300
H	-2.44062100	0.42149600	2.16727500
H	-3.81692700	1.08912700	3.05750900
H	-4.09610800	0.10890600	1.61327700
C	-4.83854200	2.68895300	1.07668600
H	-5.25449000	2.89490500	2.06881400
H	-4.88139300	3.62183100	0.50434200
H	-5.49302400	1.96102900	0.58361000
C	-2.51573600	3.18935600	1.91749800
H	-2.48779600	4.14667600	1.38642700
H	-2.91056200	3.38766400	2.91981100
H	-1.48683000	2.83252600	2.03852700
C	4.89925000	1.19015900	-0.19141000
F	5.64726800	2.30713200	-0.10105200
F	5.14416000	0.44250500	0.90599900
F	5.35301100	0.48970000	-1.25527500
Pd	-0.43189700	-0.71697700	0.12271700
C	-1.17069200	-2.70805300	-0.91976100
C	-1.34731800	-2.43880400	-2.30235400
C	-2.22535700	-2.36413100	-0.02988200
C	-2.54146800	-1.91482200	-2.77383500
H	-0.55713600	-2.68793900	-3.00208400
C	-3.44123800	-1.84469000	-0.53117100
H	-2.17515400	-2.68217500	1.00835200
C	-3.59880600	-1.62497100	-1.88975600
H	-2.66968100	-1.74713700	-3.83956500
H	-4.25819500	-1.64808800	0.15507300
H	-4.53902700	-1.24363800	-2.27695900
C	0.73943500	-2.34900800	0.50544000
C	0.05656100	-3.43115200	-0.34463400
H	1.73634400	-2.10663700	0.12353600

H	-0.31118300	-4.23013400	0.30986500
C	0.98227500	-4.05948600	-1.38523600
H	1.79266300	-4.58985500	-0.87600400
H	0.44939400	-4.78092000	-2.01489400
H	1.43656900	-3.30661300	-2.03909100
C	0.77410300	-2.64303500	2.00328600
C	1.35844000	-1.52348800	2.86190800
H	2.38988700	-1.30218100	2.56825300
H	0.76432200	-0.60737700	2.77244400
H	1.36306300	-1.81919600	3.91782100
H	-0.25373100	-2.84827500	2.34122000
O	1.55854100	-3.84395600	2.13798800
H	1.44981800	-4.15448100	3.04938100

TS6

B3LYP SCF energy in DMF: -1619.941674 a.u.

M06 SCF energy in DMF: -1619.350692 a.u.

M06 Free energy in DMF: -1618.911205 a.u.

C	2.62917800	-0.21172100	0.13921500
C	1.21522900	-2.04195000	0.19818200
C	2.27160600	-2.93729000	0.06065100
C	3.56348700	-2.42549600	-0.04785100
C	3.74190800	-1.04476200	-0.01090100
H	2.73206900	0.86696400	0.17992700
H	2.08836600	-4.00446800	0.03475800
H	4.41059700	-3.09264500	-0.16148700
C	-0.18882300	-2.47328300	0.30383900
N	-1.19214700	-1.66634100	0.21070500
C	-1.86759700	-3.85724600	0.79476300
C	-2.42905400	-2.49533500	0.31880800
H	-1.98452300	-4.01300900	1.87010900
H	-3.06938800	-2.05671500	1.08892400
O	-0.42930000	-3.76692200	0.52558700
H	-2.24474500	-4.72472600	0.25616200
N	1.39191300	-0.70241600	0.24188800
C	-3.25262100	-2.56489300	-1.00525400
C	-3.69842300	-1.15022800	-1.40261500
H	-2.84067800	-0.51492200	-1.63525100
H	-4.33728100	-1.18811000	-2.29199500
H	-4.27300400	-0.67548000	-0.60004800
C	-4.50951700	-3.41574800	-0.73343800
H	-5.14066200	-3.44529200	-1.62816000
H	-4.26780600	-4.45128700	-0.47153800
H	-5.10554600	-2.99141200	0.08288700
C	-2.43596000	-3.18418800	-2.15387300
H	-2.12520700	-4.21241300	-1.93948300
H	-3.04113000	-3.21446700	-3.06654100
H	-1.53928200	-2.59475700	-2.37569600
C	5.11738800	-0.43474700	-0.07063900
F	5.99266200	-1.23265400	-0.71345500
F	5.10492500	0.75651400	-0.70570900
F	5.61333600	-0.21528500	1.16873400
Pd	-0.47083200	0.42913300	0.57339000
C	-1.17620000	2.99127400	-0.85494400
C	-0.46727500	4.19971300	-0.78253000
C	-0.76782600	2.03728000	-1.80725000
C	0.61813100	4.44896700	-1.62556500
H	-0.76850800	4.94821300	-0.05595900
C	0.32368200	2.28334400	-2.64886100
H	-1.33306800	1.11707100	-1.92720700
C	1.02206600	3.48884200	-2.55830100
H	1.14710600	5.39575700	-1.55584400
H	0.61674100	1.53542600	-3.38095700
H	1.86455100	3.68467100	-3.21572100
C	-2.05457000	1.63017300	1.09873400
C	-2.36895400	2.72139100	0.06650900
H	-2.91117500	1.01329000	1.37684500
H	-2.53065900	3.63993500	0.64426500
C	-3.65987800	2.45296500	-0.72207500
H	-4.49989700	2.28877800	-0.03824100
H	-3.90296100	3.31633300	-1.35068700

H	-3.57575900	1.58030200	-1.37274800
C	-1.18182600	2.02783600	2.25410600
H	-0.11219200	1.59153700	1.99179000
C	-1.55326200	1.39992700	3.59776000
H	-2.48778900	1.83840500	3.96297300
H	-1.68425300	0.31926700	3.49280400
H	-0.76944600	1.57837300	4.34161900
O	-0.99990500	3.42515500	2.34284700
H	-0.36456700	3.59459000	3.05599100

13

B3LYP SCF energy in DMF: -1619.942036 a.u.

M06 SCF energy in DMF: -1619.348843 a.u.

M06 Free energy in DMF: -1618.911498 a.u.

C	-2.70512200	-0.43506000	0.00713600
C	-1.80018900	1.69235100	0.10387300
C	-3.03489300	2.29360200	-0.11724600
C	-4.14790700	1.47220000	-0.29109600
C	-3.97814600	0.09075600	-0.23233200
H	-2.53570300	-1.50381800	0.07003700
H	-3.12363800	3.37236000	-0.15811800
H	-5.12565600	1.90525600	-0.47141900
C	-0.55100700	2.45263700	0.27765700
N	0.62327700	1.91411200	0.22455100
C	0.71632800	4.17649400	0.88906900
C	1.60916600	3.03184700	0.36156500
H	0.73912500	4.26678000	1.97833800
H	2.35490300	2.74677800	1.10778300
O	-0.64197400	3.75956200	0.52173100
H	0.89294100	5.14930600	0.43529600
N	-1.63994600	0.35291700	0.17131700
C	2.35500400	3.37307900	-0.96921100
C	3.16663000	2.15526200	-1.43141300
H	2.51998200	1.30424400	-1.66006700
H	3.73275300	2.39810100	-2.33756200
H	3.88342900	1.85047100	-0.66264600
C	3.33767300	4.52575800	-0.67641300
H	3.93781400	4.73675200	-1.56795200
H	2.82902000	5.45492500	-0.39975900
H	4.02589400	4.26309600	0.13544600
C	1.37839400	3.78780800	-2.08524300
H	0.78969100	4.67248000	-1.82057300
H	1.93865900	4.03334500	-2.99378700
H	0.68566400	2.97766500	-2.33813800
C	-5.15461900	-0.84071300	-0.36427800
F	-6.12245300	-0.31371400	-1.14032100
F	-4.79601800	-2.02516300	-0.90320200
F	-5.71049300	-1.10673400	0.83966000
Pd	0.39787800	-0.25645500	0.70837700
C	2.42570400	-2.56608100	-0.66152300
C	2.49953300	-3.95693100	-0.82016800
C	1.77432900	-1.82102700	-1.65866500
C	1.93081500	-4.58857800	-1.92902200
H	3.00276600	-4.55199400	-0.06290800
C	1.19769100	-2.44885900	-2.76698600
H	1.73140300	-0.73809400	-1.57980200
C	1.27223800	-3.83691200	-2.90561800
H	2.00185000	-5.66853600	-2.02854500
H	0.69990700	-1.85061500	-3.52597600
H	0.82858300	-4.32625000	-3.76829200
C	2.15148100	-1.09150000	1.45081900
C	3.09137600	-1.88485700	0.53408000
H	2.65840000	-0.30737200	2.01583200
H	3.47367800	-2.69342200	1.17416600
C	4.30909900	-1.05967200	0.08575400
H	4.79109100	-0.57604000	0.94290800
H	5.04841300	-1.70985800	-0.39351600
H	4.03191400	-0.28689000	-0.63314000
C	1.17307900	-1.86662000	2.25083700
H	0.07571100	-1.61071800	1.72850000
C	0.98061000	-1.44426900	3.70641000

H	1.85013000	-1.76693900	4.28854400
H	0.88129900	-0.35875500	3.78264600
H	0.08283800	-1.90331400	4.13337100
O	1.29076500	-3.25074800	2.09276700
H	0.59815300	-3.67551400	2.62379100

TS7

B3LYP SCF energy in DMF: -1619.940223 a.u.

M06 SCF energy in DMF: -1619.345221 a.u.

M06 Free energy in DMF: -1618.913259 a.u.

C	2.68201400	-0.69049900	-0.00077400
C	1.97492600	1.50802100	-0.16199600
C	3.25908500	1.99908900	0.05041500
C	4.29074300	1.08558500	0.25984300
C	3.99433600	-0.27553800	0.23910300
H	2.41983000	-1.74051800	-0.04595100
H	3.44571600	3.06611800	0.05800400
H	5.30404600	1.43118800	0.43199600
C	0.80250600	2.37906900	-0.34956600
N	-0.41618000	1.95858700	-0.26579000
C	-0.29973600	4.20513200	-0.97525500
C	-1.28477300	3.17244200	-0.38637800
H	-0.34339000	4.25852200	-2.06660300
H	-2.09050600	2.95849400	-1.09290600
O	1.01916800	3.66555100	-0.62475900
H	-0.36460500	5.20638200	-0.55448000
N	1.69288200	0.18676900	-0.19653700
C	-1.92561000	3.61681700	0.97054700
C	-2.83649200	2.50599100	1.51189600
H	-2.28261800	1.58211800	1.69687900
H	-3.28908800	2.81910500	2.45926300
H	-3.65010100	2.29224300	0.81208600
C	-2.79572400	4.86042600	0.69468100
H	-3.31698400	5.15956300	1.61042200
H	-2.20817700	5.72120700	0.35951600
H	-3.55493200	4.65222200	-0.06824100
C	-0.85609300	3.95367000	2.02631600
H	-0.19408500	4.76611900	1.70882400
H	-1.34257800	4.27604500	2.95317800
H	-0.23749500	3.08291700	2.26992300
C	5.06147100	-1.30379100	0.50891700
F	6.27319500	-0.88254200	0.09433500
F	5.16430500	-1.57249700	1.83000400
F	4.79875200	-2.47295000	-0.11196800
Pd	-0.34894400	-0.26661200	-0.76042600
C	-2.84130400	-2.26704400	0.61502200
C	-3.18714600	-3.60759300	0.83446300
C	-2.12372900	-1.59741200	1.61892900
C	-2.81831300	-4.26651500	2.01039000
H	-3.74612200	-4.14378100	0.07182100
C	-1.74886400	-2.25205300	2.79549500
H	-1.85924000	-0.55240900	1.48455900
C	-2.09365700	-3.59129500	2.99561500
H	-3.09688400	-5.30669300	2.15493000
H	-1.19415400	-1.71184300	3.55854600
H	-1.80512500	-4.10117300	3.91065100
C	-2.19602500	-0.97998800	-1.55314400
C	-3.30107400	-1.55582300	-0.65719200
H	-2.51024300	-0.13494800	-2.16645500
H	-3.78990000	-2.32474500	-1.27322200
H	-4.36517400	-0.49182200	-0.34158400
C	-4.75399600	-0.04579300	-1.26402400
H	-5.20576200	-0.93935000	0.19820300
H	-3.95408600	0.30799900	0.27697900
C	-1.32038100	-1.89372200	-2.23897800
H	-0.03702100	-1.65781600	-1.43653700
C	-0.83325000	-1.60361100	-3.64466400
H	0.10201000	-2.12878800	-3.86165900
H	-1.59801700	-1.95578800	-4.34744800
H	-0.67618200	-0.53405000	-3.79317600
O	-1.48947300	-3.21835200	-1.95197100

H -0.84605400 -3.74096100 -2.45931200

M06 SCF energy in DMF: -1867.786154 a.u.

M06 Free energy in DMF: -1867.260691 a.u.

14

B3LYP SCF energy in DMF: -1619.963519 a.u.

M06 SCF energy in DMF: -1619.365893 a.u.

M06 Free energy in DMF: -1618.929356 a.u.

C	2.77241500	-0.58752000	-0.16023100
C	1.96642000	1.58124600	-0.00466000
C	3.22909900	2.08746900	0.27864300
C	4.30307400	1.20069700	0.35704800
C	4.06685900	-0.15260500	0.13948500
H	2.55642700	-1.63088400	-0.35248700
H	3.36825400	3.14951000	0.43940000
H	5.29970200	1.56313000	0.58175300
C	0.76168700	2.42576100	-0.06188300
N	-0.42480300	1.94757800	-0.21600700
C	-0.42427300	4.30860500	-0.17252200
C	-1.37261300	3.08907100	-0.07665900
H	-0.40617800	4.75233300	-1.17110600
H	-2.06162500	3.07834400	-0.92496100
O	0.90897900	3.74426200	0.07205200
H	-0.58910700	5.08589300	0.57142800
N	1.74310300	0.26259300	-0.22932900
C	-2.22610700	3.02222100	1.23061800
C	-3.06035600	1.73035600	1.23742100
H	-2.42620200	0.84187500	1.28919900
H	-3.72404200	1.71713200	2.10920900
H	-3.68822800	1.65628900	0.34180500
C	-3.18765300	4.22804000	1.22663600
H	-3.84023400	4.18831200	2.10541300
H	-2.65688200	5.18558800	1.25767400
H	-3.82612600	4.22438400	0.33539100
C	-1.34137900	3.05972300	2.49000800
H	-0.75435300	3.98166200	2.56035100
H	-1.96781700	3.00629800	3.38696200
H	-0.65091400	2.20969400	2.52272600
C	5.16672500	-1.17618100	0.25049900
F	5.09454900	-1.84775400	1.42165900
F	5.08583800	-2.09647900	-0.73465100
F	6.38759500	-0.61275200	0.18427200
Pd	-0.24408700	-0.24480400	-0.80469000
C	-2.37671800	-2.73170600	0.56160400
C	-1.39767100	-3.63747800	0.99460100
C	-3.19131300	-2.12079800	1.52844900
C	-1.22585500	-3.91924000	2.35309500
H	-0.76591000	-4.13031200	0.25923100
C	-3.02195200	-2.39827800	2.88689900
H	-3.96658500	-1.42412100	1.22058500
C	-2.03662000	-3.29752100	3.30526600
H	-0.46215100	-4.62694200	2.66461700
H	-3.66367100	-1.91542400	3.61922400
H	-1.90756900	-3.51571500	4.36177600
C	-2.25569300	-0.98778900	-1.28137500
C	-2.55192600	-2.44397700	-0.92496200
H	-2.85700500	-0.24439900	-0.76409400
H	-1.84432100	-3.07753300	-1.46616400
C	-3.97390600	-2.80497900	-1.41232000
H	-4.05815700	-2.66005500	-2.49443600
H	-4.20154200	-3.85316700	-1.19145000
H	-4.73459700	-2.18412600	-0.92769100
C	-1.83972000	-0.61037900	-2.56248700
H	0.15919100	-1.67625300	-1.10849200
C	-2.05865800	0.74673300	-3.16661000
H	-1.15467700	1.11522700	-3.66370100
H	-2.84588100	0.66009900	-3.92760700
H	-2.38005800	1.47198300	-2.42081500
O	-1.44550200	-1.57475400	-3.41988400
H	-1.11267300	-1.17101400	-4.23890300

TS8

B3LYP SCF energy in DMF: -1868.480773 a.u.

C	1.37240300	2.20574500	0.18557400
C	-0.86699000	2.68146400	-0.13243600
C	-0.65405700	4.03482700	0.13992700
C	0.62735600	4.47543000	0.45063500
C	1.65720700	3.53808400	0.47748100
H	2.15965500	1.46561000	0.18485300
H	-1.48685300	4.72567500	0.11204400
H	0.81496800	5.52229100	0.66504000
C	-2.23663500	2.20173300	-0.42441400
N	-2.63030400	0.98639400	-0.38315200
C	-4.41424700	2.49300500	-0.88197900
C	-4.07190500	0.98579800	-0.72849000
H	-4.81534800	2.75012700	-1.86343000
H	-4.17593600	0.47952400	-1.69659300
O	-3.12865700	3.16822900	-0.73582700
H	-5.07737600	2.88514400	-0.10760100
N	0.13929700	1.77350300	-0.12386900
C	-4.94646900	0.19721800	0.28938100
C	-4.53419500	-1.28604600	0.25666800
H	-3.49465300	-1.41884200	0.57057200
H	-5.16656200	-1.87232800	0.93311000
H	-4.64464300	-1.70818100	-0.74929700
C	-6.41924900	0.31408000	-0.15002000
H	-7.05873500	-0.28833000	0.50462000
H	-6.78505300	1.34575200	-0.10397500
H	-6.55825600	-0.04790100	-1.17572800
C	-4.77887300	0.73836800	1.71996100
H	-5.07494400	1.78964300	1.80602300
H	-5.40633800	0.16731600	2.41315900
H	-3.74167200	0.65128200	2.06087000
C	3.05873000	3.94684800	0.84101600
C	3.19992100	4.10677100	2.17598600
F	3.97335600	3.03125200	0.45226100
F	3.39377100	5.12225400	0.26768600
Pd	-0.21569100	-0.32742900	-0.65673400
C	0.25430300	-3.28688500	1.39566300
C	1.47236500	-3.21557800	2.08697300
C	-0.93463500	-3.23482300	2.14178900
C	1.50681300	-3.08146100	3.47816900
H	2.40468900	-3.26724500	1.52917900
C	-0.90514300	-3.10060700	3.53145600
H	-1.89394700	-3.30400500	1.63597600
C	0.31679400	-3.02103300	4.20625100
H	2.46351500	-3.02691700	3.99105200
H	-1.83785300	-3.06242300	4.08821600
H	0.33965100	-2.91770400	5.28757600
C	-0.63568600	-2.44586700	-0.83505500
C	0.23816900	-3.46886000	-0.11833500
H	-1.68357200	-2.45178600	-0.53777100
H	1.26778800	-3.36627100	-0.47160800
C	-0.23643300	-4.89377100	-0.49253400
H	-0.18146200	-5.04825800	-1.57543700
H	0.38886800	-5.65153600	-0.00801200
H	-1.27265200	-5.05943700	-0.17788900
C	-0.40303200	-1.99494800	-2.13634400
H	1.54972600	-0.62038500	-0.63543200
C	-1.50026500	-1.59279800	-3.09197700
H	-1.19166100	-0.76114000	-3.73581600
H	-1.74201900	-2.44507500	-3.74285500
H	-2.40577400	-1.30031700	-2.55828500
O	0.77734400	-2.36062100	-2.75890400
H	0.84046400	-1.88227900	-3.60080300
C	3.37673200	-1.40197100	-1.19308800
C	2.86331500	-2.08295000	-1.87120000
N	4.68382400	-1.45183100	-1.14358600
C	5.46943100	-0.56907900	-0.27600400
H	6.35152300	-0.23836200	-0.82825400
H	4.87598800	0.29518000	0.01767600
H	5.78887100	-1.11752600	0.61537600

C	5.42686900	-2.44033400	-1.93000200
H	6.00998900	-3.07333200	-1.25534200
H	4.73300500	-3.05964500	-2.49904000
H	6.10614400	-1.92417600	-2.61340800
O	2.69752000	-0.58131700	-0.47634000

15

B3LYP SCF energy in DMF: -1868.480774 a.u.

M06 SCF energy in DMF: -1867.786255 a.u.

M06 Free energy in DMF: -1867.260966 a.u.

C	1.28755100	2.23792800	0.25600400
C	-0.94099800	2.64488200	-0.19785700
C	-0.77594300	4.01067800	0.03855100
C	0.47494400	4.49458500	0.40831200
C	1.52178900	3.58571400	0.52790700
H	2.09400200	1.52061100	0.31662500
H	-1.62259600	4.67837400	-0.05699000
H	0.62409600	5.55146900	0.59979100
C	-2.28507700	2.11617600	-0.52281400
N	-2.66129200	0.90294400	-0.38393600
C	-4.43922500	2.31665900	-1.12140600
C	-4.08986400	0.84385000	-0.76994200
H	-4.76838400	2.44944100	-2.15336900
H	-4.16507100	0.21655200	-1.66692700
O	-3.17684400	3.03276100	-0.96125800
H	-5.16470600	2.78044500	-0.44982900
N	0.08725900	1.76436100	-0.11119500
C	-4.98162900	0.18094900	0.32157400
C	-4.53834300	-1.28230600	0.50401200
H	-3.50559100	-1.34632200	0.85885200
H	-5.17805500	-1.78542500	1.23780800
H	-4.61164900	-1.83829300	-0.43829800
C	-6.44254800	0.20101500	-0.16881600
H	-7.09042600	-0.31211100	0.55041300
H	-6.82664300	1.22075800	-0.28371700
H	-6.54563400	-0.30951400	-1.13361700
C	-4.86857400	0.91787700	1.66792700
H	-5.18599200	1.96425700	1.59880100
H	-5.50694400	0.43447000	2.41565300
H	-3.84110600	0.90100700	2.04683900
C	2.89044300	4.01823400	0.97936100
F	3.04155700	3.87310700	2.31530200
F	3.86658300	3.28706800	0.39359800
F	3.12656000	5.31392100	0.69190600
Pd	-0.17371800	-0.35240500	-0.64658000
C	0.31195600	-3.35895400	1.37034800
C	1.46782300	-3.12128800	2.12794700
C	-0.90664400	-3.51441100	2.05147400
C	1.41178800	-3.02717900	3.52171600
H	2.42365000	-3.01150000	1.62065300
C	-0.96753400	-3.42048200	3.44339200
H	-1.81716100	-3.71380300	1.49226700
C	0.19185500	-3.17367000	4.18507000
H	2.32186500	-2.84276600	4.08662100
H	-1.92099800	-3.54453100	3.95026600
H	0.14436700	-3.10276200	5.26822400
C	-0.51222300	-2.47917300	-0.86143700
C	0.39388700	-3.47659200	-0.14707000
H	-1.56408900	-2.54098200	-0.58339900
H	1.43126700	-3.28352000	-0.43365400
C	0.05008100	-4.91096800	-0.61417500
H	0.19327600	-5.00697700	-1.69555600
H	0.69438200	-5.64583000	-0.11913800
H	-0.99037800	-5.16547800	-0.38529800
C	-0.27265500	-1.99033200	-2.14855700
H	1.66578300	-0.56737300	-0.62339800
C	-1.36610600	-1.61950400	-3.12170200
H	-1.07521600	-0.77173600	-3.75281300
H	-1.56730600	-2.47336100	-3.78433900
H	-2.29061900	-1.36105900	-2.60292900
O	0.93404100	-2.30371600	-2.75438700

H	0.99835400	-1.80341800	-3.58330400
C	3.48052100	-1.27080900	-1.18276300
H	2.99371300	-1.98394400	-1.84636800
N	4.78529800	-1.25280000	-1.13705900
C	5.52947200	-0.31821500	-0.28543700
H	6.41021400	0.01919300	-0.83532600
H	4.90704800	0.53786100	-0.03015000
H	5.84928900	-0.82923600	0.62759800
C	5.57330700	-2.21961200	-1.90806300
H	6.18311500	-2.81312100	-1.22161300
H	4.90802300	-2.87866900	-2.46617500
H	6.22815000	-1.68285100	-2.59902300
O	2.76524200	-0.47003900	-0.47007600

16

B3LYP SCF energy in DMF: -1619.503099 a.u.

M06 SCF energy in DMF: -1618.924877 a.u.

M06 Free energy in DMF: -1618.499602 a.u.

C	1.62900700	1.30906000	0.46199100
C	-0.34014100	2.14293600	-0.39971100
C	0.22748500	3.39218100	-0.64726400
C	1.56485600	3.59001900	-0.31404400
C	2.27402800	2.53241200	0.25354100
H	2.15312700	0.46421100	0.89407200
H	-0.36372700	4.18760400	-1.08468900
H	2.04069500	4.54887100	-0.48882000
C	-1.75279300	1.84756200	-0.69389100
N	-2.32975200	0.74741100	-0.36297300
C	-3.77067900	2.17352400	-1.59610300
C	-3.75680300	0.86710900	-0.75844200
H	-3.83206300	1.98533500	-2.67093900
H	-4.00884700	0.00967000	-1.39015700
O	-2.46827100	2.78502900	-1.33386200
H	-4.53346600	2.89721700	-1.31111900
N	0.34760100	1.11306800	0.13897600
C	-4.73496700	0.85412500	0.45844100
C	-4.58447600	-0.47385900	1.22126800
H	-3.58593900	-0.57732300	1.65555400
H	-5.31544400	-0.52652300	2.03629800
H	-4.76048100	-1.33096400	0.56097100
C	-6.17369600	0.94665200	-0.08751700
H	-6.89317500	0.89544200	0.73704800
H	-6.35865000	1.88461500	-0.62210600
H	-6.39137000	0.11951700	-0.77343900
C	-4.46229300	2.02493100	1.42038800
H	-4.59076400	3.00041600	0.93847700
H	-5.16266900	1.98734000	2.26200500
H	-3.44870000	1.97857200	1.83338800
C	3.73369000	2.68190400	0.58351400
F	4.12271200	1.83656500	1.56154500
F	4.51670700	2.42748600	-0.49213600
F	4.02661400	3.93612900	0.99022300
Pd	-0.82240500	-0.89640500	0.18791000
C	2.48858300	-2.40682100	-0.49911600
C	2.95969600	-1.68080000	-1.60306600
C	3.25569100	-2.38652100	0.67843000
C	4.15053300	-0.95064100	-1.53594500
H	2.38717900	-1.68938100	-2.52812500
C	4.44671700	-1.66036600	0.75053900
H	2.92087000	-2.94579300	1.54854000
C	4.89939200	-0.93679900	-0.35726700
H	4.49186100	-0.39436200	-2.40519100
H	5.02252400	-1.66010900	1.67257000
H	5.82303700	-0.36798800	-0.30040100
C	0.14834100	-2.75429400	0.43577900
C	1.19299700	-3.20358400	-0.58841700
H	0.48273800	-2.86048800	1.47071800
H	0.77881600	-3.04610500	-1.58885100
C	1.46793400	-4.71851200	-0.43901200
H	0.54369300	-5.28811800	-0.58094800
H	2.19801100	-5.06622000	-1.17972200

H	1.86171200	-4.95556600	0.55607600
C	-1.24930400	-2.95716200	0.23507500
C	-2.15004500	-3.41959800	1.36432800
H	-3.19140600	-3.11618000	1.20657900
H	-2.13733000	-4.51802900	1.43576800
H	-1.82358500	-3.01062500	2.32501200
O	-1.63133800	-3.50187600	-1.01225700
H	-2.58087700	-3.34133300	-1.11316400

17

B3LYP SCF energy in DMF: -1960.442231 a.u.

M06 SCF energy in DMF: -1959.706599 a.u.

M06 Free energy in DMF: -1959.191978 a.u.

C	-2.20452800	-1.08187100	0.56490500
C	-0.63453600	-2.01442700	-0.82757900
C	-1.55752900	-2.91971300	-1.35424000
C	-2.86867700	-2.88309900	-0.88790800
C	-3.19766700	-1.94181500	0.08394500
H	-2.43202500	-0.34686200	1.32804100
H	-1.25651800	-3.62840100	-2.11557700
H	-3.61317800	-3.56874300	-1.27759100
C	0.75748100	-1.98359500	-1.31290400
N	1.64905200	-1.14048900	-0.93197700
C	2.46479100	-2.58080100	-2.63038800
C	2.92141500	-1.51339300	-1.60406700
H	2.41993200	-2.19484100	-3.65207900
H	3.30154500	-0.63012500	-2.12264700
O	1.09882900	-2.90696700	-2.22497900
H	3.03820100	-3.50727000	-2.61809300
N	-0.94570200	-1.11438200	0.12785900
C	4.02200400	-1.98466000	-0.60214300
C	4.36507800	-0.82575800	0.34903100
H	3.47724300	-0.48555500	0.89004300
H	5.11513800	-1.14250500	1.08162600
H	4.78174100	0.02704300	-0.19994100
C	5.28470700	-2.35101200	-1.40677400
H	6.10446000	-2.60009000	-0.72407900
H	5.12796600	-3.21736400	-2.05796000
H	5.61440100	-1.51293800	-2.03211900
C	3.55579200	-3.19940300	0.22025000
H	3.30388500	-4.05727000	-0.41295500
H	4.35496600	-3.52137700	0.89684500
H	2.68048500	-2.96034800	0.83417600
C	-4.61433800	-1.79266400	0.56603400
F	-4.67234100	-1.30576900	1.82454200
F	-5.31617800	-0.93925100	-0.21819500
F	-5.27647100	-2.96884100	0.55372600
Pd	0.92292900	0.60424900	0.43090600
C	-1.49207100	2.31878800	-1.80468100
C	-2.19911300	1.29069400	-2.44443200
C	-2.21718900	3.23564100	-1.02523200
C	-3.58363000	1.16518200	-2.29624500
H	-1.65933600	0.58095500	-3.06709600
C	-3.60032800	3.11373800	-0.87401500
H	-1.70171000	4.05771300	-0.53539200
C	-4.28946200	2.07440000	-1.50559400
H	-4.10814500	0.35540000	-2.79586900
H	-4.14050400	3.83401600	-0.26511300
H	-5.36473400	1.97734700	-1.38514900
C	0.78750300	2.55782500	-0.69990800
C	0.01186700	2.45996900	-2.00798700
H	0.38519500	3.24416400	0.03962400
H	0.35943600	1.57902200	-2.55615500
C	0.32325800	3.70257500	-2.88114800
H	1.39483500	3.76686600	-3.09320400
H	-0.21157100	3.64544200	-3.83545900
H	0.01636600	4.62526300	-2.37699100
C	2.16161200	2.34716600	-0.62194300
C	3.08721100	3.02454900	0.35499500
H	3.84455100	2.33657100	0.74490100
H	3.61384100	3.83467700	-0.16740600

H	2.54894800	3.46910500	1.19205600
O	2.78489400	1.83338900	-1.73009600
H	3.72045900	1.67952000	-1.52420700
C	0.53231800	1.57334700	2.27086500
C	-0.89700300	1.64081900	2.52600000
C	1.22472000	0.57851400	3.10357500
C	-1.53756900	0.74882500	3.33888000
H	-1.45311400	2.44011900	2.04580500
C	0.53419900	-0.38135700	3.92718800
C	-0.82139100	-0.29129900	4.02820300
H	-2.60972700	0.83247700	3.49223000
H	1.11160800	-1.12729300	4.46317000
H	-1.36391400	-0.99161200	4.65489700
H	1.03619100	2.53050500	2.16517700
N	2.54949900	0.65402600	3.21153600
N	3.67714100	0.72532200	3.31896100

TS9

B3LYP SCF energy in DMF: -1619.94144 a.u.

M06 SCF energy in DMF: -1619.350369 a.u.

M06 Free energy in DMF: -1618.907148 a.u.

C	2.80108000	-0.35647100	-0.25926500
C	1.73022300	1.69221500	-0.20179600
C	2.93279800	2.39015800	-0.16759500
C	4.12053700	1.65875300	-0.17157400
C	4.05211400	0.26892000	-0.21697700
H	2.70965700	-1.43614200	-0.30235000
H	2.94347000	3.47297500	-0.13822000
H	5.07768100	2.16735000	-0.14363200
C	0.41480700	2.35202900	-0.16493200
N	-0.70413700	1.70190800	-0.16388100
C	-1.06154100	4.02075500	-0.22153400
C	-1.79383600	2.69337000	0.07934600
H	-1.21949100	4.36699200	-1.24613100
H	-2.59074500	2.52590700	-0.64675600
O	0.36318900	3.67908400	-0.09861800
H	-1.25914200	4.83101500	0.47736500
N	1.66581200	0.34244600	-0.24943900
C	-2.41195100	2.59602200	1.51271500
C	-3.03440300	1.20523900	1.72065700
H	-2.27833900	0.41696700	1.68874600
H	-3.52478600	1.16003800	2.69943600
H	-3.79219100	0.98760900	0.95988000
C	-3.53230500	3.65211700	1.61255000
H	-4.03920200	3.56241400	2.57928100
H	-3.15333700	4.67673200	1.53847500
H	-4.28414000	3.51193000	0.82714900
C	-1.35942000	2.84664400	2.60807400
H	-0.90627500	3.84059200	2.53191200
H	-1.82998100	2.77989900	3.59476600
H	-0.55928100	2.09872900	2.57798900
C	5.30208000	-0.56988400	-0.16917500
F	6.35842600	0.07861200	-0.69899300
F	5.62935900	-0.89306400	1.10217900
F	5.15184900	-1.72917300	-0.84424100
Pd	-0.42301100	-0.36209500	-0.60822900
C	-1.44160800	-2.74540600	0.57884200
C	-0.14871800	-3.18582200	0.90950100
C	-2.37542000	-2.57756700	1.61700000
C	0.20902800	-3.43297200	2.23943000
H	0.57775400	-3.35041600	0.11694500
C	-2.02066500	-2.82748500	2.94263700
H	-3.38584300	-2.25227800	1.38498700
C	-0.72537300	-3.25191200	3.25989600
H	1.21415700	-3.77376700	2.47256500
H	-2.75679800	-2.69473700	3.73094100
H	-0.45274600	-3.44777200	4.29311000
C	-2.25408100	-1.06188500	-1.13835100
C	-1.82963100	-2.51240400	-0.88291200
H	-3.02154700	-0.69657000	-0.45211700
H	-0.91732400	-2.68021300	-1.49183500

C	-2.84634200	-3.58053100	-1.36379300
C	-2.62801200	-0.74579100	-2.58935000
H	-2.01110400	-1.37582400	-3.25044200
H	-2.42812600	-4.57906900	-1.19889600
H	-3.78198600	-3.49848700	-0.80293100
C	-2.45171900	0.71188100	-3.01414000
H	-1.40767800	1.03213000	-2.94068200
H	-3.06862200	1.37275000	-2.39799500
H	-3.07563500	-3.46369600	-2.42420400
H	-2.76644200	0.83108900	-4.05817300
O	-4.01155800	-1.12420300	-2.72531100
H	-4.24076100	-1.02653300	-3.66199600

18

B3LYP SCF energy in DMF: -1619.953241 a.u.

M06 SCF energy in DMF: -1619.362906 a.u.

M06 Free energy in DMF: -1618.924044 a.u.

C	2.74599700	-0.90047100	-0.06163300
C	2.25977000	1.36016000	-0.13422100
C	3.60382400	1.71365500	-0.12639000
C	4.55434800	0.69409000	-0.07843600
C	4.11837300	-0.62765600	-0.04168700
H	2.37183200	-1.91749000	-0.04518300
H	3.90143000	2.75469800	-0.15894500
H	5.61240800	0.93105500	-0.07299900
C	1.16442400	2.34244300	-0.14539900
N	-0.08003600	1.99454400	-0.17457300
C	0.15793800	4.32985500	-0.21690300
C	-0.89250500	3.22443900	0.04315000
H	0.11299900	4.72479300	-1.23483700
H	-1.68130900	3.26407900	-0.70955600
O	1.44979000	3.63838800	-0.08008600
H	0.15489700	5.14897200	0.49937800
N	1.83644100	0.07462000	-0.10683200
C	-1.56566600	3.27609500	1.45363300
C	-2.53495500	2.09186800	1.61657500
H	-2.00843500	1.13327400	1.60078300
H	-3.06063300	2.17176700	2.57464100
H	-3.28919600	2.08204400	0.82211900
C	-2.37793200	4.58436400	1.53160600
H	-2.91130000	4.63425000	2.48681900
H	-1.74655900	5.47651200	1.46402600
H	-3.12313400	4.63598700	0.72943000
C	-0.52389400	3.23844900	2.58664400
H	0.18268600	4.07375000	2.53298900
H	-1.02952700	3.30459900	3.55595300
H	0.04804100	2.30391100	2.57988200
C	5.10538800	-1.76091100	0.06605500
F	6.27770200	-1.45610600	-0.52587400
F	5.37689200	-2.05579800	1.35711200
F	4.63818700	-2.88950700	-0.50791500
Pd	-0.33932700	-0.08941900	-0.48222100
C	-2.35511300	-2.55815000	0.40852600
C	-1.53059400	-3.04568900	1.43021500
C	-3.74389400	-2.72883100	0.51775500
C	-2.08035000	-3.68604600	2.54415500
H	-0.45277700	-2.92020800	1.35713300
C	-4.29276500	-3.37103200	1.62892400
H	-4.39289400	-2.35845200	-0.27104200
C	-3.46313500	-3.85081300	2.64646400
H	-1.42658500	-4.05384400	3.33022000
H	-5.36993900	-3.49444700	1.70023400
H	-3.89200000	-4.34720500	3.51235900
C	-2.26167800	-0.49043500	-1.06286400
C	-1.78847700	-1.89423300	-0.83935000
H	-2.95122600	-0.12160400	-0.30280000
H	-0.61053600	-1.82637100	-0.60559000
C	-1.75901600	-2.85467400	-2.04681200
C	-2.67886000	-0.05355300	-2.45961500
H	-1.95105900	-0.41815000	-3.19727600
H	-1.27821000	-3.79534300	-1.76500400

H	-2.78190000	-3.06082400	-2.36977200
C	-2.82415100	1.45624400	-2.62521400
H	-1.85435800	1.95802500	-2.55732000
H	-3.49695400	1.87304500	-1.86841700
H	-1.20907400	-2.42793400	-2.88860500
H	-3.24329800	1.68026000	-3.61320500
O	-3.94765500	-0.70474400	-2.67590600
H	-4.18377000	-0.57149000	-3.60644000

TS10

B3LYP SCF energy in DMF: -1619.944583 a.u.

M06 SCF energy in DMF: -1619.35279 a.u.

M06 Free energy in DMF: -1618.916242 a.u.

C	-2.79563000	-0.56925600	0.15746100
C	-1.99025100	1.60209700	0.09035500
C	-3.26861200	2.13365500	-0.03450100
C	-4.35209200	1.25766800	-0.07153700
C	-4.10853100	-0.11022200	0.02224000
H	-2.57247900	-1.62494000	0.24525800
H	-3.41213100	3.20500600	-0.10303400
H	-5.36293000	1.63812900	-0.16862600
C	-0.77324500	2.42919100	0.09676300
N	0.41108200	1.92149000	0.14677400
C	0.46863700	4.27649800	0.17545200
C	1.37587000	3.04119400	-0.04074900
H	0.54052100	4.68241100	1.18761700
H	2.13476000	2.98394700	0.74217200
O	-0.89536600	3.75246400	0.01818900
H	0.59188700	5.07685900	-0.55178200
N	-1.75628000	0.27144800	0.18912000
C	2.10547400	2.99692900	-1.42307900
C	2.89757200	1.68455000	-1.55378400
H	2.23741300	0.81298700	-1.57731600
H	3.47617800	1.68959400	-2.48424000
H	3.60328600	1.56016200	-0.72485400
C	3.10150100	4.17362900	-1.46476100
H	3.65606800	4.15907400	-2.40915800
H	2.60466600	5.14688600	-1.39334500
H	3.82998700	4.10704100	-0.64829100
C	1.11424500	3.10708000	-2.59603200
H	0.56184700	4.05292300	-2.58885300
H	1.65751100	3.05691100	-3.54580900
H	0.38886900	2.28580000	-2.59048500
C	-5.23927600	-1.10184700	-0.06774600
F	-6.36559000	-0.62193100	0.49691600
F	-5.53378300	-1.39501800	-1.35397900
F	-4.93674200	-2.26508100	0.54514700
Pd	0.29721700	-0.24151300	0.57660100
C	1.96922700	-2.67971700	-0.49210000
C	0.99648300	-3.45642600	-1.14509500
C	3.22581500	-2.52643600	-1.09928800
C	1.26268400	-4.04022900	-2.38203900
H	0.02027500	-3.58956200	-0.68646100
C	3.49403200	-3.11934400	-2.33599800
H	4.00602100	-1.96348800	-0.59692900
C	2.51391900	-3.87193000	-2.98389300
H	0.49352400	-4.62677400	-2.87645600
H	4.47422800	-2.99467200	-2.78746400
H	2.72299700	-4.32991200	-3.94642600
C	2.25836700	-0.82322900	1.19678500
C	1.71064200	-2.09465000	0.87306000
H	2.90090700	-0.36493800	0.44785100
H	0.01505200	-1.73839300	0.82041800
C	1.41505200	-3.13244700	1.94871600
C	2.59367500	-0.44549100	2.63133700
H	1.76155400	-0.72676300	3.29199400
H	0.68484000	-3.86734900	1.60361200
H	2.35081600	-3.66115000	2.16233200
C	2.88018500	1.04159300	2.81860200
H	1.98484600	1.64243400	2.63337800
H	3.67787300	1.37591700	2.14672700

H	1.05342100	-2.68646700	2.87597000
H	3.20001400	1.23253300	3.84961700
O	3.75408100	-1.23272500	2.95758500
H	3.98344000	-1.03194600	3.87773800

19

B3LYP SCF energy in DMF: -1619.948072 a.u.

M06 SCF energy in DMF: -1619.355006 a.u.

M06 Free energy in DMF: -1618.918333 a.u.

C	-2.93917600	-0.66463200	-0.04128800
C	-2.01311100	1.46108700	0.05851200
C	-3.25064400	2.06740200	-0.12196400
C	-4.37458400	1.25772700	-0.27440700
C	-4.21212500	-0.12464700	-0.23656100
H	-2.77894900	-1.73330100	0.00890600
H	-3.33118500	3.14730500	-0.14114900
H	-5.35454700	1.70058200	-0.41487700
C	-0.76453900	2.22566900	0.21136500
N	0.39959700	1.67294200	0.22232200
C	0.51332400	3.98270000	0.69475300
C	1.39963900	2.77608600	0.30566800
H	0.52414800	4.18703100	1.76849100
H	2.10276900	2.54482800	1.11002800
O	-0.84787900	3.54818500	0.35507800
H	0.70905500	4.90089400	0.14426600
N	-1.86034500	0.11503100	0.10364600
C	2.21883100	2.96246600	-1.01129500
C	2.97662800	1.66351500	-1.32691600
H	2.29074800	0.83931200	-1.53627000
H	3.61173800	1.80203700	-2.20878900
H	3.62388500	1.36960000	-0.49361900
C	3.24601100	4.08722000	-0.77278900
H	3.87288400	4.21355500	-1.66197400
H	2.77150800	5.05287600	-0.56867100
H	3.90510600	3.85007400	0.07042300
C	1.31307600	3.32326000	-2.20318000
H	0.78001000	4.26845100	-2.05429200
H	1.92029000	3.43444400	-3.10805800
H	0.57380200	2.53925500	-2.40144400
C	-5.38977100	-1.04359500	-0.43539100
F	-6.51667100	-0.52095100	0.08849200
F	-5.62688900	-1.26395200	-1.74743000
F	-5.18904200	-2.24679400	0.14052900
Pd	0.09575500	-0.55141100	0.57407700
C	2.42563400	-2.17040600	-0.75163200
C	1.69305400	-2.75049500	-1.80363300
C	3.72434400	-1.70228800	-1.01236500
C	2.23226900	-2.82679300	-3.08684100
H	0.69098300	-3.12630700	-1.61861600
C	4.26901600	-1.79626800	-2.29493800
H	4.31778500	-1.28378400	-0.20567500
C	3.52322200	-2.35058300	-3.33674600
H	1.64717000	-3.26414400	-3.89089000
H	5.27874000	-1.43912300	-2.47632300
H	3.94604900	-2.41957500	-4.33492400
C	2.06242300	-1.01097000	1.45006000
C	1.87669000	-2.13293300	0.64092500
H	2.65529100	-0.19563300	1.03826900
H	-0.46744700	-1.91297200	0.91686200
C	1.49532500	-3.49003400	1.19671100
C	2.00219900	-1.04466600	2.96737300
H	1.15932500	-1.66849000	3.29414300
H	0.87656300	-4.05389900	0.49546900
H	2.42289700	-4.05961600	1.33873400
C	1.84903500	0.34612000	3.57910600
H	0.90415100	0.80665400	3.27270500
H	2.67451900	0.99846300	3.27394700
H	0.97903900	-3.43093500	2.15493900
H	1.85033900	0.28051500	4.67334000
O	3.24041100	-1.65305200	3.37271500
H	3.25636900	-1.64442100	4.34191800

TS11

B3LYP SCF energy in DMF: -1868.474874 a.u.

M06 SCF energy in DMF: -1867.7799 a.u.

M06 Free energy in DMF: -1867.255009 a.u.

C	2.21881100	0.50467000	0.96694700
C	0.92733400	2.21445400	0.09753300
C	1.90597400	3.16422200	0.38372200
C	3.09196300	2.74732000	0.98422200
C	3.24691300	1.39619300	1.28152500
H	2.31216700	-0.55270900	1.18041600
H	1.74184800	4.20667200	0.14093000
H	3.87344200	3.46245400	1.21555500
C	-0.35424600	2.58642100	-0.53613200
N	-1.34810900	1.78858500	-0.67643300
C	-1.78037900	3.93592500	-1.61316900
C	-2.43742200	2.55555700	-1.32994300
H	-1.62512100	4.12628100	-2.67717200
H	-2.68051600	2.05382200	-2.27287600
O	-0.46114700	3.84571500	-0.98718800
H	-2.29464900	4.78658700	-1.16494400
N	1.08381300	0.90123500	0.38087000
C	-3.74524600	2.60356500	-0.48246000
C	-4.28200000	1.17298100	-0.29874200
H	-3.58872400	0.55333400	0.27624900
H	-5.23647800	1.19295600	0.23934900
H	-4.45602800	0.68736300	-1.26602400
C	-4.79098800	3.42576700	-1.26161000
H	-5.74173400	3.43595800	-0.71747100
H	-4.48379500	4.46810000	-1.39967700
H	-4.97705700	2.99486800	-2.25246500
C	-3.49959200	3.23693400	0.89878800
H	-3.13050000	4.26619600	0.82635500
H	-4.43447000	3.26932400	1.46889900
H	-2.77582800	2.65778100	1.48260800
C	4.52445200	0.86424600	1.87322000
F	5.18867700	1.80766100	2.56842800
F	4.29505300	-0.17451800	2.70426900
F	5.36589800	0.41679000	0.90876600
Pd	-0.49174800	-0.52040100	-0.24974600
C	-1.88782000	-2.18379000	1.71646800
C	-1.08243100	-2.02059600	2.86159900
C	-3.28308500	-2.09595400	1.87341200
C	-1.64899500	-1.75471700	4.10709200
H	-0.00208000	-2.08475800	2.77197200
C	-3.85033900	-1.83530800	3.12309200
H	-3.93282300	-2.25569800	1.01891200
C	-3.03749400	-1.65785100	4.24392300
H	-1.00562700	-1.62372100	4.97287800
H	-4.93132500	-1.78094900	3.21913500
H	-3.47965500	-1.45571600	5.21536700
C	-1.89514000	-2.03259100	-0.80213600
C	-1.26816400	-2.48706100	0.38017600
H	-2.85005600	-1.51803800	-0.69667700
H	0.73496800	-1.38744000	-0.78225300
C	-0.29419200	-3.65067400	0.38668900
C	-1.71909900	-2.68755000	-2.15808500
H	-0.67301400	-2.99293700	-2.29617600
H	0.47154500	-3.53609800	1.15795500
H	-0.84605400	-4.57248000	0.61409200
C	-2.11249600	-1.76373500	-3.30999100
H	-1.46153200	-0.88374200	-3.34949300
H	-3.14883300	-1.42473600	-3.20082800
H	0.20867600	-3.78353600	-0.57081700
H	-2.02391300	-2.28831100	-4.26886300
O	-2.55941700	-3.85718900	-2.13564700
H	-2.49855300	-4.26685500	-3.01187500
C	2.46266400	-1.26563500	-2.18896400
H	1.81981300	-0.61626400	-2.79255900
N	3.73053900	-1.32438200	-2.56598400
C	4.70863300	-2.10743000	-1.81027200

H	5.21882000	-1.46740200	-1.08226100
H	4.20419800	-2.91785100	-1.28527300
H	5.44378100	-2.52189000	-2.50331000
C	4.22780700	-0.53053900	-3.68767700
H	4.65563200	-1.18960000	-4.44891000
H	3.41083500	0.04389500	-4.12719600
H	5.00394900	0.15808900	-3.33923500
O	1.99759200	-1.90363800	-1.20262700

20

B3LYP SCF energy in DMF: -1868.486606 a.u.

M06 SCF energy in DMF: -1867.801359 a.u.

M06 Free energy in DMF: -1867.271833 a.u.

C	2.52045400	0.89777300	0.10409300
C	0.75602100	2.00056200	1.09880400
C	1.54312300	3.10830200	1.40381800
C	2.88672000	3.09032000	1.03374700
C	3.38176200	1.96601200	0.37823900
H	2.87816600	0.00825200	-0.40312000
H	1.11647200	3.95965300	1.92003400
H	3.53111500	3.93290900	1.25797900
C	-0.66703900	1.91469900	1.47122400
N	-1.39894500	0.88605900	1.22664200
C	-2.64086500	2.63279700	2.22782200
C	-2.72199700	1.12927000	1.85731900
H	-3.17744300	3.27156800	1.52155100
H	-3.49992800	0.96502100	1.10582900
O	-1.21653300	2.95540900	2.11053400
H	-2.94789100	2.87713400	3.24374000
N	-1.23262800	0.91282700	0.45320100
C	-3.01282600	0.16707600	3.05343900
C	-3.00360100	-1.29016400	2.55826200
H	-2.01228100	-1.58736300	2.20320000
H	-3.28549300	-1.96503000	3.37450300
H	-3.71658200	-1.43983600	1.73965600
C	-4.41950800	0.49472600	3.59276000
H	-4.68018300	-0.19564000	4.40222800
H	-4.48682400	1.51087100	3.99627900
H	-5.17968700	0.39342000	2.80925300
C	-1.97079600	0.32542200	4.17611800
H	-1.95182900	1.34021700	4.58789700
H	-2.20672500	-0.35430800	5.00214100
H	-0.96179700	0.07962400	3.82693100
C	4.81288900	1.89701700	-0.08263400
F	5.60839900	2.72842900	0.62030700
F	5.31588400	0.64930600	0.04091100
F	4.93223700	2.23973500	-1.38632400
Pd	-0.35558100	-0.67296300	-0.07480700
C	1.14155800	-3.14443600	-0.30530800
C	2.48113200	-3.39018000	-0.67300900
C	0.72707600	-3.64309800	0.95236800
C	3.35687100	-4.08450700	0.16649600
H	2.85446200	-3.04237100	-1.62932200
C	1.60023400	-4.33618500	1.78815700
H	-0.29110700	-3.48415400	1.29037400
C	2.92618400	-4.56193400	1.40397000
H	4.38057000	-4.25458700	-0.15741700
H	1.24064200	-4.70364100	2.74601100
H	3.60592500	-5.10290300	2.05616700
C	-1.19630200	-2.39506300	-0.97068100
C	0.21736300	-2.37964800	-1.21408400
H	-1.55575300	-3.04222400	-0.16985100
H	-0.63247600	0.50073100	-1.64730700
C	0.76078300	-2.09223900	-2.60727200
C	-2.23743600	-2.27279000	-2.06675700
H	-1.96803800	-1.47469100	-2.77273800
H	1.67418000	-1.48949600	-2.57685600
H	1.00452300	-3.02477000	-3.13480000
C	-3.63456700	-1.97919400	-1.51929500
H	-3.66919400	-1.00763300	-1.01650200
H	-3.93861400	-2.75239300	-0.80469300

H	0.03708600	-1.55478900	-3.22069000
H	-4.37053000	-1.96061600	-2.33249700
O	-2.23614300	-3.53536300	-2.76640700
H	-2.93687000	-3.49033500	-3.43456000
C	-1.96295200	1.67402100	-2.40725600
H	-2.67208000	1.33525400	-1.65474100
N	-2.35258500	2.55634700	-3.27854000
C	-1.47227300	3.07994400	-4.32899200
H	-1.31062500	4.14692300	-4.15426600
H	-0.52049700	2.55361700	-4.32137800
H	-1.96476500	2.94298800	-5.29443600
C	-3.71778300	3.09372600	-3.24306200
H	-4.20947400	2.87500500	-4.19399700
H	-4.27642100	2.63870900	-2.42526600
H	-3.66918900	4.17606400	-3.10038700
O	-0.75680300	1.19469300	-2.41546300

21

B3LYP SCF energy in DMF: -1619.501138 a.u.

M06 SCF energy in DMF: -1618.925162 a.u.

M06 Free energy in DMF: -1618.499904 a.u.

C	-2.44748300	0.75813800	0.18472200
C	-0.76518000	2.33183200	0.30199000
C	-1.67498800	3.38253100	0.39723800
C	-3.03642000	3.08699400	0.37864800
C	-3.42637300	1.75432700	0.26777500
H	-2.72094200	-0.28851300	0.10541900
H	-1.32608400	4.40451100	0.48330300
H	-3.77387300	3.87847500	0.45163300
C	0.69149000	2.54776600	0.28600600
N	1.54196600	1.59338400	0.14764100
C	2.60546200	3.68085000	0.48712100
C	2.88908200	2.21328400	0.07257400
C	2.89514700	3.89103900	1.52001800
H	3.53320500	1.72675200	0.81131400
O	1.14814300	3.80258500	0.40928100
H	3.03068600	4.43768100	-0.17083900
N	-1.14135500	1.03558600	0.20572400
C	3.56362800	2.03838800	-1.32540800
C	3.72766100	0.53955500	-1.63524300
H	2.75933200	0.03918400	-1.73049800
H	4.27207200	0.40858400	-2.57740500
H	4.29443700	0.02992200	-0.84784100
C	4.96300500	2.68156500	-1.26027400
H	5.48232600	2.54839300	-2.21571700
H	4.91968800	3.75755500	-1.05978400
H	5.57632800	2.21758300	-0.47886300
C	2.73644700	2.70114000	-2.44185600
H	2.62722100	3.78123900	-2.29419700
C	3.23105400	2.55615400	-3.40857300
H	1.73490900	2.26380100	-2.51724500
C	-4.87968200	1.37265900	0.19052600
F	-5.67655300	2.31373400	0.73766300
F	-5.28392500	1.20746000	-1.09062500
F	-5.12613400	0.20828400	0.83020300
Pd	0.59084300	-0.45262000	0.38227300
C	-0.41754300	-3.09193300	-0.52165200
C	-1.69951300	-3.68195300	-0.50988400
C	0.26183800	-3.08550500	-1.76365300
C	-2.27277300	-4.22140900	-1.66585700
H	-2.26569400	-3.72980700	0.41324700
C	-0.30685600	-3.62704300	-2.91358000
H	1.24830300	-2.64065900	-1.83614900
C	-1.58411700	-4.19889200	-2.87766300
H	-3.26322900	-4.66641400	-1.60936900
H	0.25139700	-3.60101700	-3.84626900
H	-2.02759800	-4.61885800	-3.77612600
C	1.59641300	-2.25437100	0.79187400
C	0.18016300	-2.50645200	0.72749000
H	2.19421600	-2.57202600	-0.06442500
C	-0.60989300	-2.75421200	2.00728000

C	2.40082900	-2.35961600	2.07294900
H	1.86218400	-1.88662700	2.90635600
H	-1.62966300	-2.35953200	1.94519500
H	-0.69242300	-3.82813700	2.22923400
C	3.77947900	-1.70662500	1.96317400
H	3.69682600	-0.62612800	1.80856000
H	4.34678400	-2.13738500	1.13010800
H	-0.13577800	-2.27945600	2.86759100
H	4.35499900	-1.86634700	2.88367100
O	2.54855800	-3.77109700	2.35223100
H	3.09897600	-3.84552900	3.14649800

22

B3LYP SCF energy in DMF: -1960.431911 a.u.

M06 SCF energy in DMF: -1959.697875 a.u.

M06 Free energy in DMF: -1959.18259 a.u.

C	2.52511600	0.01160000	-0.87838800
C	1.37896600	1.94662000	-0.36569000
C	2.56364600	2.67874500	-0.27060400
C	3.77656200	2.02377400	-0.46673700
C	3.75501800	0.66604500	-0.77573600
H	2.47614100	-1.04107500	-1.13603500
H	2.53367100	3.73581200	-0.03874100
H	4.71374500	2.56228000	-0.38252600
C	0.06529100	2.59033600	-0.15227700
N	-1.05434900	1.97403500	-0.05177300
C	-1.30072300	4.34037200	0.16337200
C	-2.10562300	3.01350200	0.10367300
H	-1.57705600	5.05098300	-0.61703000
H	-2.71888900	2.99016600	-0.80574000
O	0.08064900	3.93493000	-0.07329800
H	-1.33098600	4.84016600	1.13378100
N	1.35937900	0.62922000	-0.66568000
C	-3.06667300	2.76824700	1.30249400
C	-3.85054600	1.46919900	1.04909700
H	-3.17947100	0.61080400	0.96955700
H	-4.55272200	1.27766700	1.86832800
H	-4.42996100	1.53228000	0.12007600
C	-4.06138700	3.94459900	1.36992100
H	-4.79051600	3.77744100	2.17040900
H	-3.56377700	4.89835700	1.57721800
H	-4.61631900	4.05057700	0.43028100
C	-2.29731600	2.65565300	2.63013300
H	-1.75066900	3.57394000	2.87191300
H	-2.99450600	2.46733500	3.45408200
H	-1.57600700	1.83198900	2.60792800
C	5.02260400	-0.12895000	-0.92463800
F	6.08544800	0.65445800	-1.19260300
F	5.30726100	-0.81350300	0.21106900
F	4.92873100	-1.04413600	-1.91418000
Pd	-0.55342600	-0.62492000	-0.21160200
C	0.67890200	-1.65380400	2.22487400
C	2.08209600	-1.67258100	2.07603000
C	0.16044600	-1.04431500	3.38641700
C	2.92071100	-1.07648300	3.01649400
H	2.52886300	-2.13920400	1.20502500
C	1.00073100	-0.45364300	4.33123100
H	-0.90866500	-1.04899300	3.57056700
C	2.38573800	-0.45846100	4.15005200
H	3.99544200	-1.09271400	2.85707500
H	0.56859200	0.00052100	5.21889700
H	3.03890700	0.00061500	4.88665000
C	-1.58660400	-1.98649000	1.14290800
C	-0.21070800	-2.30261000	1.20165600
H	-1.96274200	-1.26157600	1.86420700
C	0.33098200	-3.58244800	0.59062700
C	-2.65737100	-2.95354800	0.68257300
H	-2.35338800	-3.43805100	-0.25267500
H	1.27729100	-3.42776200	0.06481000
H	0.52268700	-4.31720600	1.38341000
C	-4.00998500	-2.27939600	0.46326300

H	-3.95814400	-1.53061000	-0.33244600
H	-4.35091800	-1.78934100	1.38159700
H	-0.37148600	-4.02930200	-0.11154300
H	-4.76266200	-3.02252900	0.17364000
O	-2.75789900	-3.95086300	1.72143900
H	-3.46936100	-4.55541200	1.46091700
C	-2.63556200	-0.21523800	-3.39134100
C	-1.27193400	-0.20833000	-2.96641100
C	-0.61767900	-1.35806100	-2.38051100
C	-1.34550700	-2.58006800	-2.51100100
C	-2.64746200	-2.60083500	-2.96058500
C	-3.30935000	-1.40891700	-3.36996500
H	-3.08720500	0.70351900	-3.74874600
H	0.46758800	-1.39871000	-2.39699000
H	-0.84178800	-3.50370600	-2.24980100
H	-3.17650600	-3.54643600	-3.02748700
H	-4.34055100	-1.44978700	-3.70427900
N	-0.55912400	0.90841800	-3.16986200
N	0.03833800	1.84879400	-3.35295900

TS12

B3LYP SCF energy in DMF: -1619.923668 a.u.

M06 SCF energy in DMF: -1619.335117 a.u.

M06 Free energy in DMF: -1618.896229 a.u.

C	-2.34224900	-0.72559200	0.15774600
C	-0.66715100	-2.23350000	-0.34573300
C	-1.56467100	-3.29031800	-0.44733600
C	-2.91775700	-3.03551800	-0.22117200
C	-3.30751900	-1.73718600	0.08954000
H	-2.61529600	0.29811400	0.38694100
H	-1.21648700	-4.28617100	-0.69362200
H	-3.64695000	-3.83485200	-0.28847700
C	0.78402700	-2.39792900	-0.52138400
N	1.62109100	-1.42760700	-0.36845300
C	2.69660600	-3.39361900	-1.08143000
C	2.98996100	-2.00837200	-0.45872800
H	2.83685300	-3.40856600	-2.16530600
H	3.58534500	-1.39958600	-1.14353000
O	1.26359500	-3.60148100	-0.82956800
H	3.22968900	-4.22742600	-0.62855900
N	-1.04954600	-0.96792300	-0.05384400
C	3.73081700	-2.05766500	0.91857900
C	3.90071600	-0.63416200	1.47629700
H	2.93554000	-0.15742600	1.67258100
H	4.45520600	-0.66724400	2.42077800
H	4.46614200	-0.00120600	0.78345400
C	5.13146600	-2.65545700	0.67442000
H	5.70342600	-2.65871200	1.60842300
H	5.08856000	-3.68915200	0.31532600
H	5.69260700	-2.06596400	-0.05994200
C	2.96922700	-2.91475000	1.94654000
H	2.84577800	-3.95163400	1.61640000
H	3.52495600	-2.94032300	2.89011200
C	1.97749000	-2.50256600	2.16295500
C	-4.74235300	-1.39053800	0.38672700
F	-5.58652900	-2.37331200	0.01876200
F	-4.93068900	-1.17087100	1.70794900
F	-5.12182300	-0.26302200	-0.25412700
Pd	0.63554800	0.50329000	-0.29326900
C	-0.58965900	2.18806700	-0.20285700
C	-1.35233600	2.47055100	-1.35165600
C	-1.13889400	2.45035500	1.06421100
C	-2.65409800	2.96027700	-1.23177000
H	-0.92717900	2.31395900	-2.33927400
C	-2.44292400	2.94506600	1.17802700
H	-0.55920400	2.26910400	1.96439600
C	-3.20271300	3.19988300	0.03293500
H	-3.23540800	3.16572000	-2.12668900
H	-2.85903400	3.13557300	2.16368100
H	-4.21134500	3.59255400	0.12396900
C	2.24538400	1.71215800	-0.82849000

C	1.39783400	2.81282800	-0.50355600
H	3.00890600	1.47443400	-0.09161200
H	1.03548400	3.38604100	-1.35225600
C	1.71054800	3.65364000	0.74042400
C	2.63942500	1.45690800	-2.26867700
H	1.82220500	1.67808300	-2.96256100
H	3.48530200	2.10709200	-2.53407200
H	2.96357700	0.42447800	-2.42744800
H	1.44585500	3.09208900	1.64538700
C	1.00099800	5.00576300	0.73320300
H	1.29574200	5.57940700	-0.15226800
H	-0.08612100	4.89868500	0.73602100
H	1.28018200	5.58079400	1.62333700
O	3.13552800	3.84401900	0.70475400
H	3.35243100	4.45126900	1.42840700

23

B3LYP SCF energy in DMF: -1619.943512 a.u.

M06 SCF energy in DMF: -1619.350127 a.u.

M06 Free energy in DMF: -1618.91269 a.u.

C	-2.29785400	-0.80066900	0.30638400
C	-0.50485600	-2.07918700	-0.40734600
C	-1.28054000	-3.23135300	-0.47266200
C	-2.62438100	-3.15136900	-0.11316600
C	-3.13315400	-1.91965700	0.28987700
H	-2.67062400	0.17569600	0.58893700
H	-0.83944500	-4.16831900	-0.79000100
H	-3.25685800	-4.03156500	-0.14813900
C	0.93706800	-2.08055400	-0.70205300
N	1.72503200	-1.11434200	-0.37158900
C	2.82699800	-2.75606100	-1.66106000
C	3.10729300	-1.55868900	-0.72597100
H	2.83998500	-2.48183400	-2.71919800
H	3.60437200	-0.75311100	-1.27197800
O	1.44663100	-3.13765000	-1.33436900
H	3.45422500	-3.63025100	-1.49850700
N	-1.00880500	-0.87810700	-0.03814100
C	3.98535100	-1.91056900	0.51955200
C	4.08561800	-0.69286300	1.45112000
H	3.11341300	-0.44331500	1.88562200
H	4.77300900	-0.90682800	2.27707200
H	4.46707600	0.18630300	0.92034600
C	5.39797900	-2.25686900	0.00810100
H	6.05726700	-2.47955200	0.85385100
H	5.40217500	-3.13314800	-0.64879100
H	5.83576900	-1.41858700	-0.54627200
C	3.41274100	-3.09919800	1.31456500
H	3.37464000	-4.02128400	0.72527700
H	4.04782600	-3.29972200	2.18416500
H	2.40542600	-2.88822200	1.69043700
C	-4.56525000	-1.78548500	0.73867000
F	-5.37617800	-2.62444800	0.06323700
F	-4.69878900	-2.07565900	2.05228500
F	-5.03106800	-0.53213300	0.55934300
Pd	0.40202700	0.76748700	-0.21683300
C	-1.13127100	2.03215900	-0.45907700
C	-1.64956800	2.18363900	-1.75138900
C	-1.77522300	2.64589000	0.62265400
C	-2.80941600	2.94205000	-1.95748500
H	-1.16482400	1.71310700	-2.60233500
C	-2.93535900	3.40217700	0.40868100
H	-1.38518100	2.54420800	1.63049000
C	-3.45404000	3.55287300	-0.87945200
H	-3.20544500	3.04931000	-2.96430100
H	-3.42794300	3.87465400	1.25492600
H	-4.35269900	4.14130500	-1.04200600
C	2.05764700	2.07597200	-1.00783300
C	1.56968100	2.67798100	0.13819700
H	2.90922900	1.40563000	-0.89800100
H	0.88193300	3.51312600	0.02738200
C	2.27466700	2.61227500	1.47842600

C	1.78375200	2.54320000	-2.40904200
H	0.92047300	3.20897000	-2.46450100
H	2.66598500	3.09562900	-2.76132800
H	1.64038000	1.70512600	-3.09865000
C	1.33829900	2.70236300	2.68011100
H	1.92236700	2.71744300	3.60828100
H	0.73649300	3.61626300	2.64000500
H	0.66695900	1.83898200	2.72500100
H	2.85039800	1.68265000	1.53432300
O	3.17185000	3.73721700	1.44442400
H	3.53615500	3.83536400	2.33728100

TS13

B3LYP SCF energy in DMF: -1619.93111 a.u.

M06 SCF energy in DMF: -1619.340509 a.u.

M06 Free energy in DMF: -1618.901559 a.u.

C	-2.41716100	-0.64624300	0.09448400
C	-0.66901100	-2.04874000	-0.46644700
C	-1.52853600	-3.09754000	-0.77415500
C	-2.90050600	-2.89545600	-0.62522000
C	-3.34740500	-1.65389700	-0.18326800
H	-2.73261300	0.33485300	0.42996000
H	-1.13685800	-4.04601700	-1.12133400
H	-3.60086200	-3.69021400	-0.85526100
C	0.79517300	-2.15811600	-0.55937400
N	1.58732700	-1.20433100	-0.20488300
C	2.77118400	-3.00505600	-1.13960400
C	2.97905100	-1.72655100	-0.29467300
H	2.97175600	-2.84574300	-2.20229900
H	3.57795700	-0.99441500	-0.83932400
O	1.33381100	-3.28938600	-1.01249700
H	3.30632600	-3.88663700	-0.79255500
N	-1.10530600	-0.84000200	-0.04070100
C	3.63561800	-1.97173200	1.10420900
C	3.72630300	-0.64792200	1.88329000
H	2.73722700	-0.22656700	2.08599800
H	4.22196300	-0.81425600	2.84627000
H	4.31386000	0.09631200	1.33447900
C	5.06812400	-2.49090800	0.86542300
H	5.58420000	-2.61656800	1.82338600
H	5.08447200	-3.46101400	0.35767000
H	5.65073900	-1.78492800	0.26214700
C	2.84345400	-2.99441700	1.93994600
H	2.78366500	-3.97495600	1.45569000
H	3.33491800	-3.14240800	2.90758500
H	1.82341900	-2.64955500	2.14223000
C	-4.81246900	-1.38092300	0.03231400
F	-5.58791700	-2.21517100	-0.68820800
F	-5.16022400	-1.53257000	1.33018600
F	-5.13768300	-0.11659400	-0.31555500
Pd	0.54657800	0.67312100	0.03954800
C	-0.71640800	2.32675700	0.25958900
C	-1.31581600	2.75935000	-0.93945900
C	-1.44553900	2.41153400	1.45825500
C	-2.63422200	3.21861000	-0.94257000
H	-0.74998700	2.74303700	-1.86732500
C	-2.76195100	2.88386200	1.45127800
H	-0.99200600	2.10822700	2.39705400
C	-3.35956600	3.28364800	0.25240400
H	-3.09088700	3.53819000	-1.87550600
H	-3.31700600	2.94006100	2.38386000
H	-4.38056300	3.65435500	0.24983500
C	2.11349500	2.03200400	-0.15060500
C	1.23847300	2.99090200	0.45382900
H	2.89162100	1.61944900	0.49189900
H	0.93725600	3.81627400	-0.18482200
C	1.42744500	3.37010700	1.90168800
H	2.33094500	3.99101400	1.96054800
H	0.59360700	3.95909100	2.28758100
H	1.57948900	2.49914300	2.54418800
C	2.54135400	2.26197600	-1.58990500

C	3.67432300	3.29334800	-1.66350800
H	3.97991700	3.44670100	-2.70570800
H	3.35273200	4.26145400	-1.26602300
H	4.54594400	2.95259400	-1.09428100
O	2.96628600	1.01054600	-2.14134700
H	3.34220000	1.19518400	-3.01477900
H	1.67905000	2.64628300	-2.15589000

TS14

B3LYP SCF energy in DMF: -1619.922332 a.u.

M06 SCF energy in DMF: -1619.334464 a.u.

M06 Free energy in DMF: -1618.894268 a.u.

C	-2.67169400	-0.28091000	0.37258800
C	-1.17783500	-1.74951300	-0.60514500
C	-2.18895000	-2.63714600	-0.95214500
C	-3.50317700	-2.31935200	-0.60696300
C	-3.74117300	-1.13308400	0.07720600
H	-2.83495800	0.65825300	0.88776400
H	-1.95394100	-3.55981000	-1.46882200
H	-4.31635900	-2.98975100	-0.85954500
C	0.24894900	-2.03905100	-0.81900400
N	1.18236700	-1.34950100	-0.25682900
C	2.05779800	-2.99455100	-1.69246900
C	2.46137700	-2.06332600	-0.52773800
H	2.27986800	-2.56582600	-2.67336100
H	3.21185300	-1.33826200	-0.85163500
O	0.59323800	-3.07787600	-1.58145000
H	2.44690400	-4.00928400	-1.63657200
N	-1.41723500	-0.57222700	0.02540400
C	3.01077300	-2.81321000	0.73313300
C	3.22098700	-1.82318000	1.89062300
H	2.28001600	-1.36204800	2.20595900
H	3.64112700	-2.34774500	2.75608900
H	3.91664000	-1.02694600	1.61193200
C	4.37589000	-3.42060400	0.35356900
H	4.81006600	-3.93555400	1.21740400
H	4.29751300	-4.15383900	-0.45646500
H	5.08171700	-2.64362400	0.03795300
C	2.05668400	-3.92897700	1.20076100
H	1.90523800	-4.70199600	0.44009500
H	2.47705800	-4.42383800	2.08289500
H	1.07658500	-3.53259100	1.48882000
C	-5.12650100	-0.70963400	0.48868300
F	-5.19732200	-0.47546400	1.81763000
F	-5.48912000	0.43915700	-0.12828500
F	-6.05155900	-1.63970300	0.18870200
Pd	0.33798500	0.70564700	0.14428100
C	2.12265200	1.80301200	0.04449500
C	2.47346800	2.10280100	-1.28755300
C	3.14062700	1.58613600	0.98572100
C	3.81429500	2.13388300	-1.67495900
H	1.70182300	2.31953700	-2.02014000
C	4.48260600	1.63980100	0.59703900
H	2.89479000	1.37561500	2.02112500
C	4.82232200	1.90824600	-0.73160900
H	4.07105800	2.35437000	-2.70763800
H	5.26186000	1.47281900	1.33575500
H	5.86633000	1.95440600	-1.02820100
C	-0.60758700	2.54916000	0.32257500
C	0.64611200	3.05580100	0.79802300
H	-1.35950400	2.35879000	1.09325300
H	1.10321800	3.82301000	0.18082600
C	0.88104100	3.23409000	2.27560900
H	1.92873100	3.43117900	2.50912400
H	0.30221500	4.11352200	2.58793400
H	0.53419500	2.37870400	2.86079200
C	-1.15549000	3.16854500	-0.95862700
H	-0.33293000	3.24331800	-1.68590900
C	-2.31955100	2.42759400	-1.60990800
H	-2.01128200	1.44371400	-1.97592400
H	-3.15378900	2.30067500	-0.91254400

H	-2.68262300	2.99976600	-2.47200900
O	-1.55977600	4.49436800	-0.56548300
H	-1.91409700	4.92874500	-1.35628200

TS15

B3LYP SCF energy in DMF: -1619.9256 a.u.

M06 SCF energy in DMF: -1619.336148 a.u.

M06 Free energy in DMF: -1618.896833 a.u.

C	-2.33571000	-0.72207800	0.15389100
C	-0.66608900	-2.23601900	-0.35100300
C	-1.56857900	-3.28809300	-0.45911700
C	-2.92108600	-3.02760700	-0.23592200
C	-3.30547700	-1.72867300	0.07928100
H	-2.60365400	0.30199000	0.38728500
H	-1.22458700	-4.28475500	-0.70801700
H	-3.65391900	-3.82311800	-0.30889300
C	0.78510000	-2.40626400	-0.52173900
N	1.62623700	-1.44060400	-0.36203600
C	2.69445700	-3.41096700	-1.07662200
C	2.99217800	-2.02862400	-0.44944700
H	2.83979800	-3.42413600	-2.15987900
H	3.59329500	-1.42147700	-1.13074700
O	1.25951100	-3.61169400	-0.83190000
H	3.22123700	-4.24856100	-0.62323700
N	-1.04374100	-0.96979700	-0.05613600
C	3.72816000	-2.08458000	0.93010400
C	3.90210500	-0.66293100	1.49145900
H	2.93814100	-0.18322300	1.68631600
H	4.45415900	-0.70012300	2.43722300
H	4.47166200	-0.03067500	0.80124100
C	5.12698600	-2.68791500	0.68946700
H	5.69528300	-2.69727700	1.62567400
H	5.08067200	-3.72011700	0.32648800
H	5.69382100	-2.09849600	-0.04057700
C	2.95927700	-2.94061800	1.95352900
H	2.83307700	-3.97634100	1.62078200
H	3.51125800	-2.97027000	2.89917600
H	1.96829700	-2.52503900	2.16684100
C	-4.73929000	-1.37610300	0.37408100
F	-5.58835400	-2.34825500	-0.01079200
F	-4.93302500	-1.17213600	1.69706200
F	-5.10773000	-0.23788500	-0.25416200
Pd	0.64076800	0.49680200	-0.28703300
C	-0.58692500	2.17158900	-0.20243100
C	-1.35391300	2.44486100	-1.34934100
C	-1.12176000	2.45372000	1.06510400
C	-2.65553400	2.93624000	-1.22505500
H	-0.93603900	2.27718100	-2.33842600
C	-2.42721000	2.93996700	1.18457300
H	-0.52627100	2.29426400	1.95924900
C	-3.19607800	3.18116600	0.04189400
H	-3.24356700	3.13435700	-2.11733000
H	-2.83682000	3.14214500	2.17077800
H	-4.20612500	3.56969900	0.13689500
C	2.24967500	1.71951400	-0.79712200
C	1.41673600	2.83593000	-0.49376500
H	2.99804500	1.46986600	-0.04601400
H	1.05358300	3.40482100	-1.34559600
C	1.70584100	3.70068200	0.72175800
C	2.66973700	1.46074000	-2.23126000
H	1.86555400	1.68850800	-2.93807100
H	3.52501100	2.10326700	-2.48425900
H	2.98541500	0.42507800	-2.38447100
C	3.10821600	4.31605700	0.58872600
H	3.88857300	3.55015900	0.60460200
H	3.19368600	4.88929900	-0.34048300
H	3.28659800	4.99615400	1.42953000
O	0.72669700	4.73467500	0.76773100
H	0.91591700	5.27177600	1.55056000
H	1.67251900	3.08563300	1.63219100

TS16

B3LYP SCF energy in DMF: -1619.923269 a.u.

M06 SCF energy in DMF: -1619.333402 a.u.

M06 Free energy in DMF: -1618.89319 a.u.

C	2.67163700	-0.26254500	-0.36690900
C	1.19750700	-1.77101800	0.57917800
C	2.22429700	-2.63288000	0.95157300
C	3.53319000	-2.28227000	0.62816600
C	3.75455600	-1.08681700	-0.05136900
H	2.81879100	0.68205900	-0.87087800
H	2.00249300	-3.55820600	1.46929300
H	4.35895600	-2.93385000	0.89288500
C	-0.22419100	-2.09060800	0.78455000
N	-1.17143200	-1.40150900	0.24575200
C	-2.01524900	-3.09416700	1.64172800
C	-2.43851000	-2.14064800	0.50226600
H	-2.23793100	-2.69222700	2.63376200
H	-3.19768200	-1.43463600	0.84743000
O	-0.55050100	-3.15400300	1.52100200
H	-2.39031100	-4.11279800	1.56392000
N	1.41686500	-0.59520200	-0.05506600
C	-2.98345300	-2.86611100	-0.77457200
C	-3.22334300	-1.84748200	-1.90115900
H	-2.29400200	-1.36134600	-2.21323200
H	-3.64470100	-2.35397300	-2.77680300
H	-3.92917100	-1.07177800	-1.59127900
C	-4.33384900	-3.51019600	-0.40281600
H	-4.76304000	-4.01139600	-1.27715900
H	-4.23725100	-4.26171100	0.38819500
H	-5.05263000	-2.75528000	-0.06369700
C	-2.01120900	-3.94909400	-1.28013900
H	-1.83841800	-4.73911400	-0.54190100
H	-2.42801900	-4.42832100	-2.17258800
H	-1.04145000	-3.52519600	-1.56389400
C	5.15414800	-0.65072600	-0.39335000
F	5.16828300	0.27384000	-1.37597700
F	5.77519700	-0.10286100	0.67613000
F	5.91317200	-1.69008200	-0.79872800
Pd	-0.37608700	0.64519100	-0.20692100
C	-2.15051800	1.71363300	-0.07638500
C	-2.45124600	2.02617500	1.26417800
C	-3.20043100	1.54644700	-0.99416700
C	-3.77988600	2.10427000	1.68748200
H	-1.65098500	2.21340300	1.97516200
C	-4.52800500	1.65015500	-0.57018100
H	-2.98380200	1.34815900	-2.03960500
C	-4.82009500	1.92071200	0.77030900
H	-4.00211400	2.32709100	2.72772300
H	-5.33339900	1.52268000	-1.28858800
H	-5.85319900	2.00364200	1.09589500
C	0.54549000	2.50109100	-0.56102800
C	-0.73641600	2.97044000	-0.98793800
H	1.20495300	2.17038300	-1.36849300
C	1.26351300	3.14530700	0.61277500
H	0.52345000	3.47485600	1.35446800
C	2.08803300	4.35598500	0.15759000
H	2.60762800	4.80297300	1.01387200
H	2.83708100	4.05107500	-0.58109800
H	1.45544900	5.12995200	-0.28685900
O	2.11979400	2.16074300	1.20762900
H	2.65102600	2.61465400	1.87863600
C	-1.34184600	4.28403300	-0.54694500
H	-0.80500500	5.07899000	-1.08297500
H	-2.39562300	4.34574800	-0.82478100
H	-1.24333500	4.47417500	0.52233200
H	-0.98475300	2.71409400	-2.01507500

TS17

B3LYP SCF energy in DMF: -1619.924211 a.u.

M06 SCF energy in DMF: -1619.336911 a.u.

M06 Free energy in DMF: -1618.898035 a.u.

C	-2.37268400	-0.69764200	0.06799300
C	-0.62604700	-2.08345700	-0.53948000
C	-1.48673000	-3.12260200	-0.87522200
C	-2.85838100	-2.92423900	-0.71858700
C	-3.30303900	-1.69763500	-0.23538200
H	-2.68712800	0.26901800	0.44397400
H	-1.09544400	-4.06320200	-1.24346800
H	-3.55959700	-3.71368200	-0.96425200
C	0.83834700	-2.20222300	-0.61288900
N	1.63413100	-1.25049100	-0.25735100
C	2.81855100	-3.09733500	-1.09672300
C	3.01480900	-1.81314100	-0.25949500
H	3.06412900	-2.95368100	-2.15220000
H	3.67976900	-1.11802200	-0.77522700
O	1.37262600	-3.35160500	-1.02222600
H	3.32306600	-3.98431800	-0.71835100
N	-1.06097500	-0.88713300	-0.07809200
C	3.58260800	-2.04912200	1.17987700
C	3.64603900	-0.71592500	1.94577400
H	2.65089600	-0.28524600	2.09279200
H	4.09128000	-0.87446100	2.93427900
H	4.26622400	0.01735500	1.41831000
C	5.01823200	-2.59261000	1.03212400
H	5.47055000	-2.72533300	2.02074100
H	5.04966700	-3.56321200	0.52630000
H	5.64909300	-1.89736500	0.46627500
C	2.72498700	-3.04744200	1.97967400
H	2.67707300	-4.03360900	1.50602500
H	3.15657100	-3.18935600	2.97636500
H	1.70119800	-2.68234700	2.11766500
C	-4.77160600	-1.40488000	-0.07659300
F	-5.49804000	-2.53328900	0.04620800
F	-5.01075700	-0.64309600	1.01228700
F	-5.25840000	-0.73049600	-1.14316700
Pd	0.57113800	0.62266800	0.05867500
C	-0.69483600	2.21867900	0.44799200
C	-1.35472500	2.72463400	-0.68785600
C	-1.34401800	2.26051500	1.69537100
C	-2.65846600	3.21446000	-0.58376600
H	-0.85111000	2.73971800	-1.65047200
C	-2.64305700	2.76647100	1.79634400
H	-0.83471100	1.90485900	2.58703600
C	-3.30336300	3.23926900	0.65761400
H	-3.16639200	3.58729000	-1.46929500
H	-3.13610800	2.79492700	2.76433100
H	-4.31150500	3.63569700	0.73879800
C	2.11290700	2.04078800	-0.06420800
C	1.27640100	2.90146700	0.71511700
H	2.89010700	1.51809200	0.49286100
C	2.50935500	2.44854000	-1.47597900
H	1.62203800	2.84447400	-1.99233700
C	3.09861600	1.31926000	-2.31649200
H	2.36645200	0.52361300	-2.48503000
H	3.98170600	0.89159500	-1.83057400
H	3.40419000	1.70468900	-3.29656200
O	3.47608800	3.50238500	-1.30623600
H	3.70268500	3.82413200	-2.19203300
H	1.32239300	2.72138200	1.78694900
C	1.01837000	4.34977000	0.36715400
H	0.20930200	4.76518700	0.97109800
H	1.94158200	4.89582700	0.59950200
H	0.79901400	4.50872200	-0.68885000

24

B3LYP SCF energy in DMF: -1619.944439 a.u.

M06 SCF energy in DMF: -1619.352521 a.u.

M06 Free energy in DMF: -1618.913225 a.u.

C	-2.33606000	-0.85603300	0.14558900
C	-0.40384800	-1.95494900	-0.49831400
C	-1.10497600	-3.10633700	-0.83790700

C	-2.48680600	-3.12349300	-0.65859200
C	-3.10500900	-1.98396900	-0.15217700
H	-2.79175100	0.05193900	0.51975600
H	-0.57914700	-3.96920500	-1.22784700
H	-3.06294000	-4.00686800	-0.91090000
C	1.06092500	-1.86558100	-0.59291300
N	1.73837800	-0.89991200	-0.07289300
C	3.10281100	-2.35899900	-1.32470500
C	3.18070000	-1.23897400	-0.26329500
H	3.24796100	-1.98655100	-2.34250900
H	3.68685500	-0.36255700	-0.67435700
O	1.71440700	-2.83290000	-1.23662400
H	3.75153700	-3.21488900	-1.15008500
N	-1.01098500	-0.83938200	-0.02594500
C	3.89164000	-1.65568100	1.06463000
C	3.78323700	-0.51680300	2.09083200
H	2.74630700	-0.35684700	2.39885200
H	4.36341900	-0.76069200	2.98779200
H	4.17410700	0.42362200	1.68736300
C	5.38109200	-1.89012800	0.74307100
H	5.92313800	-2.15752100	1.65663100
H	5.53154100	-2.70422200	0.02591700
H	5.84583200	-0.98700600	0.33085800
C	3.28066600	-2.93382900	1.66894900
H	3.38214500	-3.80021800	1.00698200
H	3.79319900	-3.18199900	2.60466600
H	2.21880400	-2.80314900	1.90496600
C	-4.58862900	-1.95629400	0.10980600
F	-5.25944400	-2.75301500	-0.74604800
F	-4.87806600	-2.38242500	1.35926700
F	-5.09218200	-0.70996600	-0.01040300
Pd	0.33205800	0.85380300	0.21977100
C	-1.23373900	2.10292700	0.15740600
C	-1.67293200	2.59247200	-1.07941300
C	-1.97679400	2.38146100	1.31328800
C	-2.85538300	3.34033300	-1.15916500
H	-1.10933300	2.39399300	-1.98698400
C	-3.15704800	3.13104500	1.22677200
H	-1.64687900	2.01900800	2.28374900
C	-3.59942300	3.61110400	-0.00864900
H	-3.19053900	3.70874700	-2.12564100
H	-3.72611200	3.33912200	2.12954500
C	2.03162300	2.31674400	-0.05672900
C	1.30078200	2.80275300	1.01107100
H	2.88433600	1.67652200	0.15743300
C	2.01075400	2.94421100	-1.43033200
H	1.06350300	3.46458200	-1.60253500
C	2.27318900	1.98127200	-2.58211300
H	1.50510300	1.19427800	-2.59833000
H	2.80140800	3.70957700	-1.44512700
O	3.57618300	1.41657000	-2.41234500
H	3.71197800	0.77582100	-3.12491100
H	2.21035600	2.53271400	-3.53140400
H	-4.51479000	4.19263500	-0.07352400
H	0.60224400	3.60877400	0.80262900
C	1.62629800	2.61282300	2.46454200
H	2.10535200	3.53162100	2.83137400
H	2.30879300	1.78090900	2.64073800
H	0.72123200	2.47080800	3.06381400

TS18

B3LYP SCF energy in DMF: -1619.92546 a.u.

M06 SCF energy in DMF: -1619.33769 a.u.

M06 Free energy in DMF: -1618.897675 a.u.

C	-2.38767100	-0.70576300	0.06502900
C	-0.55983600	-2.03751700	-0.40758200
C	-1.35970400	-3.13803400	-0.69684700
C	-2.74315800	-2.99881900	-0.58815700
C	-3.26065200	-1.76628100	-0.20093100
H	-2.75924000	0.26794400	0.36296100
H	-0.91434600	-4.07729000	-1.00163400

H	-3.39875300	-3.83410200	-0.80709300
C	0.91004700	-2.07691200	-0.46249400
N	1.64518200	-1.05321200	-0.18571600
C	2.94430200	-2.87818600	-0.88727200
C	3.05998400	-1.52256400	-0.15457400
H	3.17718000	-2.80287700	-1.95284900
H	3.67101200	-0.81868500	-0.72348600
O	1.51762300	-3.21905800	-0.78170400
H	3.50630800	-3.69792700	-0.44415400
N	-1.06498200	-0.83866300	-0.03399400
C	3.63999000	-1.61213800	1.29656300
C	3.62243900	-0.22216500	1.95713900
H	2.60396300	0.16363700	2.06127700
H	4.06307400	-0.28146500	2.95879600
H	4.20779400	0.50147200	1.37974500
C	5.10512300	-2.08091400	1.18829000
H	5.56619800	-2.09186700	2.18177200
H	5.19173200	-3.09270300	0.77868200
H	5.69399200	-1.40783600	0.55439800
C	2.84356800	-2.59627400	2.17319400
H	2.85768900	-3.61648900	1.77537200
H	3.28083000	-2.63550200	3.17669900
H	1.79895500	-2.28580700	2.28557000
C	-4.74183100	-1.55962700	-0.02723900
F	-5.45850400	-2.43261500	-0.76271700
F	-5.11748100	-1.72075000	1.26167000
F	-5.11478300	-0.31369000	-0.39217100
Pd	0.50248200	0.77597500	-0.01039500
C	-0.84569800	2.35533400	0.25065700
C	-1.53866400	2.74111900	-0.91320000
C	-1.51320200	2.39479500	1.48734800
C	-2.88331700	3.11076100	-0.84435000
H	-1.02494600	2.76089000	-1.87048000
C	-2.85797700	2.77315800	1.55171200
H	-0.99023600	2.12729800	2.40057600
C	-3.54603800	3.12852500	0.38788100
H	-3.41042400	3.39595300	-1.75095900
C	-3.36444700	2.79287000	2.51301400
H	1.96116200	2.23084100	-0.34363900
C	1.06794400	3.12823600	0.32966100
H	2.81041200	1.88130800	0.24169100
C	2.23958200	2.47291700	-1.81999900
H	1.30394400	2.69281700	-2.34771900
C	2.95981600	1.35779200	-2.56385300
H	2.36481300	0.43361000	-2.53587600
H	2.85703900	3.38138100	-1.89595200
O	4.24221400	1.15519600	-1.96090200
H	4.71236200	0.49643300	-2.49200800
H	3.07273400	1.65070900	-3.61757700
H	-4.58877900	3.42819700	0.44128300
H	0.67881300	3.93841100	-0.28073300
C	1.33590400	3.51637100	1.76315400
H	2.18309800	4.21493800	1.75932300
H	1.61166400	2.65942300	2.38298100
H	0.48753300	4.03000500	2.21940000

25

B3LYP SCF energy in DMF: -1619.956995 a.u.

M06 SCF energy in DMF: -1619.369436 a.u.

M06 Free energy in DMF: -1618.925645 a.u.

C	-2.73439000	-0.17561100	-0.02591200
C	-1.17172700	-1.83820600	-0.34518000
C	-2.15099600	-2.80673400	-0.54633900
C	-3.48829200	-2.42195800	-0.46907400
C	-3.78103900	-1.08867500	-0.19682200
H	-2.93322500	0.87114000	0.16960200
H	-1.87495500	-3.83333400	-0.75449100
H	-4.27935300	-3.14874800	-0.61747100
C	0.26342300	-2.16187400	-0.34238800
N	1.18568600	-1.28681300	-0.11447000
C	2.10796900	-3.38271300	-0.60811200

C	2.47264000	-2.02797000	0.03551300
H	2.37952100	-3.43408600	-1.66599700
H	3.24003300	-1.51475100	-0.54770200
O	0.63901800	-3.42445800	-0.53881800
H	2.48072300	-4.26268800	-0.08785700
N	-1.45363700	-0.53878800	-0.09680300
C	2.95399600	-2.12757200	1.52273900
C	3.17662200	-0.72281600	2.11006500
H	2.25084200	-0.14071100	2.13507800
H	3.54646200	-0.80624700	3.13833600
H	3.92185200	-0.16290300	1.53576700
C	4.30541700	-2.87150600	1.52225400
H	4.70299900	-2.92332300	2.54155800
H	4.21902100	-3.89923100	1.15430600
H	5.04416100	-2.35225700	0.90089600
C	1.94380700	-2.8844200	2.40548900
H	1.77282300	-3.91014600	2.06212700
H	2.32418000	-2.94655000	3.43082900
H	0.97729300	-2.36991600	2.44891600
C	-5.20584100	-0.62876800	-0.03570800
F	-6.04967000	-1.33532700	-0.81524100
F	-5.63026600	-0.77427800	1.24030500
F	-5.35038100	0.67541600	-0.35349200
Pd	0.50876700	0.73129500	-0.24148000
C	0.59909900	3.00103200	0.34810800
C	-0.35553900	2.95842000	-0.70369500
C	0.12125800	3.14815500	1.67691300
C	-1.73109600	3.13021300	-0.43113000
H	-0.02168300	2.98625100	-1.73675800
C	-1.23340800	3.30676500	1.92875700
H	0.82722500	3.18269400	2.49942800
C	-2.16558700	3.30897100	0.87307300
H	-2.43816600	3.14531200	-1.25539500
H	-1.57590000	3.45068300	2.94959200
C	2.31728000	1.60928700	-0.65007600
C	2.09246900	2.99549500	-0.02258600
H	3.05001900	1.02048000	-0.09706200
C	2.62574900	1.63834800	-2.14481100
H	1.79966400	2.09397900	-2.70392800
C	2.96966400	0.31097900	-2.80506300
H	2.13937600	-0.40115500	-2.69366500
H	3.48598700	2.31530300	-2.28115300
O	4.16608100	-0.20692700	-2.21197600
H	4.39272900	-1.02202700	-2.68271600
H	3.12124800	0.47915900	-3.88116700
H	-3.22051200	3.46000600	1.08283900
H	2.23700800	3.77335400	-0.78450800
C	3.04287400	3.28970500	1.13803200
H	4.07597500	3.29137100	0.77525400
H	2.96995600	2.53463300	1.92783900
H	2.84302100	4.27095800	1.58242300

26

B3LYP SCF energy in DMF: -1619.947273 a.u.

M06 SCF energy in DMF: -1619.354066 a.u.

M06 Free energy in DMF: -1618.914688 a.u.

C	2.75639900	0.08098000	0.40029600
C	1.34755800	1.57672200	-0.64397900
C	2.40676400	2.35176200	-1.09960300
C	3.70554100	1.96075700	-0.77185900
C	3.87852400	0.81423500	-0.00655000
H	2.87166700	-0.82009400	0.99210900
H	2.22243200	3.24145000	-1.68940700
H	4.55662100	2.54342700	-1.10468500
C	-0.05635400	1.94781400	-0.87694700
N	-1.04680900	1.30536900	-0.35021400
C	-1.79819300	3.01439700	-1.76612100
C	-2.28109400	2.09321200	-0.62532100
H	-2.02086900	2.61342500	-2.75816500
H	-3.06041000	1.41493300	-0.97800500
O	-0.33162100	3.01144500	-1.62382300

H	-2.12701400	4.04946100	-1.70204600
N	1.51398100	0.44909000	0.08982400
C	-2.81315500	2.85106400	0.63737400
C	-3.12543200	1.85301400	1.76556000
H	-2.22727200	1.32442500	2.09955900
H	-3.53718300	2.38860900	2.62830500
H	-3.86277100	1.10917200	1.44987900
C	-4.12275900	3.55743900	0.23208700
H	-4.54689300	4.08158000	1.09517400
H	-3.97218700	4.30007700	-0.55884300
H	-4.86809100	2.83571600	-0.12129400
C	-1.79922600	3.88905700	1.15545000
H	-1.57575000	4.66477100	0.41574000
H	-2.20994100	4.39338800	2.03667000
H	-0.85649300	3.42158800	1.46120100
C	5.24517300	0.31720500	0.38604200
F	5.32870700	0.11276700	1.71909600
F	5.52751000	-0.86395800	-0.20836900
F	6.21689500	1.18360200	0.04427800
Pd	-0.48821200	-0.65439000	0.30113700
C	-2.35853700	-1.34538000	0.07230100
C	-2.84571700	-1.45992600	-1.23823800
C	-3.21391600	-1.63659000	1.14370800
C	-4.16510500	-1.86917600	-1.47143200
H	-2.20710200	-1.22930400	-2.08655200
C	-4.53409900	-2.04082300	0.90601300
H	-2.86992800	-1.54529100	2.16991200
C	-5.01280400	-2.16141500	-0.40044500
H	-4.52529700	-1.95535800	-2.49372800
H	-5.18452200	-2.26054300	1.74911900
H	-6.03612700	-2.47796700	-0.58227200
C	0.51656800	-2.67012400	0.40332600
C	-0.10441100	-2.44706200	1.62110400
H	1.56170000	-2.38460600	0.30670300
H	-1.06765400	-2.92417000	1.78444600
C	0.57865700	-1.95168400	2.86646800
H	-0.07570700	-1.29926900	3.45365400
H	0.81601600	-2.81701300	3.50151400
H	1.51180800	-1.42390500	2.65721400
C	0.04778700	-3.65571500	-0.63851400
H	0.56230100	-4.60556100	-0.42838900
H	-1.02534700	-3.84627900	-0.54960800
C	0.37539900	-3.25304600	-2.07265900
H	-0.14488100	-2.31932400	-2.32730900
H	0.01567500	-4.03581700	-2.75705100
O	1.79052300	-3.09018900	-2.18547400
H	1.97613100	-2.77884400	-3.08245100

TS19

B3LYP SCF energy in DMF: -1619.921494 a.u.

M06 SCF energy in DMF: -1619.331878 a.u.

M06 Free energy in DMF: -1618.890729 a.u.

C	2.61172800	0.26649100	0.35488300
C	1.08193300	1.72625100	-0.58095100
C	2.07208000	2.64202300	-0.91583000
C	3.39437900	2.34480000	-0.58624200
C	3.66085400	1.14763700	0.06827700
H	2.79989300	-0.69027400	0.82660100
H	1.81402200	3.56989000	-1.41164400
H	4.19155400	3.03816000	-0.82782900
C	-0.34965900	1.99442100	-0.78878600
N	-1.27159600	1.27724100	-0.24439800
C	-2.17305300	2.94244000	-1.63945300
C	-2.56093400	1.98002200	-0.49517300
H	-2.38951100	2.53120000	-2.62909700
H	-3.30358600	1.25332200	-0.83304200
O	-0.71029100	3.04606300	-1.52712300
H	-2.57820400	3.94947800	-1.56224800
N	1.34735700	0.54228700	0.02626800
C	-3.11460100	2.69308700	0.78541600
C	-3.31349100	1.67171800	1.91782700

H	-2.36780300	1.21035100	2.21827000
H	-3.73532200	2.17035500	2.79771400
H	-4.00371100	0.87738000	1.62069000
C	-4.48589800	3.29846700	0.42536200
H	-4.92260700	3.78527800	1.30411500
H	-4.41592000	4.05454000	-0.36407500
H	-5.18572600	2.52448100	0.08961600
C	-2.16908300	3.80493200	1.27896700
H	-2.02317000	4.59598400	0.53600700
H	-2.59285700	4.27693900	2.17198500
H	-1.18608900	3.40948600	1.55815700
C	5.06219500	0.74528800	0.44250000
F	5.13787800	0.33335800	1.72472900
F	5.49828600	-0.29082400	-0.32416900
F	5.93962600	1.75048400	0.28036900
Pd	-0.39396000	-0.77328500	0.14223500
C	-2.15476100	-1.89479400	-0.02616900
C	-2.43080200	-2.20830600	-1.37277200
C	-3.22433200	-1.68645400	0.85786500
C	-3.74884800	-2.26071900	-1.83028700
H	-1.61887100	-2.42105700	-2.06170200
C	-4.54296900	-1.75860700	0.39838500
H	-3.03669000	-1.46570600	1.90294300
C	-4.80868000	-2.04058200	-0.94430400
H	-3.94740000	-2.49203600	-2.87339500
H	-5.36206800	-1.59484000	1.09351500
H	-5.83471900	-2.10107400	-1.29590600
C	0.57508100	-2.61908700	0.35792800
C	-0.69494500	-3.10584400	0.80912900
H	1.29188700	-2.39352200	1.15019000
H	-1.13359500	-3.89503000	0.20498300
C	-0.96537000	-3.24736600	2.28657000
H	-2.02000000	-3.42974500	2.50106600
H	-0.40300600	-4.12365900	2.63562500
H	-0.62590100	-2.38009300	2.85859500
C	1.17392200	-3.23722300	-0.89752500
H	1.40628100	-4.28735000	-0.66313900
H	0.43255400	-3.26143300	-1.70404000
C	2.44494600	-2.58999300	-1.42812300
H	2.24832600	-1.55176600	-1.73143800
H	2.77519300	-3.13688400	-2.32313900
O	3.44452100	-2.64655300	-0.40674300
H	4.22478800	-2.17283600	-0.72769000

27

B3LYP SCF energy in DMF: -1619.953267 a.u.

M06 SCF energy in DMF: -1619.36435 a.u.

M06 Free energy in DMF: -1618.919246 a.u.

C	2.43196900	0.46374100	0.36293200
C	0.80937200	1.88949100	-0.46504400
C	1.72105900	2.92836200	-0.61520300
C	3.04929000	2.71254900	-0.25059300
C	3.40107200	1.46609200	0.25483300
H	2.69708500	-0.52540500	0.71454000
H	1.39490600	3.88794600	-0.99711000
H	3.78460900	3.50256300	-0.35219300
C	-0.62881800	2.06352100	-0.72147700
N	-1.51533700	1.22368900	-0.31310300
C	-2.47475000	2.97022900	-1.56651900
C	-2.83929600	1.86405300	-0.55318900
H	-2.61016200	2.65411400	-2.60465300
H	-3.51223700	1.12890900	-1.00041000
O	-1.03287600	3.16560100	-1.36009700
H	-2.96077000	3.93122500	-1.40889100
N	1.16330600	0.66337600	-0.00302800
C	-3.49713300	2.39157300	0.76735300
C	-3.64881600	1.24140200	1.77695800
H	-2.67865900	0.82436900	2.06452200
H	-4.13946300	1.60682700	2.68613500
H	-4.26205700	0.43292200	1.37022300
C	-4.90010800	2.92224600	0.40959200

H	-5.41119300	3.27085600	1.31350100
H	-4.86281200	3.76380300	-0.29038700
H	-5.51720000	2.13717700	-0.04262200
C	-2.66798400	3.51569500	1.41754400
H	-2.55837100	4.38884000	0.76643500
H	-3.16638400	3.85493800	2.33204300
H	-1.66792300	3.17163800	1.70395100
C	4.82102800	1.13473400	0.62853800
F	4.88608300	0.44345200	1.78424700
F	5.40725800	0.35517900	-0.32220700
F	5.58327700	2.23348700	0.75845700
Pd	-0.40823600	-0.81047600	-0.12073700
C	-1.65335600	-2.78112800	0.16190700
C	-1.93434800	-2.37554200	-1.17190300
C	-2.68250200	-2.64329200	1.12890000
C	-3.21198100	-1.88778200	-1.52203600
H	-1.23448500	-2.60351700	-1.96951300
C	-3.94028200	-2.18847600	0.76410700
H	-2.49988500	-2.94521300	2.15413400
C	-4.21094700	-1.80957200	-0.56434600
H	-3.41252900	-1.61496000	-2.55390100
H	-4.72697800	-2.13247400	1.51073600
H	-5.20433600	-1.46547900	-0.83673000
C	0.76599400	-2.49445000	0.03246000
C	-0.32117400	-3.49966600	0.44650200
H	1.42484000	-2.25018300	0.87222800
H	-0.28428700	-4.37771400	-0.21304600
C	-0.15448100	-3.98882300	1.88581500
H	-0.94179500	-4.69661100	2.16623900
H	0.80612400	-4.50394200	1.98818900
H	-0.16694100	-3.15927300	2.60188600
C	1.55240300	-2.93086300	-1.20345800
H	1.87340700	-3.96828600	-1.01269500
H	0.90006200	-2.98337400	-2.08315400
C	2.79151800	-2.13518000	-1.58588200
H	2.52818600	-1.09542600	-1.82818600
H	3.22677700	-2.57771600	-2.49363600
O	3.72985500	-2.19021600	-0.50611400
H	4.49379200	-1.64970900	-0.75235600

28

B3LYP SCF energy in DMF: -1619.94257 a.u.

M06 SCF energy in DMF: -1619.34856 a.u.

M06 Free energy in DMF: -1618.909265 a.u.

C	-2.10443800	-1.02205300	0.26846100
C	-0.16290200	-2.08475600	-0.41318100
C	-0.78700100	-3.32632300	-0.44603700
C	-2.13084800	-3.40556700	-0.08466300
C	-2.79246600	-2.23837600	0.28524400
H	-2.59589200	-0.09116600	0.52370600
H	-0.23230400	-4.20957100	-0.73856000
H	-2.64618000	-4.35919100	-0.09453300
C	1.26901600	-1.91053700	-0.70824700
N	1.93590800	-0.85865000	-0.37217900
C	3.22203700	-2.34408600	-1.67880700
C	3.36031700	-1.13248800	-0.73159800
H	3.19487700	-2.05772400	-2.73356600
H	3.75844400	-0.26629700	-1.26618100
O	1.90031900	-2.89418800	-1.35015100
H	3.95238100	-3.13717400	-1.53146100
N	-0.81590600	-0.94747200	-0.07660700
C	4.26964600	-1.39507800	0.51350200
C	4.22673300	-0.18276300	1.45592000
H	3.22856000	-0.03982200	1.87869200
H	4.92303200	-0.33048700	2.28877900
H	4.52163900	0.73514000	0.93584000
C	5.71550600	-1.57299000	0.00761100
H	6.39093300	-1.72196500	0.85681800
H	5.82514500	-2.44024300	-0.65222700
H	6.05592400	-0.68652800	-0.53997800
C	3.83209300	-2.64956200	1.29261900

H	3.90136600	-3.56270300	0.69266200
H	4.48283000	-2.78623300	2.16293300
H	2.80577200	-2.55986000	1.66537700
C	-4.23007000	-2.26608500	0.73559500
F	-4.88763300	-3.33066300	0.23565800
F	-4.32334500	-2.33372500	2.08245500
F	-4.89411100	-1.15593800	0.34948500
Pd	0.38396300	0.85247300	-0.28717000
C	-1.28706900	1.89836700	-0.63899000
C	-1.82492600	1.80289200	-1.92967500
C	-1.99197100	2.58462400	0.35805600
C	-3.06625500	2.38450900	-2.21740300
H	-1.29032200	1.27571700	-2.71577600
C	-3.23652900	3.15821400	0.06265200
H	-1.56967600	2.70481300	1.35152400
C	-3.77654400	3.05930900	-1.22139200
H	-3.47466400	2.30377800	-3.22174600
H	-3.77670500	3.68961000	0.84257600
H	-4.74012600	3.50819600	-1.44604000
C	1.84753200	2.41369500	-0.95929900
C	1.30228700	2.87787800	0.22760700
H	2.78514200	1.86128700	-0.89479100
H	0.48720200	3.59322900	0.16234800
C	1.99757400	2.80282700	1.56433600
C	1.51046600	2.94700500	-2.32594000
H	0.55688700	3.47850200	-2.34043600
H	2.29920100	3.65023800	-2.62692600
H	1.48931200	2.15347100	-3.07984200
H	2.83965800	2.11048800	1.51534700
C	1.12440300	2.42913500	2.75766400
H	0.67338900	1.43866800	2.59466300
H	1.76026300	2.36486100	3.65277200
H	2.41624700	3.80307400	1.75358300
O	0.11543900	3.42631900	2.92712000
H	-0.42447000	3.16614300	3.68743000

TS20

B3LYP SCF energy in DMF: -1619.92251 a.u.

M06 SCF energy in DMF: -1619.334288 a.u.

M06 Free energy in DMF: -1618.894425 a.u.

C	-2.20668200	-0.99353100	0.09619100
C	-0.38469000	-2.33391000	-0.37339500
C	-1.17468300	-3.47325500	-0.48681600
C	-2.54876600	-3.34875500	-0.28648600
C	-3.06843100	-2.09168300	0.01027300
H	-2.58068500	-0.00088900	0.31661200
H	-0.72750100	-4.43051100	-0.72564100
H	-3.19719600	-4.21410800	-0.36687300
C	1.07805400	-2.35761600	-0.53198100
N	1.81687300	-1.31403900	-0.35795700
C	3.08124300	-3.15574300	-1.09010800
C	3.23609900	-1.76047900	-0.44140000
H	3.22673000	-3.13653500	-2.17327800
H	3.77754800	-1.08630800	-1.10972000
O	1.67366000	-3.50558700	-0.85127300
H	3.68915000	-3.94388900	-0.65033000
N	-0.89143900	-1.11228500	-0.08879900
C	3.96663000	-1.76372100	0.94287700
C	3.97801400	-0.34565200	1.53903300
H	2.96605500	0.01960500	1.73723800
H	4.52645000	-0.34589300	2.48763100
H	4.47751800	0.36300400	0.86929400
C	5.42561400	-2.20013500	0.69843000
H	5.98759400	-2.16221300	1.63766300
H	5.49896400	-3.22303100	0.31482200
H	5.92309300	-1.53485700	-0.01673000
C	3.29448600	-2.72460900	1.94093300
H	3.28953700	-3.76037200	1.58504200
H	3.84127100	-2.71279600	2.88996800
H	2.26126300	-2.43031200	2.15619900
C	-4.53842500	-1.90671600	0.28164900

F	-5.28478900	-2.80218600	-0.39618500
F	-4.82379600	-2.06384500	1.59411000
F	-4.96050200	-0.67301100	-0.06840500
Pd	0.64882100	0.51329500	-0.25069000
C	-0.72469100	2.07476400	-0.09792500
C	-1.53377300	2.33580400	-1.21966700
C	-1.27057200	2.23234000	1.18805900
C	-2.87331500	2.69646200	-1.05640700
H	-1.11750300	2.26319100	-2.22100600
C	-2.61363600	2.59062900	1.34691400
H	-0.65450300	2.07396500	2.06865700
C	-3.41713600	2.82246400	0.22650300
H	-3.48880200	2.88893400	-1.93116200
H	-3.02622600	2.69690000	2.34665800
H	-4.45662100	3.11179900	0.35190300
C	2.13206800	1.89723000	-0.70440900
C	1.19295100	2.92311700	-0.37956000
H	2.90867200	1.72111100	0.03973600
H	0.78323900	3.45926300	-1.22983200
C	1.40537700	3.78471600	0.85417300
C	2.57482600	1.71442400	-2.14341400
H	1.74902300	1.86339600	-2.84639300
H	3.35232500	2.45372200	-2.38405900
H	3.00494700	0.72399500	-2.31648800
H	1.30575300	3.20695800	1.77706700
C	0.53427000	5.03333700	0.91564800
H	-0.52892300	4.76921000	0.97093600
H	0.78430000	5.59214500	1.83031600
H	2.45212800	4.11609800	0.81207600
O	0.80682200	5.81265300	-0.25122800
H	0.15754700	6.52907600	-0.28165000

29

B3LYP SCF energy in DMF: -1619.958068 a.u.

M06 SCF energy in DMF: -1619.371217 a.u.

M06 Free energy in DMF: -1618.93134 a.u.

C	-2.58411100	0.21890400	0.06834300
C	-1.59260100	-1.74988200	-0.60271500
C	-2.81290000	-2.31621300	-0.95892400
C	-3.97058100	-1.56011400	-0.78251000
C	-3.85172800	-0.27617000	-0.25890000
H	-2.46032800	1.21727100	0.46978300
H	-2.85553700	-3.31984000	-1.36428400
H	-4.93937000	-1.96651700	-1.05092300
C	-0.32256700	-2.48246600	-0.71900600
N	0.82639300	-1.96506900	-0.43444700
C	1.04468600	-4.16959700	-1.22219700
C	1.82695800	-3.07053100	-0.46819400
H	1.27733800	-4.19526100	-2.28985700
H	2.68778500	-2.75226100	-1.05793800
O	-0.35907100	-3.75900900	-1.09604300
H	1.12762800	-5.17047300	-0.80269400
N	-1.47402900	-0.50000500	-0.09962000
C	2.33866800	-3.48082100	0.95134300
C	3.03314400	-2.28421600	1.62569700
H	2.33517000	-1.46143600	1.80451100
H	3.44670400	-2.59154000	2.59276200
H	3.86032800	-1.90736900	1.01414400
C	3.37825500	-4.60502100	0.76570500
H	3.80048600	-4.88474000	1.73671100
H	2.94482900	-5.50973400	0.32662600
H	4.20444400	-4.28030500	0.12276000
C	1.19100000	-3.97553500	1.85141100
H	0.67801200	-4.84704800	1.43092800
H	1.58849000	-4.27464100	2.82731100
H	0.44632600	-3.19162700	2.02991400
C	-5.06869800	0.56955600	0.00770000
F	-6.08539900	0.25965600	-0.82167400
F	-5.52027200	0.40096100	1.27155800
F	-4.80455100	1.88543200	-0.14292400
Pd	0.74758800	0.15029000	-0.06005700

C	1.08729500	2.43352500	0.20804900
C	0.03704100	3.18177600	-0.38644800
C	0.93410800	2.01754000	1.55762200
C	-1.08625400	3.53645300	0.34603500
H	0.14645000	3.51153900	-1.41589500
C	-0.22217400	2.36431600	2.28410400
H	1.76289800	1.54939900	2.07991700
C	-1.21580600	3.12983700	1.68741300
H	-1.86757400	4.13325000	-0.11553800
H	-0.31316500	2.05711700	3.32177300
H	-2.09535000	3.41846400	2.25585100
C	2.68324100	0.71023700	-0.44259400
C	2.42044300	2.21364000	-0.51986700
H	3.26104200	0.43398400	0.44537100
H	2.26534300	2.49143700	-1.56717400
C	3.57304600	3.07993600	0.03321400
C	3.24879500	0.10050500	-1.70912100
H	2.56495700	0.21363100	-2.55831000
H	4.18167300	0.61997500	-1.97821400
H	3.49340500	-0.95773500	-1.59656000
H	3.70188400	2.88762000	1.10529200
C	3.37445500	4.57624100	-0.17241600
H	2.45240100	4.90910700	0.32827100
H	4.21056600	5.11827100	0.29594600
H	4.50354500	2.77527600	-0.46234600
O	3.31643500	4.84056900	-1.57482300
H	3.10481800	5.77804500	-1.68519500

TS21

B3LYP SCF energy in DMF: -1619.939941 a.u.

M06 SCF energy in DMF: -1619.351252 a.u.

M06 Free energy in DMF: -1618.911853 a.u.

C	2.66328400	-0.11557400	0.12919000
C	1.29033100	-1.97258500	0.26293500
C	2.37368400	-2.84690500	0.26199300
C	3.65717600	-2.31010700	0.18184500
C	3.80162100	-0.92585300	0.11075500
H	2.73817500	0.96478300	0.08188600
H	2.21686700	-3.91737200	0.31601700
H	4.52488100	-2.96064900	0.17114400
C	-0.10846300	-2.42915700	0.31635100
N	-1.11910100	-1.64595000	0.13207700
C	-1.79516300	-3.81548000	0.76434300
C	-2.34232600	-2.50011400	0.16307700
H	-1.97065300	-3.89427100	1.84053400
H	-3.06928600	-2.04208200	0.83883000
O	-0.34376100	-3.71748600	0.57034700
H	-2.12818800	-4.72616400	0.27038400
N	1.43361400	-0.62999700	0.20328600
C	-3.01534100	-2.65672200	-1.23774200
C	-3.43643800	-1.27395200	-1.75785600
H	-2.56927000	-0.63101400	-1.93028100
H	-3.97330700	-1.37460700	-2.70772100
H	-4.10341000	-0.77120100	-1.04968300
C	-4.27975000	-3.52143000	-1.06253500
H	-4.80950700	-3.60355800	-2.01772700
H	-4.04957000	-4.53923100	-0.73076200
H	-4.96895100	-3.07647700	-0.33532800
C	-2.06813400	-3.31631400	-2.25660700
H	-1.76690700	-4.32527900	-1.95555800
H	-2.57080100	-3.40473000	-3.22571000
H	-1.16229000	-2.71986700	-2.41132900
C	5.16838800	-0.29500600	0.07166800
F	6.04746700	-1.05441500	-0.61323500
F	5.14111700	0.92352500	-0.50754500
F	5.67177800	-0.13122800	1.31642100
Pd	-0.48477900	0.45750600	0.41282800
C	-1.18853200	3.06477100	-0.89581200
C	-0.54914700	4.28697600	-0.64075500
C	-0.62365800	2.20383900	-1.85787200
C	0.62292400	4.64031600	-1.31452200

H	-0.97947600	4.97036100	0.08701000
C	0.55229800	2.55615300	-2.53090200
H	-1.12619600	1.27527900	-2.11681400
C	1.18079300	3.77301700	-2.25823300
H	1.09677000	5.59586200	-1.10662800
H	0.96726300	1.88231700	-3.27580100
H	2.08882300	4.04984700	-2.78643600
C	-2.12303300	1.57640800	0.90691700
C	-2.44967600	2.66253900	-0.13057500
H	-2.97405300	0.94291000	1.16562200
H	-2.76231300	3.54155200	0.45124100
C	-3.61918600	2.30794500	-1.05964000
H	-4.50482500	2.04128900	-0.47254500
H	-3.87858400	3.16853400	-1.68543200
H	-3.38658500	1.47206600	-1.72208400
C	-1.28917200	2.02774400	2.07565300
H	-0.18876100	1.77042300	1.87706000
C	-1.64808100	1.40853100	3.42127800
H	-1.68191300	0.31265800	3.32562400
H	-0.87203600	1.65679700	4.16033500
H	-1.23772300	3.12149800	2.14680200
O	-2.91396900	1.93372900	3.81009200
H	-3.12774400	1.56156400	4.67769900

30

B3LYP SCF energy in DMF: -1619.941098 a.u.

M06 SCF energy in DMF: -1619.350704 a.u.

M06 Free energy in DMF: -1618.911759 a.u.

C	-2.66546700	-0.78455400	-0.11035100
C	-2.03277300	1.41328900	0.23554900
C	-3.34627700	1.86768500	0.17419100
C	-4.35494600	0.93435700	-0.05748600
C	-4.00781700	-0.40686100	-0.20745200
H	-2.35989800	-1.81990700	-0.20856900
H	-3.57366300	2.91999600	0.29410200
H	-5.39012700	1.25071700	-0.12429900
C	-0.87793500	2.30835800	0.41842100
N	0.34755000	1.93201400	0.23689700
C	0.22347000	4.12118900	1.08634400
C	1.18763200	3.16607300	0.35417500
H	0.33951500	4.09377100	2.17321600
H	2.06097200	2.94145100	0.97027000
O	-1.10405300	3.56869000	0.78180600
H	0.23409600	5.15155200	0.73800600
N	-1.69909600	0.11140100	0.10381400
C	1.67933300	3.71066700	-1.02886600
C	2.54682100	2.65718300	-1.73240400
H	1.99299900	1.73254600	-1.92131600
H	2.89527300	3.04101700	-2.69765200
H	3.43039900	2.41761600	-1.13382200
C	2.55199400	4.95351500	-0.75732200
H	2.97073900	5.32548800	-1.69848500
H	1.98578500	5.77492800	-0.30626300
H	3.38901600	4.71423300	-0.09115200
C	0.50448900	4.09370100	-1.94822900
H	-0.13466900	4.86807600	-1.51198500
H	0.89176100	4.48933700	-2.89315100
H	-0.12182000	3.22841600	-2.19183700
C	-5.07098600	-1.45152300	-0.42212200
F	-6.07365100	-0.98507500	-1.19475100
F	-4.57616200	-2.55697300	-1.01595900
F	-5.62394500	-1.84184900	0.74859200
Pd	0.43850000	-0.23927800	0.56276000
C	2.91300000	-2.21782100	-0.76950700
C	3.26963200	-3.57141500	-0.84226600
C	2.11799900	-1.68408200	-1.79852500
C	2.84058300	-4.37427300	-1.90417400
H	3.89221800	-4.00106700	-0.06097900
C	1.68612600	-2.48245900	-2.86002500
H	1.84243600	-0.63238700	-1.77217300
C	2.04490000	-3.83282800	-2.91556300

H	3.13099900	-5.42084400	-1.93977200
H	1.07483500	-2.04833900	-3.64706500
H	1.71225800	-4.45358500	-3.74289900
C	2.26004500	-0.87456500	1.31289500
C	3.38825200	-1.34891900	0.39043900
H	2.60292100	-0.13491800	2.04042900
H	4.00079900	-1.99502200	1.03848000
C	4.30298200	-0.20991600	-0.08192200
H	4.61720100	0.41233500	0.76377100
H	5.20278600	-0.61650900	-0.55493900
H	3.80355600	0.42905800	-0.81101000
C	1.35612500	-1.91919400	1.86321500
H	0.30405500	-1.86903700	1.32620700
C	1.04450200	-1.84690900	3.35516400
H	0.75126100	-0.82074900	3.62171800
H	0.20177000	-2.51242500	3.59194200
H	1.63564300	-2.93255500	1.55509500
O	2.22656500	-2.24723500	4.03956300
H	2.02032700	-2.27104600	4.98522600

TS22

B3LYP SCF energy in DMF: -1619.931111 a.u.

M06 SCF energy in DMF: -1619.341438 a.u.

M06 Free energy in DMF: -1618.906151 a.u.

C	-2.68391000	-0.10719600	0.11858000
C	-1.53398300	1.90271500	0.16457900
C	-2.70237900	2.64111200	0.01758700
C	-3.91117300	1.95541000	-0.09938100
C	-3.89807200	0.56450900	-0.05247400
H	-2.63844300	-1.18782700	0.18063400
H	-2.66780800	3.72339000	-0.00979200
H	-4.84166000	2.49839200	-0.22000600
C	-0.20075500	2.51973900	0.26309900
N	0.89712500	1.84710600	0.18007600
C	1.28279900	4.11357400	0.72773400
C	2.01142700	2.84001900	0.23892000
H	1.37912100	4.27104100	1.80501600
H	2.73660800	2.50179900	0.98377200
O	-0.13302300	3.83630100	0.45855900
H	1.54112200	5.02871800	0.19838800
N	-1.52586300	0.55089700	0.22249500
C	2.75779000	3.00719400	-1.12275300
C	3.36871300	1.66022300	-1.53290300
H	2.59526000	0.90859200	-1.71300900
H	3.94864200	1.77170600	-2.45575400
H	4.04326200	1.28229000	-0.75774000
C	3.90126400	4.02112100	-0.91719500
H	4.48297300	4.11706100	-1.84030300
H	3.53570500	5.02013000	-0.65739300
H	4.58423300	3.69464100	-0.12428200
C	1.81528900	3.49852000	-2.23645100
H	1.38018500	4.47910000	-2.01531600
H	2.37191500	3.59573600	-3.17484500
H	0.99728900	2.79183300	-2.41418800
C	-5.16179100	-0.24036400	-0.21259100
F	-6.26227900	0.50186100	0.01488700
F	-5.26805500	-0.74665600	-1.46161800
F	-5.19129700	-1.28842700	0.63889100
Pd	0.41221600	-0.32605000	0.61864600
C	1.87023000	-2.98307800	-0.85658400
C	1.44003500	-4.30736200	-0.69779800
C	1.35966400	-2.24230500	-1.93686400
C	0.51731300	-4.87739200	-1.58139900
H	1.83576800	-4.90085000	0.12286500
C	0.44107200	-2.80923200	-2.82286100
H	1.68772100	-1.21891900	-2.09427700
C	0.01291800	-4.12897700	-2.64626600
H	0.20107600	-5.90732500	-1.43946300
H	0.06327400	-2.22135300	-3.65539100
H	-0.69917200	-4.57026200	-3.33804900
C	2.24306200	-1.41550800	1.14787800

C	2.87052100	-2.37545600	0.12341800
H	2.89835200	-0.62890900	1.52177700
H	3.24377300	-3.20717800	0.73778300
C	4.09626500	-1.77551800	-0.58155100
H	4.80204700	-1.37192300	0.15275600
H	4.61549900	-2.55126600	-1.15346500
H	3.82768100	-0.97438900	-1.27152300
C	1.22414400	-1.87097000	2.00955400
H	-0.18010200	-1.66386600	1.10115000
C	1.03193900	-1.31494300	3.40597300
H	-0.02901000	-1.35269400	3.68513800
H	1.36034300	-0.26678200	3.44660900
H	0.90865100	-2.91006900	1.90919900
O	1.81833600	-2.14234900	4.26491500
H	1.55280500	-1.94619400	5.17526100

31

B3LYP SCF energy in DMF: -1619.946871 a.u.

M06 SCF energy in DMF: -1619.348878 a.u.

M06 Free energy in DMF: -1618.911012 a.u.

C	-2.80144500	-0.34103900	0.34217200
C	-1.76844500	1.70044500	-0.04490600
C	-2.97630300	2.31480600	-0.35450000
C	-4.14071500	1.54920000	-0.32152000
C	-4.04738700	0.20319600	0.02304700
H	-2.69292400	-1.37907400	0.62777500
H	-3.00197200	3.36359200	-0.62333400
H	-5.09813900	1.99615300	-0.56605500
C	-0.47749800	2.40778600	-0.10579700
N	0.65953900	1.81523000	0.02541500
C	0.89979900	4.15669500	-0.17666600
C	1.71204300	2.84009800	-0.23295300
H	0.97740700	4.66165200	0.78944000
H	2.43855100	2.80666700	0.58279000
O	-0.49457100	3.72219700	-0.32489300
H	1.10564900	4.86373800	-0.97810000
N	-1.68499300	0.39548400	0.30788500
C	2.48496800	2.60562700	-1.57096300
C	3.17299500	1.23067000	-1.53725000
H	2.44354000	0.41726200	-1.50542100
H	3.78339900	1.09509600	-2.43696500
H	3.83601000	1.13757700	-0.66936100
C	3.57103300	3.69448800	-1.68423800
H	4.16426800	3.53406100	-2.59085400
H	3.15048500	4.70371900	-1.74566100
C	4.25516400	3.66496800	-0.82812700
H	1.54875300	2.67034600	-2.79140500
H	1.06433000	3.64689000	-2.89672000
H	2.12272000	2.49540300	-3.70776800
H	0.76875700	1.90250900	-2.74323400
C	-5.27945000	-0.66084000	0.10184100
F	-6.18790700	-0.30926800	-0.82999800
F	-4.98632000	-1.96487500	-0.08076700
F	-5.88271900	-0.55281900	1.30615500
Pd	0.25687700	-0.25200400	0.91259100
C	1.79144100	-3.03307400	-0.55017400
C	0.60303500	-3.74162900	-0.77920200
C	2.55754700	-2.64030300	-1.65933600
C	0.18477400	-4.04584300	-2.07796000
H	0.00317000	-4.06449200	0.06843100
C	2.14104800	-2.94013900	-2.95849400
H	3.48893900	-2.10063400	-1.51119100
C	0.95211700	-3.64327600	-3.17326500
H	-0.73669500	-4.60125600	-2.23124500
H	2.74939900	-2.62935800	-3.80374000
H	0.63191200	-3.88092200	-4.18388900
C	2.24786200	-1.23128400	1.18132300
C	2.23266900	-2.72037700	0.87575200
H	2.89532000	-0.62760300	0.54687000
H	1.52085500	-3.19645900	1.55819100
C	3.63673900	-3.29149900	1.18393700

H	3.89532300	-3.12657200	2.23491900
H	3.65604200	-4.36874300	0.98946700
H	4.40917000	-2.82060600	0.56740800
C	1.84322000	-0.69510700	2.39592600
H	-0.30966900	-1.53452600	1.48450000
C	2.36703600	0.61097000	2.95493400
H	1.57070700	1.16021400	3.47454600
H	1.40716300	-1.36747500	3.13524400
O	3.46698700	0.35344900	3.83181800
H	3.10699000	-0.03945400	4.64125400
H	2.75412200	1.24284100	2.15279400

32

B3LYP SCF energy in DMF: -1619.946749 a.u.

M06 SCF energy in DMF: -1619.350254 a.u.

M06 Free energy in DMF: -1618.912433 a.u.

C	-2.66180200	-0.26490300	0.86931700
C	-1.38065500	-1.35229900	-0.73258900
C	-2.50628700	-1.88351700	-1.35052700
C	-3.76031900	-1.59271000	-0.81528300
C	-3.83513300	-0.77751500	0.31039100
H	-2.68207200	0.37889700	1.73916300
H	-2.40386700	-2.51589400	-2.22383400
H	-4.65748000	-2.00108800	-1.26701800
C	-0.00970200	-1.64607200	-1.18653200
N	1.04115600	-1.26903400	-0.54281100
C	1.59309900	-2.36538000	-2.55669200
C	2.21347700	-1.89119200	-1.21962200
H	1.77875200	-1.67249500	-3.38106100
H	2.96566100	-1.11823400	-1.39872000
O	0.14615200	-2.35603200	-2.30272900
H	1.85932000	-3.37617200	-2.86048200
N	-1.45917600	-0.55202300	0.35890000
C	2.87959700	-3.02519200	-0.37276500
C	3.40217000	-2.45023400	0.95483500
H	2.58988900	-2.06443100	1.57762200
H	3.91448600	-3.23395400	1.52386600
H	4.12226900	-1.64223500	0.78292800
C	4.08131300	-3.56668900	-1.17368500
H	4.61291400	-4.32080500	-0.58346200
H	3.78110100	-4.04163500	-2.11332400
H	4.79199800	-2.76694100	-1.41262900
C	1.89131900	-4.16715800	-0.07303700
H	1.51338300	-4.64304600	-0.98422000
H	2.39073100	-4.94531800	0.51409100
H	1.03384900	-3.81666200	0.51191200
C	-5.16906200	-0.40316100	0.90295500
F	-6.07518600	-1.38721300	0.73730100
F	-5.07541300	-0.14855200	2.22425400
F	-5.67477800	0.70610300	0.31952000
Pd	0.40843800	0.24703900	1.01073600
C	1.11574700	2.81687300	-1.23418100
C	0.83244600	2.17597700	-2.44831600
C	0.33867600	3.92767200	-0.86786300
C	-0.20301900	2.62395900	-3.27378600
H	1.43305100	1.32276200	-2.75332700
C	-0.69838800	4.37559500	-1.68871400
H	0.54468600	4.45147100	0.06222600
C	-0.97477700	3.72426000	-2.89462100
H	-0.40215100	2.11446700	-4.21287900
H	-1.28790300	5.23771900	-1.38837700
H	-1.77957800	4.07585800	-3.53414200
C	1.82933100	1.98884100	1.05397400
C	2.26262500	2.32181200	-0.35937800
H	1.31706900	2.78602200	1.59015300
H	2.67243400	1.41435500	-0.81540600
C	3.40338800	3.36673600	-0.27749000
H	4.25198600	2.96966900	0.28861100
H	3.74879000	3.62182100	-1.28439400
H	3.06572900	4.28686000	0.21025900
C	2.33551200	0.92881000	1.79493400

C	2.33514000	0.90682200	3.30452500
H	1.55788000	1.58026800	3.69404500
H	3.06987000	0.27704800	1.32719500
H	-0.27250700	1.14090200	2.03129800
H	2.11995400	-0.10613500	3.67072700
O	3.63997500	1.32466700	3.71645400
H	3.73895800	1.08040500	4.64811300

TS23

B3LYP SCF energy in DMF: -1619.94049 a.u.

M06 SCF energy in DMF: -1619.346102 a.u.

M06 Free energy in DMF: -1618.909305 a.u.

C	1.89056400	-1.39388200	-0.69231900
C	0.09351500	-2.16082300	0.55345500
C	0.76809100	-3.31811500	0.92294300
C	2.06215200	-3.51405300	0.44178800
C	2.62456500	-2.54242400	-0.38102800
H	2.30483200	-0.60798300	-1.31145000
H	0.29227700	-4.04887900	1.56572700
H	2.61619000	-4.40751600	0.70660800
C	-1.28990500	-1.86967300	0.96429700
N	-1.97223200	-0.89205000	0.47039800
C	-3.13433700	-1.98778100	2.20604100
C	-3.34527000	-0.98857200	1.04387500
H	-3.00098200	-1.49407400	3.17187000
H	-3.62983300	-0.00624000	1.42975700
O	-1.86111200	-2.64607400	1.88213500
H	-3.88970700	-2.76658700	2.29180400
N	0.64908600	-1.20869900	-0.23360300
C	-4.42056100	-1.42868300	-0.00084700
C	-4.46436200	-0.41600400	-1.15581200
H	-3.52728800	-0.41076900	-1.71981300
H	-5.27139700	-0.67361700	-1.85051800
H	-4.65298900	0.59833700	-0.78718900
C	-5.79010000	-1.42638300	0.70780000
H	-6.57990900	-1.68488800	-0.00555900
H	-5.83911300	-2.15256300	1.52614100
H	-6.02218300	-0.43737800	1.11968500
C	-4.12668400	-2.82960300	-0.56782200
H	-4.12786500	-3.60329000	0.20716400
H	-4.89744500	-3.10211700	-1.29676600
H	-3.16197000	-2.86284500	-1.08614700
C	3.99653300	-2.72667500	-0.97682700
F	4.76662100	-3.52969200	-0.21643700
F	3.92771700	-3.28582300	-2.20560600
F	4.64190700	-1.54932200	-1.11473900
Pd	-0.56617400	0.55238400	-0.47233700
C	-0.34103100	2.81913900	-0.53213200
C	0.23772100	3.32975200	0.77974800
H	0.13841700	3.21131800	-1.42922000
H	-0.29405800	2.83797200	1.60072900
C	-0.05700700	4.84709300	0.86456000
H	-1.13404400	5.03673500	0.81817200
H	0.32113700	5.24879900	1.80968700
H	0.42260400	5.39326000	0.04581900
C	-1.67264700	2.37908800	-0.66675300
C	-2.36807700	2.51885000	-2.00049000
H	-1.64103700	2.38489400	-2.81574900
H	-3.14702100	1.75860800	-2.11424200
H	-2.31622500	2.41859300	0.21217700
H	0.59190200	1.40999100	-1.01862100
C	1.72455400	3.04129700	0.93933800
C	2.18667600	2.33330300	2.05749400
C	2.66260600	3.48648800	-0.00564700
C	3.54899000	2.06940200	2.22759900
H	1.47377800	1.98882900	2.80310600
C	4.02368300	3.22218700	0.16042700
H	2.33095100	4.04656000	-0.87633000
C	4.47222400	2.51181200	1.27791300
H	3.88640000	1.52036200	3.10262700
H	4.73491000	3.57535500	-0.58147400

H	5.53154600	2.30844100	1.40761600
O	-2.93989300	3.83285100	-2.03435900
H	-3.51538700	3.87115400	-2.81246300

33

B3LYP SCF energy in DMF: -1619.950879 a.u.

M06 SCF energy in DMF: -1619.359537 a.u.

M06 Free energy in DMF: -1618.920977 a.u.

C	1.47256600	-1.70493600	-0.45108800
C	-0.56988700	-2.27728800	0.47225200
C	-0.12858500	-3.54854900	0.81787200
C	1.18789000	-3.89744600	0.51119700
C	1.99576200	-2.96253400	-0.12871500
H	2.07450700	-0.95410500	-0.95006900
H	-0.79052000	-4.24417000	1.31932600
H	1.57073700	-4.87826500	0.76966000
C	-1.93081700	-1.78707000	0.74198100
N	-2.31728000	-0.59835800	0.40892900
C	-3.98801700	-1.73521000	1.59242700
C	-3.78568300	-0.52736100	0.65105200
H	-3.95068400	-1.45901800	2.64933600
H	-4.01377900	0.40807000	1.16691300
O	-2.81391200	-2.58645600	1.33037100
H	-4.87334400	-2.33690300	1.39744100
N	0.21624100	-1.37052900	-0.15548800
C	-4.62386500	-0.58715000	-0.67001000
C	-4.24340600	0.58448300	-1.59084000
H	-3.18997500	0.54533700	-1.88525000
H	-4.84717800	0.55030000	-2.50457400
H	-4.43094500	1.54761800	-1.10674700
C	-6.11008700	-0.44489100	-0.28357500
H	-6.73029400	-0.42537900	-1.18605700
H	-6.46213300	-1.27604500	0.33662100
H	-6.28960100	0.48640800	0.26587100
C	-4.40695000	-1.91070900	-1.42732200
H	-4.70904100	-2.78473300	-0.84106300
H	-5.00872500	-1.91353800	-2.34248900
H	-3.36154000	-2.04197400	-1.72761600
C	3.44318700	-3.24921800	-0.43156400
F	3.70238700	-4.57063400	-0.44931200
F	3.81003100	-2.74172600	-1.62715700
F	4.25662200	-2.69359200	0.49751300
Pd	-0.68329100	0.64751400	-0.10595500
C	2.77829200	2.60610500	0.48311700
C	3.32886500	1.45775200	1.07245600
C	3.49977900	3.23877000	-0.54157600
C	4.55986800	0.94852200	0.64891100
H	2.78608900	0.95715100	1.87126300
C	4.73338900	2.73682900	-0.96288200
H	3.09894700	4.12924700	-1.01785300
C	5.26682800	1.58813400	-0.37169100
H	4.95932200	0.04954400	1.11023000
H	5.27730000	3.24295700	-1.75604500
H	6.22477900	1.19700700	-0.70304400
C	0.32772800	2.72137900	-0.13775600
C	1.40084200	3.09597800	0.91422400
H	0.45239600	3.26803400	-1.07877200
H	1.13720500	2.56710000	1.83744200
C	1.34783700	4.60647500	1.19495800
H	0.35527400	4.89599700	1.55213600
H	2.08341500	4.87904500	1.95845200
H	1.55890900	5.19395900	0.29534400
C	-1.08732700	2.62167700	0.28635700
C	-2.13405800	3.34205900	-0.52721100
H	-2.00692900	3.12687500	-1.59837300
H	-3.13401500	3.00569200	-0.22571000
H	-1.25574300	2.70677600	1.36336600
H	0.69288600	1.63954200	-0.51967600
O	-1.97929800	4.74495900	-0.27150800
H	-2.65925500	5.20477600	-0.78596900

TS24

B3LYP SCF energy in DMF: -1619.941523 a.u.

M06 SCF energy in DMF: -1619.346302 a.u.

M06 Free energy in DMF: -1618.9085 a.u.

C	2.84064200	-0.84315800	0.60763000
C	2.11001300	0.73939500	-0.91324200
C	3.31237400	0.71061600	-1.61284100
C	4.31901600	-0.14186800	-1.16162500
C	4.07845300	-0.92861400	-0.03775300
H	2.61722700	-1.44009400	1.48518900
H	3.45979400	1.33607700	-2.48482500
H	5.27083300	-0.18854400	-1.67878900
C	0.98014100	1.60284800	-1.29829600
N	-0.08490400	1.75105300	-0.57923000
C	-0.27270900	2.85340100	-2.65591800
C	-0.95689000	2.74865200	-1.27030800
H	-0.77647200	2.26082300	-3.42344700
H	-1.95637200	2.31848000	-1.37204900
O	1.05286100	2.25724900	-2.45457800
H	-0.11721000	3.86747800	-3.01844800
N	1.87878500	-0.02447700	0.17788800
C	-1.09181400	4.10840800	-0.51326600
C	-1.81342400	3.89259900	0.82627600
H	-1.26462100	3.23034900	1.49753200
H	-1.94266600	4.85380100	1.33742600
H	-2.81187500	3.46680300	0.67245600
C	-1.95874700	5.04514100	-1.38075200
H	-2.15719700	5.97394400	-0.83532000
H	-1.47410900	5.32042500	-2.32301100
H	-2.92560200	4.58601100	-1.61825600
C	0.28338300	4.75272700	-0.26018900
H	0.83161200	4.94460600	-1.18934300
H	0.15597100	5.71659300	0.24414000
H	0.91031500	4.12576200	0.38330300
C	5.10754300	-1.91281300	0.45306300
F	6.36170000	-1.51025700	0.16564500
F	5.03039900	-2.09305300	1.78826000
F	4.93841100	-3.12620300	-0.11974300
Pd	-0.18812100	0.23563800	0.94287500
C	-3.21128800	-2.64250800	-0.64672100
C	-2.58594200	-2.91552400	-1.87215700
C	-3.78074100	-3.71450700	0.06044400
C	-2.52645700	-4.21717100	-2.37870900
H	-2.14544000	-2.09792100	-2.43871900
C	-3.72273100	-5.01613500	-0.44146700
H	-4.27537500	-3.53242100	1.01117900
C	-3.09503200	-5.27324100	-1.66400900
H	-2.03741700	-4.40309300	-3.33139500
H	-4.16995400	-5.83094600	0.12190400
H	-3.05117200	-6.28624200	-2.05439600
C	-2.44984400	-1.09316300	1.20884800
C	-3.25872900	-1.22012600	-0.10361200
H	-2.96996700	-1.61234200	2.02829800
H	-2.77779100	-0.57319000	-0.84780700
C	-4.70477500	-0.72851000	0.08794200
H	-4.72419400	0.31029800	0.43426800
H	-5.26113400	-0.77915600	-0.85382900
H	-5.23744300	-1.33675500	0.82726700
C	-2.08618800	0.32164900	1.62013300
C	-1.91992300	0.47756200	3.11526000
H	-2.87068800	0.19746600	3.60332700
H	-1.16472600	-0.24713700	3.47682900
H	-2.67999300	1.11612300	1.16612600
H	-1.50082100	-1.67567900	1.10693200
O	-1.54965600	1.81022200	3.45186400
H	-1.43531900	1.84497900	4.41244400

34

B3LYP SCF energy in DMF: -1619.951635 a.u.

M06 SCF energy in DMF: -1619.359852 a.u.

M06 Free energy in DMF: -1618.922238 a.u.

C	-3.21463400	0.82531000	0.35722400
C	-2.09405700	-0.50548100	-1.16662500
C	-3.10307900	-0.37820900	-2.11483300
C	-4.21841900	0.39349400	-1.79210700
C	-4.27385500	0.99967900	-0.53902100
H	-3.22521300	1.28378700	1.33894700
H	-3.01899100	-0.86813700	-3.07744700
H	-5.02725300	0.51406800	-2.50461800
C	-0.88157300	-1.31158600	-1.38101700
N	0.05424800	-1.40075000	-0.49526900
C	0.61194700	-2.57610200	-2.44580700
C	1.01025600	-2.44403400	-0.95762800
H	1.24017100	-1.97105700	-3.10437600
H	2.02589000	-2.05360000	-0.86811500
O	-0.74438600	-2.00640900	-2.50623600
H	0.55266500	-3.59465800	-2.82401100
N	-2.14608700	0.08713600	0.04909200
C	0.92177000	-3.76759000	-0.12787000
C	1.21885400	-3.47792000	1.35447900
H	0.46212700	-2.82385700	1.79836000
H	1.22720200	-4.41554500	1.92129200
H	2.19847400	-3.00427600	1.48064800
C	2.00272400	-4.72666200	-0.66636300
H	2.00542700	-5.65215500	-0.08052900
H	1.83293800	-5.00349100	-1.71225000
H	3.00175600	-4.28182900	-0.59271000
C	-0.46536200	-4.42593900	-0.24422700
H	-0.71213400	-4.70284800	-1.27464800
H	-0.48886300	-5.34553900	0.35049700
H	-1.25829600	-3.77277200	0.13644900
C	-5.44062800	1.87655800	-0.16647900
F	-6.60421000	1.37154300	-0.62565800
F	-5.55584600	2.02209200	1.16963300
F	-5.31158300	3.11511200	-0.69274500
Pd	-0.20744900	-0.05300900	1.12279700
C	4.01312600	1.70145700	-0.58017900
C	3.66624500	1.98860200	-1.90841000
C	5.03361200	2.46072300	0.01625600
C	4.31422000	3.00090300	-2.62232200
H	2.88227300	1.40883500	-2.39110300
C	5.68250200	3.47379800	-0.69237200
H	5.32647400	2.25947600	1.04345900
C	5.32577300	3.74813300	-2.01591700
H	4.02873900	3.20279100	-3.65144600
H	6.46928100	4.04879000	-0.21091200
H	5.83211400	4.53535800	-2.56774500
C	2.53411100	1.16714000	1.39694700
C	3.29964300	0.59144200	0.18280600
H	3.26807700	1.51364300	2.14168200
H	2.55846400	0.16008800	-0.49984000
C	4.28043200	-0.52187100	0.59339700
H	3.76527700	-1.34835300	1.09279900
H	4.79582300	-0.93061600	-0.28221000
H	5.04271500	-0.14251400	1.28343200
C	1.58199600	0.21585600	2.10697500
C	0.66700900	0.82998800	3.08284800
H	0.86479700	1.88940800	3.29070500
H	-0.40828500	1.00300000	2.50293400
H	2.00885300	-0.73248600	2.43266300
H	1.97812500	2.06000700	1.08446400
O	0.43895500	0.06358300	4.22462000
H	-0.19057000	0.53595400	4.79152200

TS25

B3LYP SCF energy in DMF: -1619.948171 a.u.

M06 SCF energy in DMF: -1619.353697 a.u.

M06 Free energy in DMF: -1618.917374 a.u.

C	3.12742000	-0.82465900	0.36342900
C	2.04073700	0.52842700	-1.16948000
C	3.06730700	0.40248200	-2.09702400

C	4.17342000	-0.37935600	-1.76248500
C	4.20194300	-0.99654300	-0.51598400
H	3.11565500	-1.29290900	1.34033400
H	3.00379000	0.90294100	-3.05568000
H	4.99338000	-0.49912100	-2.46133000
C	0.83720000	1.34251700	-1.40286900
N	-0.09702800	1.46063300	-0.52174700
C	-0.64069900	2.58336500	-2.51437100
C	-1.05465400	2.48142100	-1.02690500
H	-1.26717100	1.97117400	-3.16806700
H	-2.06805600	2.08302700	-0.94079800
O	0.71106400	2.00436100	-2.55118500
H	-0.57174000	3.59446500	-2.91128500
N	2.06780700	-0.07839200	0.04257100
C	-0.99332700	3.82545200	-0.22862700
C	-1.32134600	3.56843800	1.25311600
H	-0.57006100	2.93151200	1.72948400
H	-1.34956500	4.51864200	1.79796900
H	-2.30022000	3.09025300	1.36901100
C	-2.06722300	4.76491300	-0.81334100
H	-2.09077700	5.70250000	-0.24750300
H	-1.87287700	5.02055900	-1.86028100
H	-3.06481300	4.31452000	-0.75526900
C	0.39198600	4.48984700	-0.33070500
H	0.65839000	4.74457400	-1.36207400
H	0.39803300	5.42290000	0.24316100
H	1.18056000	3.85005700	0.08046900
C	5.34482600	-1.88814800	-0.10585600
F	6.44510000	-1.66862200	-0.85087800
F	5.67999000	-1.69968200	1.18856700
F	5.02234200	-3.19420500	-0.24189100
Pd	0.20406300	0.07722100	1.13991400
C	-3.85417000	-1.84269200	-0.55909500
C	-3.36214000	-2.27170300	-1.80052700
C	-4.94096500	-2.53683600	-0.00189700
C	-3.93391800	-3.35861500	-2.46824600
H	-2.52371000	-1.74492300	-2.25141700
C	-5.51408400	-3.62407100	-0.66444100
H	-5.34536600	-2.22605100	0.95793300
C	-5.01299900	-4.03971100	-1.90158000
H	-3.53620900	-3.67063300	-3.43045600
H	-6.35427300	-4.14678000	-0.21467400
H	-5.46041100	-4.88472400	-2.41770300
C	-2.57474500	-1.10859500	1.49169000
C	-3.21555500	-0.65864000	0.15682800
H	-3.38038800	-1.34462700	2.20360200
H	-2.40918600	-0.29096400	-0.48837600
C	-4.22335300	0.48609200	0.36471600
H	-3.75579100	1.34812000	0.85119000
H	-4.63511000	0.82437300	-0.59204500
H	-5.06105900	0.16601500	0.99460300
C	-1.65028600	-0.10052500	2.16012300
C	-0.76503400	-0.59176300	3.15862900
H	-0.76438000	-1.65792500	3.38750000
H	-2.04040500	0.90108800	2.33236600
H	-2.02272400	-2.04231300	1.33333600
H	0.56316400	-0.92366600	2.30226900
O	-0.40379800	0.23353300	4.17704600
H	0.20191200	-0.23712500	4.77229400

35

B3LYP SCF energy in DMF: -1619.95478 a.u.

M06 SCF energy in DMF: -1619.354532 a.u.

M06 Free energy in DMF: -1618.917233 a.u.

C	2.41076700	-1.67908700	0.52333200
C	2.22409000	0.10187500	-0.95235800
C	3.30240700	-0.34127000	-1.70840400
C	3.95929300	-1.50687900	-1.31546400
C	3.50779700	-2.17905300	-0.18357800
H	2.02892300	-2.17974400	1.40388700
H	3.62263800	0.21293500	-2.58205900

H	4.80687400	-1.87655700	-1.88162900
C	1.47700100	1.33133000	-1.26864100
N	0.56748300	1.81869100	-0.49606000
C	0.74743000	3.02500300	-2.51984800
C	0.11373700	3.10002900	-1.10825700
H	0.03659300	2.71116200	-3.28806400
H	-0.97724600	3.08028600	-1.17917800
O	1.75644500	1.96384200	-2.40729300
H	1.26326100	3.92686400	-2.84395900
N	1.78285100	-0.56054800	0.14524300
C	0.51497700	4.35945200	-0.27607600
C	-0.15678900	4.29612700	1.10460000
H	0.18776000	3.44093000	1.68894400
H	0.07008500	5.20443400	1.67462400
H	-1.24705700	4.22798700	1.01369800
C	-0.01065500	5.60560000	-1.01678800
H	0.18245700	6.50125600	-0.41667400
H	0.47157000	5.75629000	-1.98831500
H	-1.09248500	5.54254300	-1.18362900
C	2.04087500	4.45838100	-0.09792900
H	2.56998000	4.51619900	-1.05540400
H	2.29295900	5.36352400	0.46493700
H	2.43674900	3.60335600	0.46107900
C	4.14608700	-3.46880200	0.26455900
F	5.43235500	-3.55115600	-0.12751200
F	4.11623700	-3.59659100	1.60764700
F	3.50246300	-4.54068900	-0.24925900
Pd	0.01250900	0.23588300	1.01233400
C	-4.03364300	-1.62856400	-0.60254900
C	-3.51961200	-2.81774600	-1.13977200
C	-5.40319200	-1.57891400	-0.29323900
C	-4.34295300	-3.92502500	-1.36297400
H	-2.46233200	-2.87529500	-1.38940500
C	-6.22898400	-2.68318000	-0.51311800
H	-5.83061300	-0.66980300	0.12173400
C	-5.70205000	-3.86179600	-1.04932600
H	-3.92120400	-4.83497600	-1.78180200
H	-7.28573500	-2.62307100	-0.26601300
C	-6.34500300	-4.72061600	-1.22142800
C	-3.04905100	-0.09947700	1.14916000
C	-3.12107600	-0.43294600	-0.36173900
H	-4.02683900	0.29076600	1.46823300
H	-2.11051500	-0.72520800	-0.67588700
C	-3.54511700	0.78412800	-1.20259800
H	-2.83583300	1.61114000	-1.09000500
H	-3.58771000	0.52647800	-2.26612500
H	-4.53458200	1.14937700	-0.90501700
C	-2.00535300	0.92727700	1.54678500
C	-1.37850900	0.84106500	2.78318300
H	-1.48442900	-0.04702900	3.40118800
H	-2.08348700	1.91867300	1.10494600
H	-2.87907100	-1.02111800	1.71617000
H	-0.20112500	-1.03873000	1.82092500
O	-0.86195700	1.92976800	3.39395300
H	-0.39257100	1.65220800	4.19764900

TS26

B3LYP SCF energy in DMF: -1868.476717 a.u.

M06 SCF energy in DMF: -1867.781459 a.u.

M06 Free energy in DMF: -1867.257392 a.u.

C	-2.89987300	0.78440200	0.31646000
C	-2.30712100	-0.99277400	-1.03800800
C	-3.45711800	-0.84997400	-1.81119400
C	-4.36310000	0.15758700	-1.48902100
C	-4.08145000	0.98076100	-0.40235800
H	-2.64894800	1.41695400	1.15917400
H	-3.64045400	-1.52025400	-2.64168400
H	-5.26943900	0.29033000	-2.06905300
C	-1.33599800	-2.07541700	-1.29351900
N	-0.37314200	-2.37761900	-0.50316000
C	-0.39030600	-3.74037900	-2.45192900

C	0.30726400	-3.56531600	-1.07481900
H	0.25011100	-3.46257800	-3.29231900
H	1.36450700	-3.31725900	-1.21552300
O	-1.50413700	-2.79139400	-2.41693700
H	-0.81222400	-4.72936300	-2.63075700
N	-2.02342600	-0.17822500	0.00588300
C	0.24400200	-4.80691600	-0.13101100
C	0.94231500	-4.46824400	1.19881900
H	0.41866500	-3.67196700	1.73517100
H	0.96717100	-5.35045700	1.84861800
H	1.97758900	-4.14753900	1.03449300
C	1.00480400	-5.96243900	-0.81032900
H	1.02021500	-6.84112100	-0.15625300
H	0.54032800	-6.26733700	-1.75437100
H	2.04431600	-5.68462700	-1.02078200
C	-1.20910700	-5.22887700	0.15185200
H	-1.74387000	-5.52166900	-0.75855100
H	-1.22446600	-6.09218700	0.82609200
H	-1.77370800	-4.42360700	0.63449200
C	-4.99660500	2.11580400	-0.02842000
F	-6.26769900	1.88035700	-0.41106200
F	-5.00360200	2.33530300	1.30385200
F	-4.61368500	3.27380900	-0.61496300
Pd	-0.09366100	-0.46296600	1.03549200
C	4.25305900	1.00064000	-0.57252700
C	3.89753700	1.71371800	-1.72699700
C	5.48530100	1.29734500	0.03397400
C	4.73971200	2.69357500	-2.26057600
H	2.95151500	1.49398100	-2.21704500
C	6.32909900	2.27638200	-0.49430500
H	5.79117000	0.75753000	0.92633900
C	5.95976400	2.97952100	-1.64472600
H	4.44207900	3.23105200	-3.15719600
H	7.27727200	2.48959500	-0.00749200
H	6.61716600	3.74028800	-2.05664000
C	2.90978900	0.25615800	1.44657200
C	3.32786100	-0.07017200	-0.00907500
H	3.79663600	0.16752900	2.09225100
H	2.41231000	-0.06285100	-0.61532800
C	3.96112300	-1.46880400	-0.12799400
H	3.27225600	-2.24831600	0.21257500
H	4.22780400	-1.69055900	-1.16696000
H	4.87382000	-1.54246300	0.47483200
C	1.81900900	-0.63019200	2.02306400
C	0.91010300	-0.13688800	2.96219700
H	0.89773800	0.91708700	3.23576300
H	2.03935700	-1.69597600	2.07945400
H	2.59172700	1.30328700	1.50237200
H	-0.05854900	1.21365000	1.18265600
O	0.37786100	-0.98808000	3.90594100
H	-0.35076100	-0.53194000	4.35411300
N	0.14512800	4.23056500	-0.27870500
C	0.04025800	5.26704600	0.74835800
H	-0.08864600	4.80569800	1.72559800
H	0.95031000	5.87392200	0.74406400
H	-0.81712700	5.90916700	0.52675700
C	0.31573800	4.68678000	-1.65895200
H	0.37260100	3.82910300	-2.33029800
H	-0.53325700	5.31486500	-1.94372300
H	1.23575000	5.27288800	-1.73942300
C	0.08968000	2.94731400	0.00897200
H	0.17866100	2.25875200	-0.83523700
O	-0.06006700	2.49456400	1.18919400

36

B3LYP SCF energy in DMF: -1868.484304 a.u.

M06 SCF energy in DMF: -1867.793517 a.u.

M06 Free energy in DMF: -1867.263874 a.u.

C	3.28335300	-0.87078500	0.66492100
C	2.62880400	0.68467100	-0.90745000
C	3.78159300	0.49063300	-1.66493500

C	4.72174100	-0.43626300	-1.21818000
C	4.46817400	-1.12474800	-0.03475900
H	3.05611100	-1.38991800	1.59024600
H	3.93983100	1.05122100	-2.57825800
H	5.63193700	-0.61245000	-1.78024300
C	1.58422800	1.65140000	-1.29220700
N	0.51660400	1.85228800	-0.60549800
C	0.55793300	3.15863600	-2.58583800
C	-0.22595600	2.95923700	-1.26112800
H	0.02926300	2.76281100	-3.45621700
H	-1.24264300	2.61250300	-1.47124800
O	1.77356600	2.36129200	-2.41255400
H	0.86828500	4.18371200	-2.78532800
N	2.37975300	0.01386300	0.23855500
C	-0.34605000	4.23260400	-0.36501900
C	-1.14365200	3.88774400	0.90508200
H	-0.62853700	3.13716700	1.51265600
H	-1.28241700	4.78495800	1.51880600
H	-2.13649000	3.49726000	0.65430000
C	-1.12418400	5.30223000	-1.15820400
H	-1.29421700	6.18353000	-0.53022600
H	-0.58303800	5.63750800	-2.04934200
H	-2.10320200	4.92713600	-1.47900400
C	1.03662200	4.77951000	0.03147700
H	1.64220200	5.05057100	-0.84042800
H	0.91922700	5.68454200	0.63731200
H	1.60160100	4.05439900	0.62727400
C	5.42022600	-2.17035300	0.47963500
F	6.66188600	-2.00967300	-0.02030800
F	5.51478900	-2.13972100	1.82695700
F	5.01457900	-3.41750900	0.14471900
Pd	0.29504700	0.37812200	1.15798800
C	-4.55490700	-0.84081700	0.45796100
C	-4.55556700	-1.09942900	-0.92111100
C	-5.54291100	-1.45641700	1.24500200
C	-5.50833500	-1.94348000	-1.49939700
H	-3.80252900	-0.62923700	-1.55020300
C	-6.49517900	-2.30201500	0.67239400
H	-5.57040300	-1.27285300	2.31593900
C	-6.48245400	-2.54941800	-0.70345700
H	-5.49061000	-2.12443600	-2.57110000
H	-7.24976000	-2.76748600	1.30125900
H	-7.22486600	-3.20586600	-1.14906800
C	-2.57647900	-0.71689800	2.03219500
C	-3.50218600	0.07218000	1.07355400
H	-3.17182800	-1.00915600	2.91198000
H	-2.87716300	0.44418900	0.25174300
C	-4.14270400	1.28716800	1.76834800
H	-3.38083500	1.96465200	2.16612000
H	-4.76526500	1.85791100	1.07055500
H	-4.77916700	0.97611000	2.60478900
C	-1.33330200	0.01787200	2.51185200
C	-0.17227300	-0.70418100	2.87700700
H	-0.13687800	-1.78870000	2.74155300
H	-1.52244600	0.92787600	3.08417600
H	-2.27738100	-1.65329200	1.54736100
H	-0.20830000	-1.13506700	0.02122500
O	0.57022900	-0.25075500	3.97838200
H	1.44258300	-0.66936000	3.93697000
N	-1.20034100	-2.38726500	-2.69154000
C	-1.10369400	-3.84148200	-2.52214200
H	-0.75263900	-4.08143200	-1.52114900
H	-2.09182800	-4.27905600	-2.68435300
H	-0.40726200	-4.23669100	-3.26610300
C	-1.69409200	-1.91212000	-3.98910800
H	-1.70166100	-0.82250900	-4.00920500
H	-1.03870100	-2.29047600	-4.77751200
H	-2.70586300	-2.29354000	-4.14651200
C	-0.86680300	-1.54607900	-1.75668100
H	-0.96583200	-0.48086800	-1.95578700
O	-0.41585600	-1.94750800	-0.60985800

37

B3LYP SCF energy in DMF: -1619.497146 a.u.

M06 SCF energy in DMF: -1618.915132 a.u.

M06 Free energy in DMF: -1618.488839 a.u.

C	3.20876600	-1.02014600	0.13567600
C	2.39589900	0.85356700	-0.93553400
C	3.53358200	0.96068600	-1.73409600
C	4.54735800	0.01894200	-1.57688300
C	4.38109100	-0.98545300	-0.62456200
H	3.05144200	-1.78723600	0.88592500
H	3.62123800	1.76121700	-2.45870300
H	5.44691700	0.07045800	-2.18037400
C	1.27568200	1.80651700	-1.02575700
N	0.22916200	1.74079900	-0.28312400
C	0.09701100	3.51650000	-1.85596400
C	-0.62436300	2.90744100	-0.62242900
H	-0.43862400	3.33819700	-2.79150700
H	-1.61184400	2.53349900	-0.91075700
O	1.36575100	2.79192600	-1.93126800
H	0.33479500	4.57695800	-1.77251200
N	2.23000300	-0.12286700	-0.01608000
C	-0.83246200	3.88676600	0.57576900
C	-1.55508000	3.14873700	1.71685600
H	-0.95654100	2.31751800	2.10180100
H	-1.75416400	3.83775100	2.54576700
H	-2.51633200	2.74510600	1.37905900
C	-1.73038300	5.04482900	0.09575300
H	-1.94691600	5.72333000	0.92818000
H	-1.25920200	5.63904600	-0.69451000
H	-2.68769900	4.67312500	-0.28822700
C	0.50703200	4.44178300	1.09246100
H	1.04369400	5.01390100	0.32749900
H	0.33171600	5.11743800	1.93687900
H	1.16567900	3.63995000	1.44346200
C	5.42044500	-2.05808100	-0.44684400
F	6.66483100	-1.59509800	-0.69089400
F	5.41266600	-2.56544600	0.80453900
F	5.21438600	-3.09495000	-1.29263900
Pd	0.14104800	-0.23590200	0.90702900
C	-4.51007400	-1.38985000	-0.60177600
C	-4.40984200	-1.14002800	-1.97868100
C	-5.50371400	-2.28267900	-0.16486800
C	-5.26965300	-1.75706300	-2.89192100
H	-3.64989800	-0.45007900	-2.33929700
C	-6.36448800	-2.90236500	-1.07309600
H	-5.60799300	-2.49587100	0.89580800
C	-6.25168600	-2.64191200	-2.44197200
H	-5.17204800	-1.54414600	-3.95339700
H	-7.12546100	-3.58912300	-0.71117700
H	-6.92273500	-3.12276700	-3.14855000
C	-2.61634300	-1.76026800	1.03495500
C	-3.55657900	-0.71924300	0.37851400
H	-3.23796300	-2.43214600	1.65005200
H	-2.92280000	-0.03514500	-0.20055700
C	-4.31394400	0.11461000	1.42773000
H	-3.61974300	0.66208900	2.07263500
H	-4.97223900	0.84757400	0.94842100
H	-4.93460000	-0.52017300	2.07113600
C	-1.49422800	-1.19660600	1.89655200
C	-0.28167800	-1.91872400	2.04095400
H	-0.14060700	-2.85075700	1.48292400
H	-1.82475100	-0.64554900	2.77902300
H	-2.18250100	-2.38661200	0.24552100
O	0.33274400	-1.94034400	3.31051100
H	1.25783500	-2.19253100	3.17854000

38

B3LYP SCF energy in DMF: -1960.435188 a.u.

M06 SCF energy in DMF: -1959.698226 a.u.

M06 Free energy in DMF: -1959.184099 a.u.

C	3.66859900	0.21441700	-0.15846700	H	2.09644900	-0.85369500	-2.75214000
C	2.07685200	1.87178900	-0.10537700	N	-2.32216200	-2.88616800	2.05872600
C	2.99596200	2.84780700	-0.49754800	1-s			
C	4.31393700	2.46314500	-0.72843300	B3LYP SCF energy in DMF: -1457.612694 a.u.			
C	4.65489200	1.12263200	-0.55902200	M06 SCF energy in DMF: -1457.114751 a.u.			
H	3.90510600	-0.83401500	-0.00805900	M06 Free energy in DMF: -1456.804711 a.u.			
H	2.68708000	3.87876300	-0.61891800	C	2.51108700	-0.03854200	-0.27060300
H	5.05595100	3.19315600	-1.03356100	C	1.04177100	-1.67855100	0.43682200
C	0.66348200	2.21021500	0.15318400	C	2.06696700	-2.60404000	0.60520400
N	-0.26051200	1.35681100	0.42607000	C	3.37220700	-2.21273700	0.31099300
C	-1.12577100	3.54682500	0.23953700	C	3.59463000	-0.91226700	-0.13484600
C	-1.48805300	2.13229700	0.74892200	H	2.64892000	0.98111300	-0.61145600
H	-1.53911400	3.75637000	-0.75106700	H	1.84905600	-3.60679900	0.95196800
H	-2.32169200	1.72184200	0.17275200	H	4.19320100	-2.91201400	0.42412700
O	0.33057100	3.50954000	0.10630900	C	-0.37282700	-1.99851000	0.69974300
H	-1.37233900	4.36373900	0.91625000	N	-1.32909700	-1.17249300	0.46174300
N	2.40536400	0.57673900	0.06642200	C	-2.11850000	-3.16393700	1.46734600
C	-1.87105600	2.05144600	2.26226600	C	-2.60461200	-1.85539900	0.78734100
C	-2.08978800	0.58015800	2.65848300	H	-2.24924400	-3.15066000	2.55172200
H	-1.15785400	0.01034400	2.59711900	H	-3.14793100	-1.23517100	1.50717900
H	-2.45341800	0.51786500	3.69038800	O	-0.67454600	-3.19746300	1.20573100
H	-2.83271500	0.09856800	2.01370200	H	-2.54308500	-4.08080100	1.05987200
C	-3.19311800	2.82035900	2.45641200	N	1.26071600	-0.41402500	0.00679100
H	-3.51839100	2.75095400	3.50019200	C	-3.52951500	-2.04696200	-0.45473100
H	-3.09447300	3.88451000	2.21636100	C	-3.83831800	-0.66986900	-1.06928700
H	-3.99030700	2.40628300	1.82845100	H	-2.93842700	-0.22376700	-1.50458700
C	-0.77882500	2.65678400	3.16275400	H	-4.58506200	-0.76771700	-1.86503600
H	-0.60967900	3.71938000	2.95834000	H	-4.23735600	0.02193800	-0.31814900
H	-1.07590600	2.57385400	4.21400500	C	-4.84461200	-2.68441400	0.03320900
H	0.17552400	2.13070000	3.05023400	H	-5.53573400	-2.81178900	-0.80693000
C	6.05084700	0.64535000	-0.84935400	H	-4.68572400	-3.67205000	0.47993600
F	6.34320400	-0.49683400	-0.19133200	H	-5.33797000	-2.05248700	0.78086100
F	6.22335800	0.39449200	-2.16889900	C	-2.87587700	-2.94195700	-1.52271400
F	6.97697700	1.56418900	-0.50223700	H	-2.67837300	-3.95427500	-1.15428700
Pd	0.16039300	-0.85309400	-0.01626300	H	-3.54222300	-3.03768300	-2.38690000
C	0.59321000	-2.88416200	0.27789900	H	-1.93129500	-2.51879000	-1.88224300
C	2.02441500	-3.10035100	0.18080800	C	4.98721800	-0.41962700	-0.42730000
C	0.11146800	-2.73197800	1.65724000	F	5.79172900	-1.41745200	-0.84597400
C	2.84580800	-3.04372100	1.27305100	F	4.98919700	0.53511900	-1.38173100
H	2.43006900	-3.31733000	-0.80236800	F	5.56193500	0.12057700	0.67140900
C	0.98615000	-2.69468400	2.80375100	Pd	-0.56590400	0.84436600	-0.11985500
C	2.32515800	-2.83884100	2.59764000	C	-1.56121000	2.76981300	-0.17804200
H	3.91386600	-3.19872700	1.15143700	C	-1.99121800	3.35647300	1.08044000
H	0.55481800	-2.57016800	3.79117800	C	-0.15948400	2.82392500	-0.61671900
H	3.00488300	-2.82275400	3.44332300	C	-1.05096700	3.94430500	1.87311100
H	-0.03580700	-3.44135800	-0.41194100	H	-3.04169000	3.31777600	1.34739100
N	-1.20799800	-2.81209800	1.87360900	C	0.73816500	3.53209800	0.26457900
C	-4.65870200	-0.28181900	-1.19589400	C	0.32177100	4.03790700	1.46623000
C	-5.34790200	0.04829400	-0.01771200	H	-1.35536300	4.37538700	2.82185800
C	-5.20540600	0.14217100	-2.41812200	H	1.76369400	3.66895100	-0.06625300
C	-6.53748000	0.78054300	-0.05360100	H	1.02560200	4.55483800	2.11113000
H	-4.94923200	-0.27928100	0.93943900	H	0.05817500	2.82734800	-1.68395500
C	-6.39291500	0.87764500	-2.45851200	N	-2.52645100	2.60851200	-1.13553900
H	-4.70697600	-0.10277800	-3.35162400	N	-3.33473700	2.47015900	-1.90253300
C	-7.06418900	1.20135900	-1.27692800	TS1-s			
H	-7.05063600	1.02166300	0.87371000	B3LYP SCF energy in DMF: -1457.609012 a.u.			
H	-6.79400600	1.19696100	-3.41693700	M06 SCF energy in DMF: -1457.109822 a.u.			
H	-7.98727000	1.77353600	-1.30959300	M06 Free energy in DMF: -1456.79997 a.u.			
C	-2.27611400	-0.58545100	-2.05393600	C	2.39407300	-0.34157700	-0.34131400
C	-3.38652700	-1.12040800	-1.11946600	C	0.74000900	-1.74440800	0.45657500
H	-2.62058100	-0.68416500	-3.09425800	C	1.65013100	-2.76214600	0.72342900
H	-3.01321000	-1.04500000	-0.08989100	C	2.99656000	-2.54218200	0.43373500
C	-3.71151500	-2.60392400	-1.38669800	C	3.37147900	-1.31512100	-0.10506000
H	-2.83871300	-3.24540400	-1.22645500	H	2.65272100	0.62647400	-0.75633500
H	-4.50400100	-2.95247200	-0.71626200	H	1.31562600	-3.70171800	1.14623500
H	-4.05578900	-2.75211900	-2.41719700	H	3.73281800	-3.31445600	0.62489400
C	-0.94562900	-1.30095700	-1.96796700	C	-0.70356900	-1.88041400	0.71955200
C	0.24961500	-0.67314700	-2.27874300	N	-1.56311400	-0.96927000	0.42176100
H	0.30295300	0.40508900	-2.42779200				
H	-0.96591000	-2.38038900	-2.10339200				
H	-2.13200000	0.48696100	-1.87916800				
O	1.29394000	-1.39640400	-2.79215100				

C	-2.56894600	-2.78679300	1.54811800
C	-2.91077900	-1.50408200	0.74738200
H	-2.68681300	-2.65645800	2.62642400
H	-3.42130600	-0.77988700	1.38890800
O	-1.14041000	-3.00412600	1.29195300
H	-3.09577500	-3.68504700	1.22933100
N	1.10637400	-0.55335000	-0.06926700
C	-3.80017000	-1.72818400	-0.51619700
C	-4.00159400	-0.38443600	-1.23713100
H	-3.05812900	0.01008500	-1.62728300
H	-4.68887400	-0.50825900	-2.08161500
H	-4.43210900	0.36396100	-0.56333500
C	-5.17392700	-2.24131400	-0.04073400
H	-5.84106100	-2.37415300	-0.89916000
H	-5.10392300	-3.20657000	0.47199000
H	-5.64730900	-1.52865400	0.64463300
C	-3.16734700	-2.74142800	-1.48718700
H	-3.04396100	-3.73252300	-1.03727300
H	-3.81010700	-2.86483200	-2.36553400
H	-2.18764300	-2.40383600	-1.84319000
C	4.81278900	-0.99153100	-0.39603900
F	5.56590100	-2.10281600	-0.51243400
F	4.94093700	-0.28780200	-1.54190700
F	5.35766300	-0.24019900	0.58805800
Pd	-0.59463700	0.92334300	-0.19763900
C	-0.98562300	3.12034800	-0.02239000
C	-0.89691200	3.72190900	1.27244500
C	0.17045800	2.84606200	-0.83593900
C	0.34409900	4.10598800	1.71356600
H	-1.80117100	3.88787800	1.84760100
C	1.42457700	3.29840300	-0.31629900
C	1.50944900	3.88902700	0.92264800
H	0.43478900	4.60165100	2.67494100
H	2.30862400	3.17967000	-0.93482000
H	2.47146300	4.22180000	1.29943100
H	0.05370600	2.70001400	-1.90873300
N	-2.20954900	2.75325600	-0.52148500
N	-3.28857200	2.81117700	-0.89097300

2-s

B3LYP SCF energy in DMF: -1457.610118 a.u.

M06 SCF energy in DMF: -1457.111786 a.u.

M06 Free energy in DMF: -1456.802941 a.u.

C	-2.46373900	-0.06711300	0.19549600
C	-0.97102900	-1.77074400	-0.26080300
C	-1.96977500	-2.73788300	-0.21509700
C	-3.27677800	-2.33063900	0.05296800
C	-3.52496500	-0.97735600	0.26252100
H	-2.62203000	0.99488000	0.35184600
H	-1.73275000	-3.78141900	-0.38277500
H	-4.08031000	-3.05718400	0.09818200
C	0.44494200	-2.09462200	-0.51196000
N	1.38742600	-1.21873100	-0.45393400
C	2.19623900	-3.33281000	-1.13381000
C	2.67354100	-1.93267700	-0.66845900
H	2.28135400	-3.47187300	-2.21416800
H	3.21550400	-1.42889300	-1.47400300
O	0.76587600	-3.35652100	-0.80570100
H	2.65969800	-4.17381100	-0.62045200
N	-1.21407600	-0.45541100	-0.06067600
C	3.59166800	-1.93339300	0.59438300
C	3.94564100	-0.48425200	0.96958100
H	3.06071500	0.08305300	1.27026600
H	4.65257500	-0.47452600	1.80685200
H	4.41737900	0.03851800	0.12975800
C	4.89242700	-2.67905300	0.23438200
H	5.58648900	-2.65154500	1.08140600
H	4.71768400	-3.73252100	-0.00901300
H	5.39342100	-2.21351600	-0.62251300
C	2.90636700	-2.61678500	1.79150900
H	2.66216000	-3.66566800	1.59011300

H	3.57185300	-2.60178100	2.66140800
H	1.98366400	-2.09906200	2.07571200
C	-4.91734000	-0.46299500	0.51466000
F	-5.74617800	-1.43833100	0.93534700
F	-4.92301200	0.51104900	1.45032600
F	-5.45815700	0.06785500	-0.60592500
Pd	0.58669700	0.85146800	-0.36859300
C	0.46752400	2.97003300	-0.40603400
C	0.23808800	3.69531900	0.83340300
C	1.80855000	2.51446900	-0.80110300
C	1.30459300	3.92204700	1.65180900
H	-0.76467900	4.03663500	1.06666500
C	2.87132700	2.87168100	0.10282100
H	2.04455200	2.42222200	-1.85964500
C	2.63040500	3.51648300	1.28652900
H	1.14780700	4.44770800	2.58880600
H	3.88706200	2.63042500	-0.19535900
H	3.45551700	3.76497600	1.94667600
N	-0.45715100	3.17297500	-1.40766500
N	-1.22944700	3.34896800	-2.20106600

TS2-s

B3LYP SCF energy in DMF: -1457.60808 a.u.

M06 SCF energy in DMF: -1457.109447 a.u.

M06 Free energy in DMF: -1456.799836 a.u.

C	-2.51141300	0.07531200	0.17852300
C	-1.10034600	-1.70774500	-0.23913100
C	-2.14607000	-2.62311400	-0.18517700
C	-3.43331900	-2.14753000	0.06539000
C	-3.61656000	-0.78045700	0.25064600
H	-2.61828600	1.14683600	0.31306000
H	-1.95967900	-3.67961200	-0.33515500
H	-4.27175700	-2.83306500	0.11530900
C	0.29827100	-2.10502300	-0.48255000
N	1.28338500	-1.27700200	-0.44071600
C	1.98310000	-3.43988700	-1.08660900
C	2.53100800	-2.05887900	-0.64300700
H	2.05723800	-3.59942300	-2.16494200
H	3.09861700	-1.59544300	-1.45505500
O	0.55428100	-3.38626200	-0.75479700
H	2.40498600	-4.29507200	-0.56106200
N	-1.28147200	-0.37950600	-0.06107400
C	3.44646800	-2.08758400	0.62149200
C	3.87017200	-0.65236000	0.97692600
H	3.01170100	-0.03678000	1.25996800
H	4.57015000	-0.66399300	1.81999000
H	4.37403200	-0.16777800	0.13347600
C	4.70850900	-2.90119100	0.27186700
H	5.40471000	-2.89476100	1.11751800
H	4.48191000	-3.94827100	0.04413800
H	5.22916300	-2.47315800	-0.59279700
C	2.72820400	-2.72057000	1.82725000
H	2.42883500	-3.75733400	1.63820600
H	3.39546100	-2.73128900	2.69589800
H	1.83435400	-2.15266500	2.10817000
C	-4.98468300	-0.19524900	0.48096300
F	-5.86456700	-1.12398200	0.90309700
F	-4.95369300	0.78936000	1.40504500
F	-5.48637800	0.34713600	-0.65191700
Pd	0.55865300	0.84185800	-0.39301600
C	0.78846100	3.03442600	-0.34944500
C	0.85982600	3.73248000	0.90154700
C	1.94035900	2.42632300	-0.97396000
C	2.09128700	3.85751200	1.48940100
H	-0.04123900	4.15900500	1.32804300
C	3.18992500	2.63444800	-0.30965800
H	1.93393200	2.23061500	-2.04444200
C	3.26079600	3.30721000	0.88632500
H	2.17838800	4.40608300	2.42206600
H	4.09000500	2.26373200	-0.78904900
H	4.22095100	3.45178400	1.37142900

N	-0.40834500	2.96383200	-1.01473300
N	-1.39899600	3.19751200	-1.52610800

3-s

B3LYP SCF energy in DMF: -1457.683861 a.u.

M06 SCF energy in DMF: -1457.175467 a.u.

M06 Free energy in DMF: -1456.864792 a.u.

C	2.77853300	-0.49511800	0.21563300
C	1.49941000	1.31017800	-0.46481600
C	2.61942100	2.08803900	-0.72779900
C	3.87738800	1.53001300	-0.49673100
C	3.95491600	0.22610200	-0.01655800
H	2.80495500	-1.51446300	0.58449200
H	2.51451200	3.10064100	-1.09855900
H	4.77602100	2.10671600	-0.68606800
C	0.12013500	1.79014900	-0.63629200
N	-0.91085900	1.07619800	-0.30562400
C	-1.56158600	3.06821100	-1.34091000
C	-2.12201300	1.93604900	-0.45267500
H	-1.73333100	2.89473100	-2.40608400
H	-2.88848100	1.37083500	-0.98608200
O	-0.10223000	2.99664200	-1.13143000
H	-1.87494700	4.07409700	-1.07128200
N	1.57711400	0.03965800	-0.00391400
C	-2.71664400	2.41339800	0.91369800
C	-3.11744500	1.20366200	1.77498400
H	-2.25133100	0.59471600	2.04993900
H	-3.58705600	1.55258700	2.70131500
H	-3.83689500	0.56289400	1.25644500
C	-3.98836400	3.22852300	0.59963200
H	-4.46119300	3.55245100	1.53272500
H	-3.77774100	4.12797700	0.01152500
H	-4.71790400	2.62636600	0.04607000
C	-1.72047200	3.28366900	1.70302500
H	-1.43227400	4.19053100	1.16129400
H	-2.18039900	3.60358500	2.64403000
H	-0.80984200	2.73092200	1.96018300
C	5.29000900	-0.43691300	0.20596700
F	5.23001300	-1.36185300	1.18579600
F	5.71531600	-1.06736500	-0.91116400
F	6.23893300	0.45801700	0.54346900
Pd	-0.42717000	-0.91621100	0.01472400
C	-2.30120500	-1.60753500	-0.20876600
C	-2.94724900	-1.43236600	-1.43767900
C	-2.93949600	-2.29638900	0.82873500
C	-4.24234200	-1.93531000	-1.61998300
H	-2.45832400	-0.90566200	-2.25286400
C	-4.23597700	-2.79135400	0.63973800
H	-2.44348500	-2.44809600	1.78365400
C	-4.88857800	-2.61111100	-0.58246400
H	-4.74136000	-1.79478900	-2.57548700
H	-4.73003300	-3.32051000	1.45061800
H	-5.89344700	-2.99823400	-0.72635100
N	0.51873000	-3.86491100	0.37463500
N	0.15518500	-2.82598900	0.25651000

4-s

B3LYP SCF energy in DMF: -1457.611411 a.u.

M06 SCF energy in DMF: -1457.11248 a.u.

M06 Free energy in DMF: -1456.804753 a.u.

C	-2.49218800	-0.09176600	0.14835200
C	-0.95561500	-1.70408200	-0.46663500
C	-1.95062900	-2.64969400	-0.69423500
C	-3.27799100	-2.28112500	-0.47969500
C	-3.55059400	-0.98475200	-0.05050700
H	-2.66785700	0.92595700	0.47913000
H	-1.69419700	-3.64850500	-1.02570100
H	-4.07877100	-2.99425000	-0.64061400
C	0.47857300	-1.99900900	-0.63893000
N	1.40756200	-1.15461500	-0.35433800

C	2.28763200	-3.15084200	-1.26989300
C	2.71330600	-1.82420300	-0.58369100
H	2.49040700	-3.15767900	-2.34315700
H	3.29437700	-1.20929900	-1.27760000
O	0.83002600	-3.19904200	-1.10446300
H	2.69257800	-4.05390200	-0.81489900
N	-1.22130200	-0.44419600	-0.05328900
C	3.56018600	-1.99314100	0.71731400
C	3.88347200	-0.60778500	1.30510800
H	2.97969900	-0.09462000	1.64534900
H	4.55594000	-0.71369700	2.16372800
H	4.38236400	0.03163500	0.56766700
C	4.88377300	-2.68320800	0.33179000
H	5.52772200	-2.77460200	1.21308900
H	4.72950000	-3.69196900	-0.06583900
H	5.42926400	-2.10384100	-0.42236800
C	2.81730100	-2.83159400	1.77263600
H	2.60784900	-3.84919700	1.42527700
H	3.42825200	-2.91880300	2.67773000
H	1.86837300	-2.36594400	2.06046100
C	-4.96713200	-0.51793700	0.15548500
F	-5.78229000	-1.53375700	0.50471900
F	-5.04694200	0.42143300	1.12210900
F	-5.47651800	0.03152600	-0.97044700
Pd	0.60533900	0.85382600	0.10929000
C	1.94395800	2.44579800	0.29203200
C	2.72292500	2.78214900	-0.87434700
C	0.57654200	2.98809600	0.31022300
C	2.19829600	3.50256100	-1.91356500
H	3.76035900	2.46090300	-0.89436000
C	0.05709000	3.80070600	-0.77856500
C	0.85873900	4.01380500	-1.85981600
H	2.81193000	3.73181000	-2.77923800
H	-0.94244300	4.21365400	-0.69700100
H	0.48154100	4.60521100	-2.68847100
H	2.46518700	2.29742700	1.23549800
N	-0.53298100	3.30828400	2.52210500
N	-0.02213300	3.15757900	1.53465100

TS3-s

B3LYP SCF energy in DMF: -1457.609463 a.u.

M06 SCF energy in DMF: -1457.110033 a.u.

M06 Free energy in DMF: -1456.801407 a.u.

C	-2.49854800	-0.07739400	0.23469100
C	-0.97224300	-1.63907300	-0.52828800
C	-1.97637600	-2.53473400	-0.88017300
C	-3.30314500	-2.16572400	-0.65749500
C	-3.56593200	-0.92235000	-0.08963800
H	-2.66422200	0.89750300	0.68261000
H	-1.72936300	-3.49545800	-1.31544800
H	-4.11185200	-2.83870900	-0.91862300
C	0.46220500	-1.93248600	-0.70196600
N	1.39147700	-1.12183500	-0.33204900
C	2.27591800	-3.02688000	-1.41024400
C	2.69538400	-1.78717300	-0.57707100
H	2.48238400	-2.90821500	-2.47647300
H	3.31433700	-1.11725700	-1.18099100
O	0.81631100	-3.09215100	-1.25848000
H	2.67983600	-3.97668800	-1.06335400
N	-1.23162600	-0.42682200	0.01392800
C	3.47716600	-2.09507500	0.73907400
C	3.77441800	-0.77604400	1.47581800
H	2.85496700	-0.27971800	1.80017600
H	4.38357700	-0.97263800	2.36522000
H	4.33221300	-0.08114400	0.83741600
C	4.81488900	-2.75641500	0.35341100
H	5.41432600	-2.93686300	1.25221100
H	4.67520100	-3.72151000	-0.14515600
H	5.39975100	-2.11310000	-0.31449300
C	2.68038200	-3.02924300	1.66742600
H	2.47383800	-4.00050600	1.20480400

H	3.25275900	-3.22277800	2.58105400
H	1.72569700	-2.58291900	1.96643200
C	-4.97551600	-0.44405100	0.13716800
F	-5.85414100	-1.46451500	0.17817900
F	-5.08560500	0.23877900	1.29720700
F	-5.37654600	0.39055500	-0.84906200
Pd	0.57685800	0.86139700	0.22695600
C	2.00025100	2.46786700	0.45447000
C	2.95285800	2.72967600	-0.58373300
C	0.69611300	3.06725300	0.27029800
C	2.61425200	3.45346000	-1.70091500
H	3.96455000	2.35856100	-0.45306000
C	0.34331000	3.82615100	-0.89528500
C	1.30826400	4.00970900	-1.84962300
H	3.35487300	3.63634000	-2.47301300
H	-0.65287600	4.24658200	-0.97658200
H	1.07766300	4.60475100	-2.72777600
H	2.35369000	2.24340900	1.45866100
N	-0.22861500	2.89228300	1.26566200
N	-1.02017600	3.03995700	2.07242900

6-s

B3LYP SCF energy in DMF: -1619.962665 a.u.

M06 SCF energy in DMF: -1619.375757 a.u.

M06 Free energy in DMF: -1618.936115 a.u.

C	2.65516400	-0.20637100	0.04581900
C	1.60981000	1.76956200	-0.51168200
C	2.81677600	2.40241600	-0.79063800
C	3.99789500	1.67704000	-0.63362600
C	3.91261500	0.35579700	-0.20892800
H	2.55829600	-1.23516700	0.37273900
H	2.83286500	3.43317800	-1.12292800
H	4.95786700	2.13560100	-0.84173200
C	0.31706200	2.46367300	-0.61520800
N	-0.81868700	1.89076800	-0.39215600
C	-1.09819500	4.12826500	-1.05699800
C	-1.85892500	2.95970800	-0.38970700
H	-1.30405300	4.20946100	-2.12738500
H	-2.69331300	2.64442400	-1.01862400
O	0.31622400	3.76104000	-0.91615000
H	-1.22823500	5.09878400	-0.58200800
N	1.52482900	0.48357600	-0.09894300
C	-2.42298200	3.27168100	1.03558900
C	-3.10752000	2.02223000	1.61792100
H	-2.39756700	1.20508900	1.77383500
H	-3.55822900	2.26389400	2.58702400
H	-3.90690100	1.66254800	0.96055200
C	-3.48668900	4.37836100	0.88402200
H	-3.95103900	4.58205000	1.85477900
H	-3.06412000	5.32099800	0.52109000
H	-4.28002900	4.07497900	0.19114400
C	-1.31563000	3.74047200	1.99714600
H	-0.81421200	4.64766000	1.64333800
H	-1.74818100	3.97161800	2.97654600
H	-0.55596100	2.96582600	2.15065000
C	5.14130400	-0.48678800	0.00940900
F	6.24551500	0.08414500	-0.50964700
F	5.37397200	-0.69039900	1.32588300
F	5.00802000	-1.70711700	-0.55608200
Pd	-0.67879800	-0.24410300	-0.14840500
C	-1.00187300	-2.52898000	0.05575400
C	0.07254700	-3.23779300	-0.54416000
C	-0.87447700	-2.13784600	1.41590000
C	1.19549900	-3.58193500	0.19357500
H	-0.01649500	-3.54376200	-1.58291900
C	0.27970500	-2.47832000	2.14888600
H	-1.72025400	-1.69887000	1.93630300
C	1.29760600	-3.20647600	1.54646600
H	1.99683100	-4.14773100	-0.27251000
H	0.35064600	-2.19502800	3.19482900
H	2.17588700	-3.48960000	2.11958800

C	-2.58219700	-0.81657900	-0.65064600
C	-2.33237000	-2.32523400	-0.67902000
H	-3.22760700	-0.51129500	0.17683100
H	-2.18902600	-2.64475600	-1.71808800
C	-3.47841500	-3.17248600	-0.08758300
C	-3.00693900	-0.21644000	-1.97551400
H	-2.27448000	-0.41346000	-2.76721100
H	-3.95241700	-0.68387800	-2.28488600
H	-3.17407400	0.86162100	-1.91957300
H	-3.59559900	-2.90041900	0.97360000
C	-3.22664200	-4.67454700	-0.19453400
H	-3.09501600	-4.97068600	-1.24113100
H	-2.33808700	-4.97789100	0.36857400
H	-4.07886900	-5.23012200	0.21417800
O	-4.65392900	-2.79770700	-0.81337600
H	-5.39161500	-3.30953400	-0.45089400

7-s

B3LYP SCF energy in DMF: -1619.952348 a.u.

M06 SCF energy in DMF: -1619.355759 a.u.

M06 Free energy in DMF: -1618.918676 a.u.

C	2.31687900	-0.82001000	-0.11855600
C	0.42590800	-2.00424500	0.50255300
C	1.17461300	-3.11818800	0.86418000
C	2.55950400	-3.06927900	0.71187400
C	3.13353600	-1.90734000	0.20433600
H	2.73265300	0.10261000	-0.50266000
H	0.68407300	-4.00414900	1.24837900
C	3.17136200	-3.92408200	0.97810000
H	-1.04505900	-1.98666000	0.55968200
N	-1.75253300	-1.01042300	0.10311500
C	-3.09453200	-2.66309900	1.10368000
C	-3.17620600	-1.44982300	0.14912700
C	-3.33138300	-2.40410700	2.13885700
H	-3.77892100	-0.65282200	0.59187400
O	-1.67485000	-3.04383200	1.06987500
H	-3.66984000	-3.53544900	0.80028400
N	0.99029700	-0.86688300	0.02760300
C	-3.76112200	-1.77206900	-1.26713900
C	-3.70134400	-0.52008600	-2.15945200
H	-2.67364500	-0.17735500	-2.31246700
H	-4.12814700	-0.74404900	-3.14325400
H	-4.28159300	0.30353800	-1.72905300
C	-5.24025300	-2.16957700	-1.08431700
H	-5.70307200	-2.34272300	-2.06177700
H	-5.35778900	-3.08843800	-0.50073600
H	-5.80567700	-1.37569200	-0.58254000
C	-2.99470700	-2.91758800	-1.95430000
H	-3.02973400	-3.84912700	-1.37944600
C	-3.44175800	-3.12587000	-2.93226000
H	-1.94405000	-2.65840500	-2.12568700
C	4.62789700	-1.78243200	0.05204000
F	5.20195700	-2.97283300	-0.21326100
F	4.95830300	-0.93628100	-0.94569100
F	5.19993400	-1.30770700	1.18120700
Pd	-0.42643900	0.78486300	-0.14845100
C	1.05228600	2.09242600	-0.46017100
C	1.77018800	2.68309700	0.58837100
C	1.45758700	2.31253900	-1.78402700
C	2.88801700	3.48096300	0.31219400
H	1.46965100	2.52649600	1.62049600
C	2.57569900	3.11253700	-2.05376000
H	0.91217800	1.86539700	-2.61153100
C	3.29236800	3.69833400	-1.00718100
C	3.43891500	3.93246400	1.13365500
H	2.88158100	3.27498200	-3.08438100
H	4.15870300	4.31898100	-1.21869400
C	-2.09207300	2.27021500	-0.45190300
C	-1.56180300	2.45725200	0.81493200
H	-0.85760800	3.27159000	0.97299200
C	-2.20766200	1.92642500	2.07253900

H	-2.86282800	1.08259500	1.81685500
H	-2.94174600	1.59640500	-0.53711900
C	-1.89141500	3.19833400	-1.61681500
H	-1.02853400	3.85329300	-1.48418000
H	-2.78778500	3.82602100	-1.71406200
H	-1.78475300	2.65142300	-2.55870100
C	-3.04980000	3.02940200	2.72535500
H	-3.50200400	2.65473000	3.65137000
H	-2.43116400	3.89930500	2.96950000
H	-3.86063500	3.34935700	2.06321800
O	-1.16393400	1.49409800	2.95331600
H	-1.57711200	1.27300600	3.80143100

TS5-s

B3LYP SCF energy in DMF: -1619.920786 a.u.

M06 SCF energy in DMF: -1619.331107 a.u.

M06 Free energy in DMF: -1618.892031 a.u.

C	-2.23841100	-0.95262200	0.18183600
C	-0.39829700	-2.09210000	-0.62836200
C	-1.16227200	-3.19905000	-0.98386700
C	-2.53163000	-3.16670800	-0.72546100
C	-3.07307200	-2.03140700	-0.12712100
H	-2.62758300	-0.05020900	0.63784300
H	-0.69727000	-4.06506000	-1.43916300
H	-3.15804900	-4.01449100	-0.98000000
C	1.06349500	-2.04102500	-0.79175900
N	1.80047300	-1.14221200	-0.22845700
C	3.04930100	-2.51838300	-1.67738200
C	3.21850600	-1.50055900	-0.52704100
H	3.14919100	-2.06204000	-2.66581400
H	3.73829500	-0.60432200	-0.87569300
O	1.65520300	-2.96421300	-1.54959000
H	3.68128000	-3.40199700	-1.61370900
N	-0.92847800	-0.98238300	-0.06825100
C	3.98947700	-2.05729500	0.71405200
C	3.98774100	-1.01175600	1.83921100
H	2.97598500	-0.82484100	2.20991300
H	4.59165900	-1.36642500	2.68173400
H	4.41438100	-0.06206500	1.49945800
C	5.44825100	-2.31283400	0.28403400
H	6.03036400	-2.67324800	1.13893800
H	5.52605100	-3.06746200	-0.50567800
H	5.92226000	-1.39370100	-0.07981500
C	3.36406000	-3.36253200	1.24010000
H	3.38500400	-4.16628400	0.49705700
H	3.92615500	-3.71398100	2.11198300
H	2.32659700	-3.21510900	1.55983800
C	-4.55256200	-1.92827200	0.13396000
F	-5.09838600	-3.13348300	0.39525200
F	-4.82217400	-1.12079900	1.18129000
F	-5.20725300	-1.42030900	-0.93531800
Pd	0.57814200	0.63756600	0.23303700
C	-0.81335100	2.18663000	0.32162000
C	-1.69443400	2.29385500	-0.76832300
C	-1.28305700	2.47276600	1.61751800
C	-3.03141500	2.63874800	-0.55790700
H	-1.34187300	2.10724800	-1.77674300
C	-2.62394100	2.80864500	1.82220800
H	-0.60460000	2.43877800	2.46474700
C	-3.49926400	2.89478300	0.73501500
H	-3.70670800	2.71276300	-1.40625600
H	-2.97948400	3.01366700	2.82847500
H	-4.53846800	3.16912400	0.89332300
C	2.02997400	2.11252900	0.49274000
C	1.06852200	3.02707600	-0.04289300
H	0.75406400	3.82668600	0.62258700
C	1.13942900	3.48102900	-1.49288500
H	1.03306000	2.61807600	-2.16521700
H	2.80116500	1.76064000	-0.19437900
C	2.47512500	2.30224300	1.92901300
H	1.66453700	2.69276400	2.55104500

H	3.29428800	3.03487500	1.96066000
H	2.84599900	1.38141600	2.38066600
C	2.49167200	4.15923900	-1.76045200
H	2.50127400	4.55644100	-2.78199500
H	2.65087100	4.99090100	-1.06610900
H	3.32315100	3.45515700	-1.66582500
O	0.08131600	4.41558600	-1.69832500
H	0.13497400	4.70917700	-2.61945800

8-s

B3LYP SCF energy in DMF: -1619.956022 a.u.

M06 SCF energy in DMF: -1619.368928 a.u.

M06 Free energy in DMF: -1618.926817 a.u.

C	2.68548200	0.12829000	0.37696900
C	1.29664000	1.58737500	-0.74416900
C	2.36744800	2.26026500	-1.32500700
C	3.65955100	1.83775700	-1.01589400
C	3.81797200	0.76648000	-0.14142500
H	2.77753900	-0.71693300	1.04692900
H	2.19660200	3.10058600	-1.98687400
C	4.51964600	2.34435000	-1.43946700
H	-0.09806800	2.02191200	-0.92309500
N	-1.07871300	1.56179900	-0.21620500
C	-1.82896200	3.05310700	-1.87102300
C	-2.27778300	2.38428600	-0.55428100
H	-2.15624000	2.50617000	-2.75926700
H	-3.12760000	1.71922400	-0.72743800
O	-0.36264200	2.96324500	-1.82682100
H	-2.08666300	4.10542700	-1.97056000
N	1.44813000	0.52337400	0.07621300
C	-2.66550100	3.39582500	0.57619100
C	-2.98917100	2.63894700	1.87412000
H	-2.12175200	2.08840100	2.24975800
H	-3.29641400	3.34741900	2.65129200
H	-3.81311700	1.93364000	1.72517200
C	-3.93588000	4.14150800	0.11984700
H	-4.26798400	4.82652300	0.90733600
H	-3.77118000	4.73842400	-0.78306700
H	-4.75544400	3.44193100	-0.08165600
C	-1.53765000	4.40743200	0.85313100
H	-1.29559300	5.01783700	-0.02322200
H	-1.84727200	5.09397000	1.64841100
H	-0.62106800	3.91191300	1.19159600
C	5.18826100	0.25303000	0.21266300
F	6.11424900	1.23246000	0.17487600
F	5.21507000	-0.28777500	1.44933400
F	5.59461400	-0.70913100	-0.64713100
Pd	-0.60925300	-0.43917200	0.48853000
C	-0.77302600	-2.71775200	0.08977900
C	-0.03007800	-3.01076900	-1.08658400
C	-0.06555500	-2.64292600	1.32268200
C	1.32763300	-3.28123300	-1.01555000
H	-0.54371100	-3.08686300	-2.03667200
C	1.31759900	-2.92835900	1.37664800
H	-0.61430600	-2.55538400	2.25502600
C	2.00609600	-3.25242900	0.21878500
H	1.87016500	-3.53770100	-1.92120000
H	1.82549000	-2.91414400	2.33654300
H	3.06525600	-3.48926900	0.25915300
C	-2.52242700	-1.14804700	0.63228000
C	-2.30951700	-2.58587000	0.13509100
H	-2.68211000	-3.30304500	0.87897300
C	-2.02939700	-2.90342900	-1.18119900
H	-2.65817800	-2.22327800	-1.96568400
H	-3.06604200	-0.52675800	-0.08446100
C	-3.09332600	-1.03885100	2.03505700
H	-2.54510800	-1.65538300	2.75434400
H	-4.13183100	-1.40540800	2.02847000
H	-3.11016100	-0.01329900	2.40646500
C	-4.54661500	-2.74830700	-1.07320300
H	-5.01766000	-3.03798200	-2.01986600

H	-4.94551200	-3.39300100	-0.28241100
H	-4.84126300	-1.71500500	-0.86548500
O	-2.69423500	-4.25753400	-1.50918800
H	-3.14153000	-4.47177100	-2.34109000

9-s

B3LYP SCF energy in DMF: -1619.948856 a.u.

M06 SCF energy in DMF: -1619.353226 a.u.

M06 Free energy in DMF: -1618.914268 a.u.

C	2.72254000	0.12965200	0.39376600
C	1.30674300	1.62029700	-0.64533600
C	2.35739300	2.43539200	-1.05084700
C	3.65379100	2.07343300	-0.68648400
C	3.83328200	0.91214000	0.05712100
H	2.84945400	-0.79185300	0.94589100
H	2.16593200	3.33456000	-1.62381100
H	4.49924500	2.68802700	-0.97431400
C	-0.10061000	1.97515200	-0.88129900
N	-1.08176000	1.32352900	-0.34680400
C	-1.85699300	3.01715400	-1.76892000
C	-2.32509500	2.09929600	-0.61973900
H	-2.07592800	2.60536600	-2.75741000
H	-3.10074400	1.41208200	-0.96309200
O	-0.38994300	3.03378700	-1.62914300
H	-2.19882900	4.04834200	-1.71240000
N	1.48157400	0.47196000	0.05048700
C	-2.85714200	2.86375000	0.63894800
C	-3.14354600	1.87606100	1.78238100
H	-2.23362900	1.36867100	2.11691500
H	-3.55798900	2.41621500	2.64096600
H	-3.86994400	1.11535700	1.48278900
C	-4.18148600	3.54388000	0.23708000
H	-4.60373900	4.07613200	1.09613700
H	-4.05142200	4.27527200	-0.56789800
H	-4.91983400	2.80516400	-0.09529600
C	-1.85567800	3.92406300	1.13620700
H	-1.65223800	4.69686400	0.38760700
H	-2.26614000	4.42942900	2.01696100
H	-0.90213300	3.47550400	1.43686000
C	5.19615700	0.50179400	0.54961500
F	6.18229800	1.03375100	-0.19898600
F	5.39963200	0.90519300	1.82450800
F	5.34866400	-0.84004300	0.53372200
Pd	-0.49651600	-0.67087100	0.18231200
C	-2.38590400	-1.33058600	0.07347100
C	-2.97131000	-1.46143000	-1.19435800
C	-3.15307800	-1.59532600	1.21329400
C	-4.31033800	-1.85362100	-1.31704700
H	-2.39379000	-1.26040800	-2.09335200
C	-4.49291600	-1.98718200	1.08550800
H	-2.72669300	-1.48986300	2.20589200
C	-5.07402600	-2.11907900	-0.17746800
H	-4.75087800	-1.95228400	-2.30618500
H	-5.07859400	-2.18592000	1.97976400
H	-6.11202000	-2.42543700	-0.27309200
C	0.43799600	-2.51568200	1.10397400
C	0.00583300	-2.86480100	-0.16292100
H	1.46919300	-2.19109200	1.21063600
H	-0.94229900	-3.38820700	-0.25113300
C	0.87293700	-3.00063600	-1.39422200
C	-0.22506100	-2.94542500	2.38354800
H	-1.23951200	-3.31510200	2.22632500
H	0.36996700	-3.76130600	2.81649600
H	-0.24288000	-2.14067500	3.12574300
C	1.04631600	-4.48956600	-1.73039100
H	1.54086200	-5.01631700	-0.90774400
H	0.07906200	-4.96487700	-1.92245300
H	1.65823000	-4.59656600	-2.63302600
H	0.36224500	-2.51638500	-2.24018800
O	2.13310700	-2.37824800	-1.15746300
H	2.64662900	-2.44583500	-1.97533900

TS6-s

B3LYP SCF energy in DMF: -1619.920622 a.u.

M06 SCF energy in DMF: -1619.331083 a.u.

M06 Free energy in DMF: -1618.892114 a.u.

C	2.83706300	-0.07275200	0.30009000
C	1.57078500	1.62350000	-0.62774700
C	2.70198600	2.34543500	-0.99158900
C	3.95648100	1.82456500	-0.67688500
C	4.02029700	0.60039100	-0.01960600
H	2.86466900	-1.03485600	0.79680800
H	2.60290300	3.29350300	-1.50591700
H	4.85906700	2.36259000	-0.94350300
C	0.20532100	2.11495400	-0.87031000
N	-0.84051200	1.53884600	-0.38673000
C	-1.40784700	3.33470200	-1.79920400
C	-2.00099100	2.41441400	-0.70878900
H	-1.62698100	2.98678000	-2.81220900
H	-2.80369900	1.79583600	-1.11788300
O	0.04433400	3.21555800	-1.60824300
H	-1.66375300	4.38882000	-1.70938600
N	1.63431100	0.42668700	0.00620800
C	-2.55658800	3.16619100	0.54547600
C	-2.99171400	2.14555800	1.60974100
H	-2.14330800	1.56235700	1.97965200
H	-3.43948000	2.66469400	2.46473900
H	-3.73801800	1.45011100	1.21370500
C	-3.79192500	3.97317800	0.09820600
H	-4.23966800	4.48087000	0.95945500
H	-3.54105000	4.74261500	-0.63971700
H	-4.55601100	3.32082800	-0.34009300
C	-1.50949000	4.11526500	1.15704000
H	-1.19382400	4.89716900	0.45847500
H	-1.93426500	4.61802900	2.03263400
H	-0.61810200	3.57466500	1.49415700
C	5.33601200	-0.01184700	0.38375000
F	6.36698100	0.50984700	-0.30848000
F	5.59291200	0.18593300	1.69625900
F	5.34064000	-1.34775300	0.18135500
Pd	-0.30036800	-0.56786400	0.20909900
C	-2.20535800	-1.46722600	0.23510500
C	-3.00006300	-1.26980300	-0.90797600
C	-2.83123800	-1.54182700	1.49524000
C	-4.38430400	-1.11493300	-0.78793000
H	-2.54823900	-1.23247300	-1.89440100
C	-4.21337200	-1.38790400	1.60937400
H	-2.24198500	-1.73971100	2.38565600
C	-4.99444900	-1.17721500	0.46810600
H	-4.98445500	-0.95543500	-1.67971000
H	-4.68145800	-1.44431800	2.58838800
H	-6.07213600	-1.07328700	0.55620600
C	0.44667700	-2.45983700	0.62461400
C	-0.78121900	-2.94658000	0.07030600
H	1.30526000	-2.51031000	-0.04325300
H	-1.40428000	-3.51884000	0.75039700
C	-0.81649700	-3.45681800	-1.37919100
C	0.76166200	-2.66801100	2.09045000
H	-0.13080100	-2.60207600	2.71934900
H	1.19610000	-3.66772800	2.23398800
H	1.49661200	-1.94331100	2.45547400
C	-1.90763200	-4.50810400	-1.57254800
H	-1.72896200	-5.36598300	-0.91546400
H	-2.89821900	-4.09861800	-1.35259600
H	-1.91356000	-4.86222100	-2.60922100
H	-0.98905100	-2.62056900	-2.06598100
O	0.47930500	-4.01411400	-1.64666300
H	0.47152500	-4.30167500	-2.57193500

10-s

B3LYP SCF energy in DMF: -1619.960778 a.u.

M06 SCF energy in DMF: -1619.373223 a.u.

M06 Free energy in DMF: -1618.933651 a.u.

C	-2.73198500	0.07597800	0.08105900
C	-1.51531100	-1.81051100	-0.47587600
C	-2.66596500	-2.51639400	-0.81396100
C	-3.90180600	-1.88718600	-0.68214000
C	-3.93076700	-0.57076100	-0.23035700
H	-2.72934300	1.10514300	0.41871900
H	-2.59332400	-3.53498700	-1.17496000
H	-4.81655600	-2.41161300	-0.93520200
C	-0.17292700	-2.40593000	-0.57438100
N	0.90030400	-1.76931900	-0.26406200
C	1.37798700	-3.91426100	-1.11114100
C	2.01978200	-2.74291900	-0.32935300
H	1.61966400	-3.89342000	-2.17709400
H	2.83874600	-2.29946200	-0.90190300
O	-0.06565600	-3.67233100	-0.98931000
H	1.57597700	-4.90655800	-0.70918400
N	-1.54653500	-0.53099900	-0.02565300
C	2.56568300	-3.11741400	1.08864700
C	3.05014900	-1.84733000	1.80930600
H	2.23076000	-1.14064200	1.97815500
H	3.47207700	-2.11028400	2.78592100
H	3.82934200	-1.33464300	1.23606200
C	3.76475700	-4.06685200	0.89747300
H	4.19932100	-4.32325800	1.86975200
H	3.47808700	-5.00519000	0.41065400
H	4.55029600	-3.59913000	0.29266700
C	1.49001000	-3.80350800	1.95107200
H	1.13404500	-4.74050000	1.50993200
H	1.90530800	-4.04734800	2.93488700
H	0.62569200	-3.15068400	2.11515300
C	-5.23591400	0.15279600	-0.02528200
F	-6.19282800	-0.30085600	-0.85921300
F	-5.69643800	-0.00833700	1.23601200
F	-5.10914900	1.48086200	-0.23113700
Pd	0.43026000	0.40991900	0.13915000
C	2.04565500	2.04010100	-0.30829700
C	1.65805100	1.68308600	-1.62920900
C	3.30776200	1.59672700	0.16193500
C	2.51819900	0.92395200	-2.44254300
H	0.74930500	2.09371100	-2.05832100
C	4.15398000	0.85835200	-0.65585900
H	3.61964600	1.87148100	1.16578600
C	3.75948000	0.52093700	-1.96119700
H	2.21643500	0.67898600	-3.45664200
H	5.12654700	0.54736600	-0.28631000
H	4.43070600	-0.04785000	-2.59829800
C	-0.14502100	2.26908800	0.73937600
C	1.17928700	3.00246600	0.51833800
H	-0.93523200	2.59836700	0.05637400
H	1.67650000	3.14417700	1.48515700
C	1.02836800	4.39334400	-0.12823300
C	-0.60777300	2.18621800	2.18144400
H	0.17167700	1.77573200	2.83417700
H	-0.83277600	3.19976300	2.54454600
H	-1.51313500	1.58368300	2.30363200
C	2.36011600	5.11583400	-0.31599200
H	2.87180200	5.24145300	0.64470500
H	3.02294900	4.57091000	-0.99586900
H	2.19292900	6.10980200	-0.74764600
H	0.54327300	4.26955200	-1.10964500
O	0.16416600	5.12696100	0.74619600
H	0.03778800	6.00446700	0.35686000

11-s

B3LYP SCF energy in DMF: -1619.952481 a.u.

M06 SCF energy in DMF: -1619.356162 a.u.

M06 Free energy in DMF: -1618.917466 a.u.

C	2.80964800	-0.01981000	-0.05355500
C	1.38786000	1.74087400	-0.48777000

C	2.44228500	2.60452700	-0.76421200
C	3.74401900	2.11536000	-0.66715400
C	3.92674800	0.78552800	-0.30191900
H	2.93304900	-1.06163500	0.21511600
H	2.24998600	3.63210300	-1.04770900
H	4.59114700	2.75929400	-0.87597000
C	-0.01505300	2.18254300	-0.52367000
N	-1.00347200	1.42096900	-0.18640900
C	-1.75667300	3.49602400	-0.97668500
C	-2.22981800	2.26879400	-0.16825600
H	-2.01641900	3.43271200	-2.03653300
H	-3.02769400	1.74212200	-0.69540400
O	-0.28815600	3.42959300	-0.89165200
H	-2.05922500	4.46211500	-0.57868700
N	1.56176000	0.44306300	-0.14278600
C	-2.72440600	2.59823600	1.28049200
C	-3.02960000	1.29937500	2.04604700
H	-2.13185100	0.68959300	2.18251600
H	-3.42389400	1.54058600	3.03954400
H	-3.77872100	0.69459500	1.52655400
C	-4.03088600	3.40747500	1.15145500
H	-4.43175600	3.62676600	2.14684100
H	-3.88373500	4.36519200	0.64089800
H	-4.79348800	2.84504200	0.60035100
C	-1.68294000	3.41232000	2.07153300
H	-1.46969500	4.38247400	1.61115700
H	-2.06088800	3.61025900	3.08025500
H	-0.73853900	2.86745900	2.18092300
C	5.30929800	0.21308300	-0.12544300
F	6.20304300	0.81045600	-0.93833600
F	5.75169200	0.37595000	1.14157700
F	5.33847300	-1.111104100	-0.38738900
Pd	-0.47558700	-0.65697400	-0.19403000
C	-2.35192300	-1.21141400	-0.61741000
C	-2.80465300	-0.94297200	-1.91673100
C	-3.22884400	-1.78490100	0.31150500
C	-4.12140500	-1.25032800	-2.28261400
H	-2.13940400	-0.49730300	-2.65199400
C	-4.54625100	-2.08651300	-0.05911600
H	-2.90395200	-1.99606600	1.32560500
C	-4.99519100	-1.82260400	-1.35487600
H	-4.45836300	-1.03992400	-3.29472100
H	-5.21767100	-2.52944300	0.67243700
H	-6.01621700	-2.06135900	-1.63943100
C	0.44618600	-2.62162500	-0.82543000
C	-0.08676200	-2.77882000	0.44350300
H	1.49454200	-2.33585800	-0.90449400
C	-0.14237200	-3.20258400	-2.08084000
H	-0.05939800	-2.51273100	-2.92638400
H	0.43536500	-4.09919700	-2.34421500
H	-1.18650900	-3.49439600	-1.95567100
H	-1.05676000	-3.26300000	0.53459200
C	0.72397600	-2.76883500	1.71702000
H	1.65267200	-2.20518700	1.56435700
C	1.08309000	-4.20632600	2.11422200
H	1.71311400	-4.67730100	1.35296100
H	1.64189100	-4.20455800	3.05764700
H	0.17988600	-4.81093800	2.24776300
O	-0.07148100	-2.14305400	2.73061200
H	0.41173000	-2.22385300	3.56650800

TS7-s

B3LYP SCF energy in DMF: -1619.920915 a.u.

M06 SCF energy in DMF: -1619.330673 a.u.

M06 Free energy in DMF: -1618.892084 a.u.

C	2.85311100	-0.25470400	0.12857400
C	1.66309100	1.64482400	-0.44119800
C	2.82550800	2.37597200	-0.66183000
C	4.05402200	1.74891900	-0.46333500
C	4.06432400	0.41849500	-0.05273500
H	2.83453500	-1.29495600	0.43027200

H	2.77034400	3.41165900	-0.97407300
H	4.97991700	2.28982800	-0.62504100
C	0.31928900	2.23759100	-0.54400400
N	-0.74104300	1.62616600	-0.14056700
C	-1.25636800	3.68757500	-1.14899300
C	-1.85886300	2.60669000	-0.22381200
H	-1.52540900	3.54312300	-2.19884500
H	-2.71816700	2.12414800	-0.69587300
O	0.19424300	3.46900400	-1.04303500
H	-1.45242900	4.71738400	-0.85650000
N	1.67429000	0.34152200	-0.06939900
C	-2.30214600	3.13437200	1.18261600
C	-2.73127900	1.95843000	2.07621100
H	-1.90414500	1.26529700	2.25848200
H	-3.07377700	2.33373400	3.04709200
H	-3.55483200	1.39813300	1.62508700
C	-3.51803000	4.05855800	0.97154700
H	-3.87808000	4.43075000	1.93679600
H	-3.27985600	4.93073800	0.35320300
H	-4.34396700	3.52157400	0.49087900
C	-1.17223600	3.91056800	1.88646700
H	-0.85390900	4.79416100	1.32368700
H	-1.52029800	4.26038500	2.86438600
H	-0.29396900	3.27942200	2.06180400
C	5.36125800	-0.29056800	0.23638500
F	6.36086000	0.16529500	-0.54498600
F	5.74568300	-0.11097100	1.52034000
F	5.26051900	-1.62169500	0.03709200
Pd	-0.30698700	-0.58663500	-0.14341900
C	-2.22407600	-1.29564400	-0.54446100
C	-2.50972600	-1.29505200	-1.92387400
C	-3.26132900	-1.07574800	0.37222100
C	-3.79972100	-1.00856800	-2.37564200
H	-1.72817600	-1.52241000	-2.64360500
C	-4.55315900	-0.79863800	-0.08543800
H	-3.06822600	-1.11593000	1.43797100
C	-4.82413600	-0.75938500	-1.45595800
H	-4.00683000	-0.99539600	-3.44245800
H	-5.34968600	-0.62140400	0.63241500
H	-5.83157200	-0.55183800	-1.80571900
C	0.35126300	-2.55836100	-0.26452200
C	-0.99716100	-2.95892100	-0.03243600
H	1.01347400	-2.59628700	0.60298400
C	1.00868300	-2.87660100	-1.59230800
H	1.89138100	-2.25695700	-1.77205200
H	1.33880900	-3.92478700	-1.59897000
H	0.31455800	-2.74296800	-2.42749300
H	-1.49386700	-3.47204400	-0.85133600
C	-1.44516400	-3.46082300	1.33081600
H	-1.31585600	-2.67114900	2.08412800
C	-0.60667700	-4.68262100	1.73840200
H	0.44337900	-4.42018700	1.89538700
H	-0.99441600	-5.08992700	2.67918400
H	-0.66575200	-5.46508000	0.97451400
O	-2.81751200	-3.83171200	1.21604100
H	-3.10479400	-4.13775600	2.08851300

12-s

B3LYP SCF energy in DMF: -1619.957045 a.u.

M06 SCF energy in DMF: -1619.370395 a.u.

M06 Free energy in DMF: -1618.929963 a.u.

C	-2.67114000	-0.14587100	0.13157000
C	-1.31484100	-1.93036600	-0.44280500
C	-2.40093100	-2.79425000	-0.53763500
C	-3.67514100	-2.29959700	-0.26638800
C	-3.80624300	-0.95918900	0.08441000
H	-2.75192500	0.90493600	0.38179800
H	-2.24939000	-3.83257200	-0.80592600
H	-4.54138400	-2.94906300	-0.32427900
C	0.07364800	-2.39230300	-0.60242900
N	1.09141400	-1.67783300	-0.26858400

C	1.73812200	-3.72669900	-1.23093700
C	2.28034000	-2.57080500	-0.36255900
H	1.95236000	-3.59078200	-2.29473600
H	3.08352800	-2.03987300	-0.87905500
O	0.28117200	-3.62759800	-1.06902600
H	2.03416200	-4.72726800	-0.92111800
N	-1.44967500	-0.61741200	-0.13282900
C	2.80838600	-3.00850900	1.04565900
C	3.16686800	-1.76752000	1.88044500
H	2.29377600	-1.13271000	2.05946600
H	3.56350100	-2.07521400	2.85458800
H	3.93295300	-1.16451700	1.38529000
C	4.08745500	-3.84089100	0.82829100
H	4.51013200	-4.13844000	1.79404900
H	3.89745800	-4.75699500	0.25894700
H	4.85071800	-3.26416000	0.29291300
C	1.76912700	-3.84617900	1.81489800
H	1.50306200	-4.77020800	1.29133800
H	2.17759000	-4.13428500	2.78953400
H	0.84968700	-3.28078900	2.00326200
C	-5.14416000	-0.37529100	0.45562400
F	-6.15999800	-1.04540200	-0.12263300
F	-5.34600800	-0.41791600	1.79177700
F	-5.24222300	0.91918900	0.08324000
Pd	0.37690400	0.52592600	-0.32139800
C	1.86198000	2.35589300	-0.31086600
C	2.15744600	1.67598600	-1.52335700
C	2.77640000	2.22521600	0.76641000
C	3.35620300	0.94513100	-1.66593700
H	1.54643200	1.85723500	-2.40314500
C	3.95870900	1.51860500	0.60509500
H	2.58287600	2.74426900	1.69686900
C	4.25693000	0.88174100	-0.61396000
H	3.57785000	0.46548800	-2.61469200
H	4.66800000	1.46795700	1.42602100
H	5.19497600	0.34671000	-0.72922200
C	-0.55193300	2.33944600	-0.44020900
C	0.63870500	3.29357000	-0.29725900
H	-1.17849800	2.32649700	0.45911000
C	-1.36335900	2.50291800	-1.71354400
H	-2.16287500	1.76224800	-1.80572500
H	-1.83461000	3.49743500	-1.72246400
H	-0.73396100	2.43895800	-2.60734500
H	0.71272700	3.93939200	-1.18227100
C	0.53894900	4.21972700	0.92206700
H	0.48190200	3.60156700	1.83333300
C	-0.68990200	5.12730700	0.86585700
H	-1.62250900	4.55464500	0.88139200
H	-0.70141600	5.79378200	1.73620100
H	-0.67270900	5.74688600	-0.03732700
O	1.73671300	5.00508400	0.93717100
H	1.68709100	5.59183600	1.70613400

13-s

B3LYP SCF energy in DMF: -1619.949035 a.u.

M06 SCF energy in DMF: -1619.353903 a.u.

M06 Free energy in DMF: -1618.916207 a.u.

C	-2.36979600	-0.77621600	0.14935200
C	-0.53005600	-1.99086800	-0.55600600
C	-1.31663300	-3.07864300	-0.91694500
C	-2.69357700	-3.00210200	-0.71716600
C	-3.22173600	-1.83641300	-0.17034500
H	-2.75317500	0.15052000	0.55631600
H	-0.85930700	-3.96462000	-1.33981800
H	-3.33541600	-3.83381400	-0.98535000
C	0.93554700	-2.00230900	-0.67486600
N	1.68680900	-1.09330500	-0.15491700
C	2.92588100	-2.62753500	-1.44813100
C	3.09715100	-1.52558700	-0.37828000
H	3.08249000	-2.25932100	-2.46536800
H	3.66130400	-0.68243300	-0.78368200

O	1.50952600	-3.00383400	-1.34146800	C	-3.18431900	1.14805900	2.04324500
H	3.51544800	-3.52805100	-1.28748000	H	-2.29199600	0.52195600	2.13623800
N	-1.04927800	-0.84936800	-0.04207700	H	-3.56427100	1.34108300	3.05272000
C	3.80700800	-2.00065100	0.93090400	H	-3.95176300	0.58076700	1.50642600
C	3.79700300	-0.86532200	1.96620700	C	-4.19150300	3.28150400	1.22547300
H	2.77991600	-0.63097700	2.29199700	H	-4.62401000	3.43108400	2.22066600
H	4.37156800	-1.15863400	2.85195500	H	-4.04543300	4.27227800	0.78219500
H	4.25116400	0.04607200	1.56196000	H	-4.92978100	2.74595200	0.61727400
C	5.27026300	-2.33064600	0.57579900	C	-1.86056400	3.27034900	2.18706700
H	5.81091000	-2.64446100	1.47523100	H	-1.64187500	4.25767200	1.76718700
H	5.34939300	-3.14398000	-0.15341100	H	-2.26299400	3.42972600	3.19324200
H	5.78564900	-1.45542900	0.16352800	H	-0.91579200	2.72643400	2.29715200
C	3.12453000	-3.24048500	1.53796200	C	5.22968500	0.36992100	-0.01386800
H	3.15875300	-4.10721700	0.86967700	F	6.12787800	1.00639000	-0.79263800
H	3.63653400	-3.52660100	2.46295400	F	5.64239300	0.51389500	1.26619100
H	2.07745100	-3.04356500	1.79340800	F	5.29770900	-0.94730200	-0.30432400
C	-4.69713700	-1.71128800	0.10931400	Pd	-0.54281900	-0.63420500	-0.18892400
F	-5.42809000	-2.44460500	-0.75398200	C	-0.73472900	-2.88584900	0.43636900
F	-5.00305000	-2.14019000	1.35404500	C	0.17310800	-2.90642400	-0.65635200
F	-5.11602700	-0.43180700	0.01731900	C	-0.20988200	-3.04668200	1.74574200
Pd	0.40864900	0.74171400	0.19605400	C	1.54666500	-3.15860300	-0.44166500
C	-1.07333600	2.09008700	0.22776400	H	-0.20926600	-2.91906800	-1.67361900
C	-1.52987700	2.63806900	-0.97775900	C	1.14221400	-3.28591300	1.94022200
C	-1.74602300	2.38619200	1.42142700	H	-0.88068400	-3.02847800	2.59775500
C	-2.66098200	3.46507300	-0.98815700	C	2.02468400	-3.35540900	0.84459700
H	-1.01878900	2.42348300	-1.91245700	H	2.21600900	-3.21970100	-1.29467600
C	-2.87513900	3.21523500	1.40377400	H	1.52045700	-3.44063900	2.94668400
H	-1.40094500	1.97753500	2.36795500	H	3.07664200	-3.56918600	1.01023200
C	-3.33558000	3.75512900	0.20001400	C	-2.41603400	-1.40598200	-0.47764700
H	-3.01145700	3.87945700	-1.93027100	C	-2.24047100	-2.80781000	0.12647900
H	-3.39063100	3.43727300	2.33498500	H	-3.07400800	-0.77242000	0.12029400
H	-4.21133300	4.39801400	0.18876000	H	-2.44620700	-3.57366200	-0.63232700
C	2.17911600	2.08041700	-0.13333100	C	-3.15635300	-3.06944800	1.32204300
C	1.55117500	2.61777800	0.97290600	H	-4.20156900	-3.03928300	0.99834500
H	3.00179200	1.38287100	0.01507900	H	-2.97007100	-4.05569100	1.76125100
H	0.89297000	3.46493600	0.79904900	H	-3.03031800	-2.31545600	2.10645300
C	1.93621700	2.40264600	2.40686700	C	-2.82918700	-1.38164600	-1.94400200
H	2.46413000	3.30085100	2.75664500	C	-4.26315800	-1.89834000	-2.12777900
H	1.05395700	2.29004100	3.04517600	H	-4.54211500	-1.85768500	-3.18804200
H	2.59444100	1.54477300	2.54586100	H	-4.36376900	-2.93868100	-1.80331900
C	2.12042400	2.72829700	-1.49680700	H	-4.97061500	-1.28414400	-1.56046100
C	3.36244800	3.59942200	-1.71804300	O	-2.72956300	-0.03224100	-2.42139600
H	3.33290700	4.04569600	-2.71903300	H	-3.08642400	-0.02074100	-3.32191500
H	3.40380100	4.41501000	-0.98907500	H	-2.15091500	-2.02697800	-2.52319000
H	4.27788700	3.00435700	-1.63167100				
O	2.05007600	1.68375600	-2.47569100				
H	2.09924600	2.10414500	-3.34728700				
H	1.22511200	3.36227300	-1.55304800				

14-s
B3LYP SCF energy in DMF: -1619.96253 a.u.
M06 SCF energy in DMF: -1619.373757 a.u.
M06 Free energy in DMF: -1618.930267 a.u.

C	2.73626200	0.07471900	-0.00763700
C	1.28153600	1.81405500	-0.41724400
C	2.32016700	2.71079100	-0.64870800
C	3.63073100	2.24873900	-0.53980200
C	3.83865400	0.91313500	-0.20749700
H	2.86754200	-0.97283800	0.23360800
H	2.10934700	3.74183300	-0.90511900
H	4.46591300	2.91875800	-0.71181600
C	-0.13203000	2.21984400	-0.45111400
N	-1.09973400	1.42074500	-0.15034900
C	-1.90538500	3.50492300	-0.86010500
C	-2.35100400	2.22742600	-0.11330800
H	-2.16154000	3.48531700	-1.92255400
H	-3.11404700	1.69560300	-0.68335100
O	-0.43708600	3.47600600	-0.77176700
H	-2.23635600	4.44222600	-0.41774100
N	1.48121300	0.51186900	-0.10990500
C	-2.87732200	2.48232900	1.33964800

15-s
B3LYP SCF energy in DMF: -1619.947566 a.u.
M06 SCF energy in DMF: -1619.355178 a.u.
M06 Free energy in DMF: -1618.916522 a.u.

C	2.39656900	-0.68221900	-0.15064400
C	0.66614400	-2.11787800	0.40046800
C	1.52648400	-3.20392500	0.50304800
C	2.88449900	-3.00761300	0.24976400
C	3.31906100	-1.73200500	-0.09041800
H	2.70623700	0.32667100	-0.39396300
H	1.14293300	-4.18152500	0.76805200
C	3.58146700	-3.83526500	0.31444000
H	-0.78986400	-2.24528000	0.57550000
N	-1.61422900	-1.28250100	0.33913300
C	-2.71338400	-3.18459900	1.18608700
C	-2.98701000	-1.85517600	0.44707800
H	-2.86297000	-3.10829800	2.26612400
H	-3.59905000	-1.19270200	1.06355400
O	-1.27970500	-3.42153800	0.96552800
H	-3.24834900	-4.05010100	0.80015000
N	1.09755900	-0.86961600	0.08999700
C	-3.69511800	-2.01938100	-0.93824900
C	-3.82952800	-0.64989400	-1.62464700
H	-2.85332900	-0.20151700	-1.82866800
H	-4.35238900	-0.76094900	-2.58113900
H	-4.41068600	0.04685800	-1.01081800

C	-5.10939400	-2.57564400	-0.67688000
H	-5.65614000	-2.66316100	-1.62191100
H	-5.09069000	-3.57015400	-0.21865100
H	-5.68245400	-1.91132100	-0.01958100
C	-2.92271500	-2.97425300	-1.86723900
H	-2.83105800	-3.98258300	-1.45001900
H	-3.45145100	-3.06742600	-2.82183100
H	-1.91661000	-2.60040400	-2.08724400
C	4.76099400	-1.44458000	-0.42055900
F	5.56629300	-2.47481800	-0.10137000
F	4.92166300	-1.19827500	-1.74000400
F	5.20913800	-0.35365100	0.23836100
Pd	-0.45943500	0.65532500	0.26792600
C	0.90848500	2.10973500	0.12100300
C	1.62711000	2.56292300	1.23602700
C	1.26534300	2.56087100	-1.15775100
C	2.69499400	3.45404900	1.07000700
H	1.37077700	2.22487000	2.23654200
C	2.33326900	3.45367900	-1.31677000
H	0.72376000	2.22119200	-2.03627500
C	3.05025900	3.90153100	-0.20453300
H	3.24745800	3.79464000	1.94228200
H	2.60127300	3.79457200	-2.31378800
H	3.87853900	4.59324500	-0.33020700
C	-2.21949400	2.01204800	0.37958200
C	-1.63593400	2.00268000	1.63861900
H	-0.97458500	2.82945100	1.88920600
C	-2.11102300	1.18870400	2.80726200
H	-1.27792600	0.79854700	3.40049100
H	-2.68701300	1.85230900	3.46803400
H	-2.76112900	0.36411100	2.50826300
H	-3.05082100	1.33387400	0.19545400
C	-2.18316300	3.23092400	-0.52371600
H	-1.23575400	3.76469800	-0.37532200
C	-2.36488300	2.90378300	-2.00348100
H	-2.36291600	3.82665800	-2.59550100
H	-1.55816400	2.26752500	-2.37835200
H	-3.31875100	2.39293200	-2.16956000
O	-3.27319600	4.04285800	-0.04829000
H	-3.40035000	4.75239600	-0.69639400

TS9-s

B3LYP SCF energy in DMF: -1619.916336 a.u.

M06 SCF energy in DMF: -1619.327982 a.u.

M06 Free energy in DMF: -1618.88892 a.u.

C	2.30880800	-0.71867500	-0.35149600
C	0.57449300	-2.03509500	0.42523300
C	1.40359400	-3.14049200	0.58795900
C	2.74847900	-3.01252900	0.24434700
C	3.20278500	-1.78705800	-0.23841400
H	2.63131000	0.25467700	-0.70157000
H	1.00762700	-4.07477800	0.96700300
H	3.42584300	-3.85212800	0.35383900
C	-0.87001400	-2.06372700	0.70751600
N	-1.69587900	-1.16808800	0.27459900
C	-2.73173300	-2.68819200	1.75080300
C	-3.06217000	-1.63337300	0.67408400
H	-2.74413900	-2.27916900	2.76482100
H	-3.60468400	-0.79040500	1.10968500
O	-1.34296800	-3.06100600	1.45532800
H	-3.32816700	-3.59751000	1.71328200
N	1.02192700	-0.84226800	-0.02160500
C	-3.90205400	-2.19362100	-0.52173300
C	-4.08154800	-1.10354700	-1.58669800
H	-3.12515400	-0.79676500	-2.01726300
H	-4.71203300	-1.47409300	-2.40263800
H	-4.57033500	-0.21998600	-1.16451400
C	-5.29416600	-2.57591400	0.02173100
H	-5.92943300	-2.92874600	-0.79783700
H	-5.25155400	-3.37681000	0.76723300
H	-5.79113700	-1.71396600	0.48193500

C	-3.23822100	-3.42461900	-1.16714800
H	-3.13192500	-4.26090200	-0.46846300
H	-3.85311400	-3.77741300	-2.00208200
H	-2.24817700	-3.18648800	-1.57143900
C	4.63331100	-1.60599800	-0.67242600
F	5.46820300	-2.41648500	0.00872000
F	4.79038400	-1.88723000	-1.98605600
F	5.05470300	-0.33658400	-0.48771800
Pd	-0.51903200	0.74687600	0.05054200
C	0.88163500	2.26587900	0.40691100
C	1.74473200	2.06318200	1.49972800
C	1.38833900	2.86720300	-0.76176800
C	3.08791500	2.43495500	1.41669400
H	1.37303200	1.61168900	2.41388400
C	2.73776800	3.22097400	-0.84472200
H	0.73349400	3.06659300	-1.60411100
C	3.58844700	3.01098300	0.24473200
H	3.74307500	2.27246300	2.26822200
H	3.11918400	3.67320500	-1.75619800
H	4.63328900	3.30166100	0.18403600
C	-1.92123200	2.28270900	0.18201900
C	-0.95544400	2.95561600	1.00743300
H	-0.62801700	3.92325300	0.63811400
C	-1.05416500	2.88330700	2.51059800
H	-0.15265200	3.24949000	3.00544700
H	-1.88264200	3.53932600	2.80910600
H	-1.27808900	1.87561800	2.86982400
H	-2.75582600	1.80495000	0.70142300
C	-2.30002600	3.01282700	-1.10313700
H	-1.38640600	3.45146900	-1.52986900
C	-2.98299200	2.17628700	-2.17532300
H	-3.21308100	2.80373200	-3.04507200
H	-2.33656600	1.36110900	-2.51459500
H	-3.91993000	1.75473900	-1.80336700
O	-3.16665100	4.07756000	-0.66389700
H	-3.41253800	4.58513300	-1.45225300

16-s

B3LYP SCF energy in DMF: -1619.949855 a.u.

M06 SCF energy in DMF: -1619.363184 a.u.

M06 Free energy in DMF: -1618.921985 a.u.

C	-2.62580000	0.19345500	-0.53870600
C	-1.19402900	1.68039100	0.49404700
C	-2.23244700	2.54318100	0.82953100
C	-3.52774000	2.20178300	0.44174300
C	-3.72294600	1.01559200	-0.25932000
H	-2.74899000	-0.74527600	-1.06434500
H	-2.03387200	3.45948300	1.37224000
H	-4.36275100	2.85012700	0.68206400
C	0.21527600	1.97538200	0.80144100
N	1.20566500	1.33722100	0.26886500
C	1.92594200	2.84284500	1.93308900
C	2.45439400	2.00049500	0.75144200
H	2.04001200	2.34088600	2.89757300
H	3.14245100	1.22847800	1.10489900
O	0.48374800	2.94734300	1.67272800
H	2.32020000	3.85508100	1.99560300
N	-1.38756200	0.51367000	-0.16121700
C	3.18377300	2.82962900	-0.35452100
C	3.54541200	1.91085600	-1.53020200
H	2.65047400	1.52182500	-2.02196000
H	4.12460100	2.46403300	-2.27795700
H	4.15422600	1.06378600	-1.19735500
C	4.48693300	3.38212400	0.25771000
H	5.04814600	3.93800000	-0.50105400
H	4.30180500	4.06513000	1.09330900
H	5.12918800	2.57148300	0.62126900
C	2.31521400	3.99144200	-0.87166900
H	2.06194300	4.70897100	-0.08416400
H	2.85930300	4.54216500	-1.64671000
H	1.38369400	3.63208500	-1.32278000

C	-5.08662300	0.61456600	-0.75621900
F	-6.07231000	1.20170300	-0.04915500
F	-5.26223100	0.96297200	-2.05120700
F	-5.26892300	-0.72195200	-0.68065700
Pd	0.52119100	-0.70200400	-0.26972000
C	0.47158400	-2.69675000	0.95719600
C	-0.22646600	-2.50026900	2.17789300
C	-0.29936100	-2.95653200	-0.21508500
C	-1.60837600	-2.60300700	2.23032300
H	0.32888500	-2.30013600	3.08742500
C	-1.70808300	-3.06169900	-0.13886000
H	0.18830200	-3.28153200	-1.12780900
C	-2.35769500	-2.88597300	1.07112500
H	-2.11821700	-2.47589100	3.18133700
H	-2.26885600	-3.30494200	-1.03672700
H	-3.43838400	-2.97378500	1.13149800
C	2.31338100	-1.68382100	-0.23384700
C	2.00944200	-2.73213100	0.85328900
H	2.30412700	-3.72918700	0.50099000
C	2.73899500	-2.46178800	2.16914000
H	2.48458700	-3.20310500	2.93411000
H	3.81965000	-2.51097800	2.00371500
H	2.50569900	-1.46769900	2.56662000
H	3.03800800	-0.93103700	0.09132800
C	2.73187000	-2.29685100	-1.57460500
H	2.08543600	-3.15990800	-1.78603200
C	2.68965500	-1.36871600	-2.78462900
H	2.96768600	-1.92328200	-3.68919000
H	1.68139000	-0.96487800	-2.93558600
H	3.38775700	-0.53765500	-2.66828200
O	4.07112800	-2.77709300	-1.34624800
H	4.30031600	-3.34801800	-2.09495400

17-s

B3LYP SCF energy in DMF: -1619.948472 a.u.

M06 SCF energy in DMF: -1619.355455 a.u.

M06 Free energy in DMF: -1618.916855 a.u.

C	-2.80130800	-0.06755600	0.27911500
C	-1.40125700	-1.64064300	-0.65782900
C	-2.46594500	-2.41737500	-1.09738000
C	-3.76331800	-1.98584800	-0.81761200
C	-3.92931400	-0.79895500	-0.11504300
H	-2.91102900	0.86451300	0.82196300
H	-2.28746100	-3.33867100	-1.63852900
H	-4.61899400	-2.56805300	-1.13928200
C	-0.00032900	-2.04896000	-0.84221100
N	0.99235800	-1.40023700	-0.32681900
C	1.73795200	-3.18974700	-1.64270500
C	2.21620500	-2.22432900	-0.53714200
H	1.98809200	-2.84209400	-2.64813100
H	3.01674300	-1.57928300	-0.90437100
O	0.26879200	-3.15182800	-1.53129200
H	2.04424200	-4.22666200	-1.52152400
N	-1.56039800	-0.47496400	0.01571200
C	2.70569200	-2.93195400	0.77096200
C	3.02280700	-1.88818200	1.85567000
H	2.13074200	-1.32928400	2.15491700
H	3.41425900	-2.39021400	2.74752200
H	3.77699800	-1.17221200	1.51590600
C	4.00414600	-3.68945300	0.42627800
H	4.40498800	-4.17052300	1.32478200
H	3.84621900	-4.47499400	-0.32057300
H	4.77040600	-3.00728900	0.04059300
C	1.65589000	-3.91779900	1.31749000
H	1.42949500	-4.72377900	0.61196300
H	2.03458900	-4.38727300	2.23167200
H	0.71902300	-3.41266900	1.57777500
C	-5.29369700	-0.25824500	0.22521400
F	-5.41125000	-0.02145400	1.55043000
F	-5.52698400	0.91609700	-0.40291100
F	-6.27706800	-1.10724500	-0.12614900

Pd	0.45850600	0.59950400	0.21417500
C	2.34279100	1.24408100	-0.03073400
C	2.82738600	1.29499600	-1.34601500
C	3.20452500	1.56076200	1.02745800
C	4.15372500	1.66815700	-1.59766600
H	2.18039500	1.04587700	-2.18291600
C	4.53194800	1.92863200	0.77061800
H	2.86196700	1.51748100	2.05716200
C	5.00933700	1.98693700	-0.54036500
H	4.51288000	1.70642600	-2.62316400
H	5.18872900	2.16895000	1.60305500
H	6.03810000	2.27594300	-0.73656800
C	-0.48124100	2.61536700	0.26107500
C	0.08890700	2.41543700	1.50778500
H	-1.53906900	2.38932900	0.13256900
H	1.06300600	2.86456400	1.68588400
C	-0.63901000	1.96254300	2.74098700
H	-0.01640900	1.30697800	3.35820500
H	-0.86672000	2.84892200	3.35011400
H	-1.58049200	1.45650600	2.51773500
C	0.05900300	3.59410600	-0.76346800
H	1.15007000	3.66336500	-0.66642800
C	-0.31150400	3.21519100	-2.19527400
H	0.12853500	2.25476500	-2.47940800
H	-1.39993400	3.14561600	-2.30222200
H	0.05524900	3.97222200	-2.89830900
O	-0.54229700	4.84821300	-0.39556400
H	-0.36422700	5.47009800	-1.11743000

18-s

B3LYP SCF energy in DMF: -1619.954002 a.u.

M06 SCF energy in DMF: -1619.367207 a.u.

M06 Free energy in DMF: -1618.924272 a.u.

C	-2.47077100	-0.51037400	0.36981500
C	-0.86820000	-1.92593700	-0.51229300
C	-1.79035300	-2.95218000	-0.68071800
C	-3.11224000	-2.73619100	-0.29144600
C	-3.44889800	-1.50188800	0.25275900
H	-2.71726000	0.46463600	0.77089400
H	-1.47741400	-3.90329400	-1.09387400
H	-3.85480100	-3.51723300	-0.40739100
C	0.56822400	-2.09919100	-0.77828900
N	1.45705100	-1.26745900	-0.35538300
C	2.41137500	-2.98737900	-1.64782600
C	2.78048600	-1.90253400	-0.61339000
H	2.54090900	-2.64922100	-2.67965600
H	3.45166700	-1.15869600	-1.04881400
O	0.96986700	-3.18776500	-1.43863800
H	2.89805800	-3.95126600	-1.51240600
N	-1.21006600	-0.70863100	-0.01940600
C	3.44417200	-2.45631900	0.69314800
C	3.59657700	-1.32672700	1.72539300
H	2.62617400	-0.92106700	2.02773600
H	4.09525400	-1.70787600	2.62360600
H	4.20253600	-0.50675400	1.33113400
C	4.84707200	-2.97544500	0.31856300
H	5.36232600	-3.34256800	1.21266200
H	4.80917300	-3.80136300	-0.39981600
H	5.46036000	-2.17889900	-0.11843300
C	2.62022400	-3.59593500	1.32289900
H	2.51410200	-4.45774300	0.65623800
H	3.12053600	-3.94958800	2.23086000
H	1.61878500	-3.26173900	1.61612500
C	-4.84311900	-1.19310200	0.73164600
F	-4.90697000	-1.16229700	2.08127100
F	-5.25381300	0.01877600	0.29319100
F	-5.73596900	-2.10523900	0.30494100
Pd	0.36367100	0.75028100	-0.13265600
C	1.54028200	2.76208900	0.32331700
C	1.92657600	2.36799800	-0.98785800
C	2.49737500	2.63538900	1.36246100

C	3.23986400	1.91342900	-1.24617300
H	1.28786800	2.59431800	-1.83632900
C	3.78884100	2.21354700	1.08777800
H	2.23272200	2.92229300	2.37397000
C	4.16741400	1.85266000	-0.21981500
H	3.52045000	1.65259300	-2.26237500
H	4.51935700	2.16762800	1.89030200
H	5.18650600	1.53528000	-0.41970600
C	-0.83862400	2.40439600	-0.02544700
C	0.16698400	3.43200700	0.51824700
H	-1.59222400	2.14037200	0.72485800
H	0.14632100	4.33287400	-0.10820000
C	-0.13632600	3.85488700	1.95608600
H	0.59538600	4.57886500	2.33034200
H	-1.12160500	4.32895900	1.99362600
H	-0.15044200	2.99780500	2.63930400
C	-1.51003600	2.84073100	-1.33211300
H	-0.72930900	3.16732700	-2.03512200
C	-2.38489500	1.80702300	-2.03634300
H	-1.80253400	0.93545800	-2.35091400
H	-3.20581400	1.47221200	-1.39486700
H	-2.82595000	2.25282200	-2.93600400
O	-2.30066100	3.98690500	-0.95771000
H	-2.60377500	4.40355300	-1.77832800

19-s

B3LYP SCF energy in DMF: -1619.952474 a.u.

M06 SCF energy in DMF: -1619.355516 a.u.

M06 Free energy in DMF: -1618.917367 a.u.

C	2.82131200	-0.09410900	0.09426500
C	1.49095700	1.70919400	-0.44749400
C	2.58919200	2.53587600	-0.65771700
C	3.86403000	2.00449400	-0.46864600
C	3.97798200	0.67459100	-0.07632400
H	2.89155500	-1.13602700	0.38146900
H	2.45137400	3.56804100	-0.95633600
H	4.74485100	2.61794400	-0.62227500
C	0.10792300	2.20075600	-0.54475800
N	-0.91627500	1.48452300	-0.21279500
C	-1.57285800	3.56352200	-1.07064200
C	-2.10685400	2.38174200	-0.23411300
H	-1.80980500	3.47242300	-2.13387100
H	-2.92109500	1.87358100	-0.75438000
O	-0.10916200	3.44723000	-0.94839600
H	-1.84877200	4.55311700	-0.71299700
N	1.59936500	0.40676900	-0.09311000
C	-2.59908800	2.77284100	1.20002500
C	-2.95768000	1.51022500	2.00194900
H	-2.08448300	0.87092600	2.16280600
H	-3.34856400	1.79635700	2.98483100
H	-3.72616200	0.91870700	1.49579100
C	-3.87287000	3.62622200	1.03518000
H	-4.26917500	3.89795900	2.01941700
H	-3.68581500	4.55777400	0.49065900
H	-4.65441400	3.07415700	0.50044700
C	-1.53384300	3.57149400	1.97535200
H	-1.27559800	4.51568000	1.48500100
H	-1.91409300	3.81946400	2.97202600
H	-0.61351000	2.99340400	2.11486800
C	5.32566000	0.06450700	0.20836500
F	6.29302200	0.62376600	-0.54543600
F	5.67974900	0.23414300	1.50180000
F	5.33379100	-1.26373600	-0.03294700
Pd	-0.45724200	-0.61018900	-0.22710300
C	-2.37113800	-1.11861600	-0.52886300
C	-2.92673300	-0.83842500	-1.78565700
C	-3.17811700	-1.67148000	0.47255800
C	-4.27850900	-1.10771600	-2.03562100
H	-2.31723200	-0.40927200	-2.57718300
C	-4.53051500	-1.93665500	0.21676000
H	-2.76474500	-1.89450300	1.45141700

C	-5.08380400	-1.65696600	-1.03467800
H	-4.69614800	-0.88723700	-3.01494600
H	-5.14847000	-2.36238000	1.00369100
H	-6.13199400	-1.86655300	-1.22916900
C	0.32805600	-2.66828200	0.18278600
C	0.03923600	-2.61407400	-1.17083400
H	1.34211100	-2.44659400	0.51187500
H	-0.90596200	-3.04552300	-1.49418500
C	1.03510400	-2.37311100	-2.27102500
H	1.28439600	-3.34213700	-2.72549800
H	0.61314000	-1.75044200	-3.06631800
H	1.96183700	-1.91997300	-1.91292400
C	-0.47028800	-3.47237100	1.17875700
C	0.21775800	-4.81793600	1.43537800
H	-0.34922500	-5.39113500	2.17866400
H	0.26604000	-5.41451000	0.51880400
H	1.23510600	-4.67253200	1.81406100
O	-0.55284200	-2.70385100	2.38615300
H	-0.95194800	-3.27150800	3.06283100
H	-1.47420600	-3.65849100	0.77665800

TS11-s

B3LYP SCF energy in DMF: -1619.929318 a.u.

M06 SCF energy in DMF: -1619.338176 a.u.

M06 Free energy in DMF: -1618.898271 a.u.

C	-2.70787800	-0.19834400	0.08700300
C	-1.21286800	-1.85612700	-0.52038800
C	-2.23442400	-2.75921700	-0.79165400
C	-3.55397400	-2.34791200	-0.60843400
C	-3.78791700	-1.05315500	-0.15615000
H	-2.85014000	0.81130000	0.45400200
H	-2.00170000	-3.75935200	-1.13628900
H	-4.37545400	-3.02443200	-0.81513400
C	0.21029900	-2.21186400	-0.62949100
N	1.15459500	-1.42100500	-0.25138600
C	2.00377400	-3.37711200	-1.24587000
C	2.42753100	-2.18486300	-0.35832700
H	2.22784400	-3.21596000	-2.30382600
H	3.16656500	-1.56435900	-0.87131900
O	0.53943800	-3.40975400	-1.11718800
H	2.37993400	-4.34928100	-0.93320700
N	-1.44357300	-0.58785100	-0.09953100
C	3.01038300	-2.58097400	1.03804500
C	3.26328300	-1.31345800	1.87141500
H	2.33266700	-0.78273900	2.09324800
C	3.73080700	-1.58218800	2.82551200
H	3.93617700	-0.62350300	1.35311100
C	4.35795600	-3.29142600	0.80105500
H	4.82267300	-3.54212900	1.76080600
H	4.24461700	-4.22501600	0.23977900
H	5.05386700	-2.64828300	0.25000000
C	2.06000300	-3.51196800	1.81369300
H	1.89474100	-4.46481500	1.30004400
H	2.49069700	-3.74521900	2.79351100
H	1.08585300	-3.04268100	1.99054200
C	-5.18455500	-0.55891000	0.11276600
F	-6.10443500	-1.25321200	-0.58600300
F	-5.50777800	-0.67201300	1.42100400
F	-5.32104500	0.74492100	-0.21371400
Pd	0.34453500	0.66473000	-0.12121000
C	2.13264600	1.74451700	-0.35473200
C	2.94116300	1.37757500	-1.44525900
C	2.74629300	2.18849600	0.83249200
C	4.33331600	1.42442600	-1.33856000
H	2.48703000	1.05784200	-2.37832400
C	4.13786300	2.23379300	0.93478800
H	2.13758700	2.51844500	1.66969100
C	4.93397800	1.85532400	-0.15115600
H	4.94763600	1.13428500	-2.18674400
H	4.59926900	2.57722100	1.85671500
H	6.01655400	1.90610500	-0.07668400

C	-0.59463900	2.51566500	-0.20800700
C	0.58166200	2.99384900	-0.87421700
H	-1.45156200	2.30495800	-0.85348200
H	1.12535000	3.77730200	-0.35504500
C	0.58824200	3.14045100	-2.37572200
H	-0.00996700	4.02848600	-2.61896900
H	1.59308700	3.30113300	-2.77062100
H	0.13630200	2.28345200	-2.88206800
C	-0.96133100	3.12308500	1.13428100
C	-1.73901200	4.43022200	0.94907900
H	-2.01640500	4.84927300	1.92396400
H	-1.13225600	5.17687100	0.42678800
H	-2.65449800	4.25791800	0.37285100
O	-1.74997300	2.16554000	1.85419800
H	-2.13132600	2.61738600	2.62174400
H	-0.03888100	3.33641700	1.69392100

20-s

B3LYP SCF energy in DMF: -1619.961647 a.u.

M06 SCF energy in DMF: -1619.371514 a.u.

M06 Free energy in DMF: -1618.929881 a.u.

C	-2.45939500	-0.57609400	0.02726000
C	-0.70143900	-1.89103700	-0.70626500
C	-1.56171700	-2.88479300	-1.16036100
C	-2.93483700	-2.70331200	-1.00457500
C	-3.38332200	-1.53818200	-0.39061500
H	-2.77346500	0.33233400	0.52553400
H	-1.16308400	-3.78156600	-1.61859200
H	-3.63344400	-3.45724100	-1.34918200
C	0.76180800	-2.03985400	-0.74087800
N	1.56232600	-1.18781600	-0.20174100
C	2.73320300	-2.92497300	-1.27378400
C	2.92011000	-1.79502800	-0.23576900
H	3.03779900	-2.62708300	-2.28078700
H	3.63315400	-1.05140700	-0.59938700
O	1.27906600	-3.13368300	-1.30683000
H	3.19300700	-3.87769300	-1.01665800
N	-1.14440300	-0.74074400	-0.13950800
C	3.39238500	-2.27607600	1.17745300
C	3.39795800	-1.09257700	2.16114900
H	2.39914600	-0.66326000	2.28891300
H	3.74634800	-1.42712000	3.14470800
H	4.07111000	-0.29859300	1.82430500
C	4.83370800	-2.80499800	1.03678600
H	5.21777400	-3.11003000	2.01624700
H	4.89577100	-3.67737500	0.37708900
H	5.50404400	-2.03408400	0.63947100
C	2.48570500	-3.38799500	1.73861100
H	2.47760100	-4.28222600	1.10676900
H	2.84832100	-3.69486700	2.72562800
H	1.45254500	-3.04596700	1.86456700
C	-4.84797600	-1.30939100	-0.12709700
F	-5.62276500	-2.02428600	-0.96670300
F	-5.18663400	-1.66807800	1.13210900
F	-5.18300200	-0.00856700	-0.26806900
Pd	0.40734800	0.75220000	0.11175200
C	1.28681300	2.77776300	-0.71514800
C	1.78037200	2.56329100	-2.02828300
C	2.12764700	2.44401500	0.38134300
C	3.07249300	2.10165400	-2.23028000
H	1.15758100	2.80749800	-2.88186600
C	3.44692100	1.99029700	0.15593300
H	1.83119600	2.72234200	1.38947200
C	3.91583300	1.82372800	-1.13729200
H	3.44440100	1.97539700	-3.24317200
H	4.09552700	1.80346800	1.00516600
H	4.93570000	1.49357200	-1.31131800
C	-0.86441400	2.34776200	0.28469000
C	-0.06047400	3.45287400	-0.41514500
H	-1.74442300	2.05960900	-0.30003200
H	0.14205900	4.27358400	0.28468900

C	-0.77608300	4.03410200	-1.63439500
H	-1.70271100	4.52316800	-1.31797800
H	-0.15786800	4.78155100	-2.14353600
H	-1.04195500	3.25641300	-2.35889300
C	-1.23693900	2.62931800	1.73357000
C	-2.26534200	3.76233300	1.84055200
H	-2.52382500	3.93891300	2.89206400
H	-1.86994900	4.70104900	1.44063000
H	-3.18087000	3.50655500	1.29664200
O	-1.77100700	1.41915400	2.29317500
H	-2.13181800	1.63495100	3.16604800
H	-0.33414400	2.92446700	2.29007000

21-s

B3LYP SCF energy in DMF: -1619.947851 a.u.

M06 SCF energy in DMF: -1619.351644 a.u.

M06 Free energy in DMF: -1618.91386 a.u.

C	-2.28925700	-0.78643400	0.29369300
C	-0.51473700	-2.09409900	-0.41491700
C	-1.30708800	-3.23499000	-0.47602900
C	-2.64988300	-3.13378300	-0.11773200
C	-3.14024200	-1.89388900	0.28257500
H	-2.64695600	0.19585400	0.57493000
H	-0.87977300	-4.17975500	-0.78892200
H	-3.29534000	-4.00456500	-0.14962600
C	0.92884500	-2.11763100	-0.69833800
N	1.71847600	-1.14221000	-0.40169300
C	2.83189000	-2.85172000	-1.58696600
C	3.10275100	-1.61037900	-0.70774300
H	2.87025000	-2.63142600	-2.65703800
H	3.61633800	-0.83570600	-1.28289100
O	1.44166600	-3.20644400	-1.27181600
H	3.44888200	-3.72056500	-1.36576900
N	-1.00211600	-0.88372600	-0.05275700
C	3.94774800	-1.90220600	0.57532300
C	4.05436000	-0.62951200	1.42897700
H	3.07757900	-0.32858500	1.81816400
H	4.71370000	-0.80701200	2.28591200
H	4.47323300	0.20353800	0.85405700
C	5.36313300	-2.31095500	0.12118800
H	6.00022700	-2.48095800	0.99567800
H	5.36383300	-3.23472700	-0.46702900
H	5.82898800	-1.52513000	-0.48472300
C	3.32783800	-3.02447400	1.42908900
H	3.27321200	-3.97765400	0.89281800
H	3.94165100	-3.19008300	2.32092000
H	2.32053600	-2.76282200	1.77155000
C	-4.56851100	-1.73894300	0.73643300
F	-5.39237200	-2.57494300	0.07298300
F	-4.69886500	-2.01502100	2.05345900
F	-5.02102000	-0.48216300	0.54752000
Pd	0.42461800	0.74053700	-0.25182000
C	-1.09886900	2.02500100	-0.45456600
C	-1.69344100	2.13981900	-1.71749300
C	-1.65883800	2.69370800	0.64197400
C	-2.85132600	2.91256400	-1.87874600
H	-1.27129900	1.62882000	-2.57877800
C	-2.81975600	3.45963600	0.47286400
H	-1.18429400	2.63752600	1.61691400
C	-3.41823600	3.57062700	-0.78490300
H	-3.30775600	2.99319800	-2.86225200
H	-3.24941400	3.97436700	1.32889600
H	-4.31687800	4.16779200	-0.91228600
C	2.09664000	2.03332600	-1.05664600
C	1.59729400	2.67665800	0.06013900
H	2.95153800	1.37255000	-0.91826000
H	0.89083900	3.48936900	-0.08878200
C	2.25648900	2.65852700	1.41781300
C	1.82068800	2.44699500	-2.47539600
H	0.94263100	3.09142100	-2.55488600
H	2.69046200	3.00511100	-2.84865400

H	1.69365200	1.58140100	-3.13319200
C	3.00455000	3.97723000	1.64474100
H	3.80923100	4.10356000	0.91318500
H	2.32311000	4.83109400	1.56864800
H	3.45704900	3.98263200	2.64341600
O	1.23057700	2.47849500	2.40411900
H	1.64569100	2.58837200	3.27279400
H	2.97221500	1.83150400	1.46397600

22-s

B3LYP SCF energy in DMF: -1619.962602 a.u.

M06 SCF energy in DMF: -1619.375886 a.u.

M06 Free energy in DMF: -1618.934985 a.u.

C	2.65450700	-0.19085100	0.06854800
C	1.59863600	1.77644300	-0.49891100
C	2.80295400	2.41920400	-0.76594900
C	3.98843300	1.70363900	-0.59746900
C	3.90970500	0.38206800	-0.17295800
H	2.56280000	-1.22002000	0.39532400
H	2.81390600	3.45035300	-1.09710100
H	4.94668700	2.17024700	-0.79545600
C	0.30176200	2.46095800	-0.60935300
N	-0.83027000	1.88085700	-0.38527200
C	-1.12436900	4.11205900	-1.06413400
C	-1.87775900	2.94331400	-0.38931000
H	-1.32753300	4.18193600	-2.13586600
H	-2.71016800	2.61932500	-1.01634900
O	0.29232200	3.75676800	-0.91601000
H	-1.26333300	5.08570300	-0.59824600
N	1.51987600	0.48905300	-0.08899100
C	-2.44365000	3.26157200	1.03380800
C	-3.11967300	2.01197400	1.62542400
H	-2.40470500	1.20018100	1.78609800
H	-3.57058000	2.25729500	2.59348500
H	-3.91787600	1.64363300	0.97145200
C	-3.51530800	4.35943500	0.87396900
H	-3.98163800	4.56656900	1.84303200
H	-3.09961200	5.30257200	0.50450900
H	-4.30596200	4.04517200	0.18284700
C	-1.33958600	3.74519800	1.99184900
H	-0.84342200	4.65227200	1.63052800
H	-1.77409500	3.98206300	2.96899700
H	-0.57536100	2.97651300	2.15241300
C	5.14298400	-0.45043600	0.05776400
F	6.24746500	0.12994400	-0.45002200
F	5.36402900	-0.65266900	1.37641300
F	5.02559000	-1.67161800	-0.50939900
Pd	-0.67510400	-0.25478600	-0.15792300
C	-0.98959000	-2.54180500	-0.00488500
C	0.05367100	-3.21786500	-0.69086000
C	-0.78680400	-2.19772600	1.35761700
C	1.21384200	-3.59018100	-0.02901800
H	-0.09226000	-3.48335000	-1.73435900
C	0.40288800	-2.56829100	2.01527600
H	-1.60282400	-1.77903900	1.93888200
C	1.38510200	-3.27416400	1.33211200
H	1.98925100	-4.13539900	-0.55912500
H	0.52987000	-2.32663500	3.06636300
H	2.28949000	-3.58398800	1.84798500
C	-2.58070200	-0.82021400	-0.66225200
C	-2.36347600	-2.33391300	-0.65852700
H	-3.22841400	-0.48126600	0.15065900
H	-2.29001700	-2.69390500	-1.69154400
C	-3.47044000	-3.15022400	0.03693900
C	-2.97130400	-0.23463200	-2.00663400
H	-2.23638400	-0.47605900	-2.78314000
H	-3.93153800	-0.66146100	-2.33258800
H	-3.09614900	0.84991800	-1.97485000
C	-4.82743000	-3.01340900	-0.64931200
H	-5.18887500	-1.98042400	-0.62608200
H	-4.77027300	-3.34303700	-1.69242300

H	-5.57271400	-3.63268200	-0.13620200
O	-3.02588900	-4.51009400	0.02165100
H	-3.69164000	-5.03629900	0.48788700
H	-3.56065700	-2.79661800	1.07669500

23-s

B3LYP SCF energy in DMF: -1619.950482 a.u.

M06 SCF energy in DMF: -1619.354501 a.u.

M06 Free energy in DMF: -1618.915812 a.u.

C	-2.36645200	-0.78404100	0.06677700
C	-0.49620500	-2.00891500	-0.53601000
C	-1.26388700	-3.11299600	-0.88745000
C	-2.64798900	-3.03782100	-0.73916200
C	-3.20163900	-1.86041400	-0.24509400
H	-2.76728100	0.14957400	0.43955700
H	-0.78776700	-4.01174900	-1.25987300
H	-3.27486300	-3.88442400	-0.99643000
C	0.97440200	-2.01644500	-0.58499600
N	1.69010600	-1.05691000	-0.10994200
C	3.01710800	-2.70211100	-1.14084600
C	3.10961000	-1.50183600	-0.17074100
H	3.25497000	-2.43133200	-2.17286800
H	3.69987400	-0.69604300	-0.61031600
O	1.59353500	-3.07261500	-1.11214900
H	3.58610800	-3.58308600	-0.85038200
N	-1.04061900	-0.85500400	-0.07716300
C	3.70022600	-1.84853000	1.23680500
C	3.63258000	-0.61694700	2.15682000
H	2.60115200	-0.29322600	2.32483400
H	4.06978300	-0.85692900	3.13233100
H	4.19658100	0.22485900	1.74108200
C	5.18110800	-2.23193900	1.04057900
H	5.64867200	-2.42849500	2.01141400
H	5.30181100	-3.13428800	0.43207600
H	5.73986500	-1.42164300	0.55792700
C	2.94436700	-3.01283300	1.90392200
H	2.98860500	-3.93443400	1.31417900
H	3.39130500	-2.23319200	2.87936400
H	1.89086700	-2.76653500	2.07739300
C	-4.69350900	-1.70544900	-0.09638500
F	-5.29425900	-2.88644100	0.15025800
F	-5.00924900	-0.86602700	0.91187500
F	-5.25098200	-1.20198900	-1.22068000
Pd	0.40606300	0.76676000	0.11159100
C	-1.06042300	2.09130500	0.42920600
C	-1.81110800	2.64508100	-0.61714600
C	-1.43044800	2.35381500	1.75551000
C	-2.92610200	3.44504200	-0.33689300
H	-1.53965800	2.45720700	-1.65276200
C	-2.54681200	3.15519100	2.03000700
H	-0.85996900	1.93724900	2.58185400
C	-3.29614400	3.70218500	0.98573000
H	-3.50212300	3.86681300	-1.15691800
H	-2.82570100	3.34862200	3.06294200
H	-4.16077000	4.32394100	1.20086900
C	2.13665000	2.16582700	0.43923500
C	1.52636800	2.54629700	-0.74349300
H	0.83895000	3.38719200	-0.72092300
H	2.97244200	1.47676000	0.36544100
C	2.02982400	2.92916000	1.73169600
H	1.17948600	3.61398500	1.74180800
H	2.94636500	3.52159800	1.85799000
H	1.96287300	2.26329200	2.59741200
C	2.01707800	2.22033400	-2.13520700
H	1.15751800	1.91225200	-2.74943800
C	2.62465900	3.48319900	-2.76464800
H	3.47896100	3.83517900	-2.17731800
H	1.88429800	4.28707200	-2.82773100
H	2.96627600	3.26131700	-3.78179400
O	2.97741200	1.16855200	-2.06909400
H	3.23934500	0.96055400	-2.97760500

TS13-s

B3LYP SCF energy in DMF: -1619.919606 a.u.

M06 SCF energy in DMF: -1619.330075 a.u.

M06 Free energy in DMF: -1618.889836 a.u.

C	-2.25078600	-0.94529700	0.15624300
C	-0.39600600	-2.08548800	-0.61884300
C	-1.15010900	-3.20108200	-0.96805400
C	-2.52238000	-3.17295100	-0.72429700
C	-3.07623900	-2.03303100	-0.14645100
H	-2.64998800	-0.03876000	0.59542300
H	-0.67580900	-4.07053900	-1.40702200
H	-3.14146100	-4.02759000	-0.97387200
C	1.06719900	-2.02722500	-0.76663700
N	1.79077700	-1.11522000	-0.20692400
C	3.06676900	-2.49677200	-1.62607200
C	3.21504900	-1.45965300	-0.48973100
H	3.17232100	-2.05479100	-2.62036600
H	3.72485700	-0.56181300	-0.84884200
O	1.67526900	-2.95417600	-1.50596800
H	3.70648400	-3.37297000	-1.54167500
N	-0.93830400	-0.97111200	-0.07960800
C	3.98410300	-1.98672800	0.76499100
C	3.96114300	-0.92286000	1.87267300
H	2.94499700	-0.74525800	2.23600200
H	4.56687100	-1.25373600	2.72362200
H	4.37410600	0.02764200	1.51867200
C	5.44877700	-2.23009500	0.34859600
H	6.02949800	-2.57094200	1.21243700
H	5.54117400	-2.99489200	-0.42974100
H	5.91382600	-1.31035100	-0.02509900
C	3.37115300	-3.29149000	1.30645700
H	3.40890800	-4.10616800	0.57596000
H	3.93006300	-3.62232300	2.18840400
H	2.32904000	-3.15269500	1.61472600
C	-4.55851100	-1.93515900	0.10120600
F	-5.10059300	-3.14081900	0.36775500
F	-4.84038100	-1.12082000	1.14009400
F	-5.20681400	-1.43867500	-0.97720200
Pd	0.56610200	0.65182200	0.23512600
C	-0.81966300	2.22649900	0.32592800
C	-1.73614600	2.35311200	-0.73359000
C	-1.25937700	2.48141800	1.64053800
C	-3.06624500	2.69851500	-0.47932800
H	-1.42513900	2.17756400	-1.75837300
C	-2.59456500	2.80697200	1.88923000
H	-0.56140200	2.43160200	2.47013900
C	-3.50026500	2.92277100	0.83013700
H	-3.76239400	2.79139800	-1.30858400
H	-2.92178800	2.98427800	2.91023300
H	-4.53409300	3.19419700	1.02350300
C	2.01363700	2.13134800	0.50572900
C	1.03146800	2.99580400	-0.08330400
H	0.72676900	3.83455800	0.53644000
H	2.80364100	1.78451900	-0.15755100
C	2.43067000	2.37416900	1.94051500
H	1.61460200	2.78681900	2.53977100
H	3.25039500	3.10693200	1.95616000
H	2.79824000	1.47031300	2.42897900
C	1.09931500	3.33050900	-1.58251700
H	0.54681000	2.57944900	-2.15848200
C	0.52218400	4.71549100	-1.86835400
H	1.09553800	5.48300500	-1.33736900
H	-0.52401500	4.78187700	-1.55430100
H	0.56485200	4.93233100	-2.94142400
O	2.48335500	3.26785100	-1.95811900
H	2.51916200	3.43758600	-2.91136000

24-s

B3LYP SCF energy in DMF: -1619.954965 a.u.

M06 SCF energy in DMF: -1619.367761 a.u.

M06 Free energy in DMF: -1618.926082 a.u.

C	-2.71151200	-0.03506000	0.41204000
C	-1.38006300	-1.54471100	-0.71350400
C	-2.47808600	-2.19789000	-1.26558300
C	-3.75307000	-1.73886300	-0.93818100
C	-3.86889400	-0.65199800	-0.07595200
H	-2.76879400	0.82181000	1.07151800
H	-2.34109100	-3.05128000	-1.91869400
H	-4.63336800	-2.22989700	-1.33801700
C	0.00095900	-2.01401500	-0.91376600
N	1.00096400	-1.59053600	-0.21136300
C	1.69459600	-3.06123600	-1.91133300
C	2.17971300	-2.42299400	-0.59173700
H	2.01805800	-2.50672300	-2.79627400
H	3.03374600	-1.76487500	-0.77093900
O	0.23149800	-2.94215000	-1.84091700
H	1.92953800	-4.11673600	-2.03258500
N	-1.49048400	-0.46598400	0.09358600
C	2.58047900	-3.45800400	0.51152000
C	2.93511400	-2.72502900	1.81502900
H	2.07385200	-2.18846200	2.22331800
H	3.26728400	-3.44635800	2.56981200
H	3.74936400	-2.00976100	1.65903800
C	3.83445100	-4.20593200	0.01595400
H	4.17456100	-4.91181000	0.78130900
H	3.64726000	-4.78093600	-0.89704500
H	4.65718600	-3.50994300	-0.18525800
C	1.44871300	-4.46395400	0.79312000
H	1.18861800	-5.06131600	-0.08710100
H	1.76416000	-5.16292400	1.57515400
H	0.54130600	-3.96486600	1.15055200
C	-5.21977900	-0.10086200	0.29605800
F	-6.16820900	-1.05923300	0.29256100
F	-5.20964800	0.46059100	1.52372100
F	-5.62113600	0.85623400	-0.57172200
Pd	0.59277800	0.42795400	0.50258600
C	0.88272300	2.67365800	-0.00250200
C	0.25870000	2.84726100	-1.26830200
C	0.06099000	2.74357400	1.15673500
C	-1.09208500	3.15320700	-1.35630600
H	0.84767200	2.77658000	-2.17575800
C	-1.31014500	3.06106400	1.04940500
H	0.51884500	2.72647400	2.14101900
C	-1.87981300	3.27532500	-0.19660300
H	-1.54129700	3.31296500	-2.33235100
H	-1.90432900	3.15771300	1.95337500
H	-2.93071100	3.53593100	-0.28069200
C	2.52018900	1.05897000	0.72324300
C	2.39908500	2.50093200	0.20920900
H	2.70385000	3.19958000	0.99947800
H	3.09320800	0.42184700	0.04561000
C	2.97617100	0.93567400	2.16599200
H	2.38290100	1.56341300	2.83920900
H	4.01843100	1.28294800	2.23982600
H	2.94469400	-0.09055900	2.53610800
C	3.28748000	2.79512200	-1.00855100
C	2.95402000	2.18071000	-1.85993600
H	3.29365000	4.26999400	-1.40998900
H	3.65907700	4.88390700	-0.57958400
H	2.29989800	4.62846100	-1.69364700
H	3.95722200	4.42684400	-2.26869100
O	4.60538900	2.38491100	-0.61813400
H	5.19210300	2.56120100	-1.36787200

25-s

B3LYP SCF energy in DMF: -1619.951429 a.u.

M06 SCF energy in DMF: -1619.354815 a.u.

M06 Free energy in DMF: -1618.915613 a.u.

C	-2.73423000	0.11685400	-0.42348500
C	-1.31774600	1.60715100	0.61831300

C	-2.37028600	2.41778200	1.02726000	H	2.63496600	3.28774800	-1.51516000
C	-3.66763300	2.05114200	0.66928100	H	4.88929700	2.33682100	-0.97860500
C	-3.84743900	0.89117200	-0.07598700	C	0.23526000	2.12504700	-0.86318800
H	-2.85666400	-0.80308300	-0.98293600	N	-0.81042000	1.55801900	-0.36865800
H	-2.18046200	3.31692000	1.60085500	C	-1.37705700	3.36013500	-1.77288100
H	-4.51365500	2.66162800	0.96408100	C	-1.96609500	2.44579600	-0.67546700
C	0.08997800	1.96441300	0.85319300	H	-1.60991200	3.01313400	-2.78318500
N	1.07276200	1.31819100	0.31497400	H	-2.78016100	1.83525800	-1.07395000
C	1.84423400	3.01153000	1.73995900	O	0.07610000	3.22858600	-1.59731800
C	2.31336600	2.09723600	0.58824500	H	-1.62283900	4.41650300	-1.68128500
H	2.06716700	2.59917600	2.72723500	N	1.65798500	0.41822300	-0.01263500
H	3.09165800	1.41162200	0.92903900	C	-2.49839800	3.20399200	0.58509300
O	0.37644900	3.02166800	1.60372500	C	-2.93291700	2.18977200	1.65567700
H	2.18105800	4.04441600	1.68400400	H	-2.08751700	1.59651300	2.01643300
N	-1.49274500	0.46048000	-0.08096200	H	-3.36337200	2.71581500	2.51535100
C	2.83989300	2.86445100	-0.67122600	H	-3.69251800	1.50327400	1.26970400
C	3.12270700	1.87825700	-1.81695100	C	-3.73026600	4.02386700	0.15164200
H	2.21138000	1.37215200	-2.14994300	H	-4.16303300	4.53594700	1.01788700
H	3.53530100	2.41918300	-2.67592400	H	-3.47987200	4.79076800	-0.58907500
H	3.84919800	1.11664900	-1.51990300	H	-4.50567500	3.37928300	-0.27814500
C	4.16469700	3.54591300	-0.27340100	C	-1.43428200	4.14240500	1.18339700
H	4.58214500	4.08129300	-1.13286100	H	-1.11900400	4.92054100	0.48053100
H	4.03645000	4.27481600	0.53415700	H	-1.84342200	6.64975800	2.06376500
H	4.90579500	2.80767200	0.05382000	H	-0.54445500	3.59292600	1.51013700
C	1.83512900	3.92407100	-1.16348700	C	5.35998000	-0.04840500	0.33072400
H	1.63380100	4.69615500	-0.41355700	F	6.38934700	0.47155600	-0.36515500
H	2.24159900	4.43050300	-2.04547100	F	5.62708000	0.13906400	1.64270400
H	0.88088100	3.47482200	-1.46091900	F	5.35514300	-1.38314000	0.11962200
C	-5.21131400	0.47070200	-0.55793100	Pd	-0.29195600	-0.55949700	0.20294800
F	-6.19547100	0.99979000	0.19437100	C	-2.20355900	-1.40771200	0.21970000
F	-5.42443100	0.86583000	-1.83330300	C	-2.95794100	-1.21002600	-0.94949000
F	-5.35306400	-0.87231000	-0.53351800	C	-2.86537000	-1.48021900	1.45971200
Pd	0.49183400	-0.67924000	-0.21510900	C	-4.34099700	-1.02990800	-0.87175000
C	2.36909700	-1.36033500	-0.05796400	H	-2.46994100	-1.19656900	-1.91884900
C	2.89254600	-1.55356600	1.22885600	C	-4.24973900	-1.31320800	1.53134700
C	3.19087400	-1.57040600	-1.17085100	H	-2.30230000	-1.68294400	2.36660500
C	4.22496300	-1.95208400	1.39652900	C	-4.98956700	-1.08560400	0.36619000
H	2.27186700	-1.39757900	2.10698100	H	-4.91345800	-0.86441200	-1.78068000
C	4.52283700	-1.97122300	-0.99764200	H	-4.75043700	-1.36770200	2.49430900
H	2.81394300	-1.41904200	-2.17735100	H	-6.06791500	-0.96493500	0.42089300
C	5.04304700	-2.16344400	0.28397500	C	0.43051500	-2.46590900	0.60159800
H	4.61690800	-2.09858000	2.40005600	C	-0.80869200	-2.97855600	0.10788400
H	5.15024200	-2.12905900	-1.87147100	H	1.27131900	-2.51567000	-0.09306500
H	6.07564700	-2.47510300	0.41467100	H	-1.43179500	-3.50132900	0.82769100
C	-0.35402200	-2.51035900	-1.25435900	C	-0.90152900	-3.57696900	-1.28603700
C	-0.16867600	-2.80066900	0.08812600	C	0.79093100	-2.65239800	2.06219200
H	-1.32699000	-2.12954600	-1.56288800	H	-0.08772400	-2.56988800	2.70940100
H	0.71551700	-3.36795800	0.37375700	H	1.22237800	-3.65216800	2.21265400
C	-1.28392900	-2.82732300	1.10843400	H	1.53591300	-1.92475000	2.39826000
C	0.47854100	-3.05809200	-2.37716800	C	0.05119200	-4.77753900	-1.40079900
H	1.43305700	-3.45942700	-2.03438400	H	1.09801600	-4.47367900	-1.31273600
H	-0.08706600	-3.87536000	-2.84593900	H	-0.16843300	-5.52119900	-0.62755400
H	0.65638300	-2.31124500	-3.15733800	H	-0.07959600	-5.25134300	-2.38052600
C	-1.71829200	-4.27620700	1.35777700	O	-2.24758100	-4.00488200	-1.47925100
H	-2.11179700	-4.73137400	0.44320900	H	-2.30336100	-4.37891600	-2.37050900
H	-0.87739800	-4.87848800	1.71721700	H	-0.61913300	-2.82342400	-2.03446100
H	-2.51215500	-4.30196800	2.11349400				
O	-0.79386200	-2.22755600	2.31384400				
H	-1.47669200	-2.34539700	2.99141800				
H	-2.14567900	-2.26394800	0.72835800				

TS14-s

B3LYP SCF energy in DMF: -1619.922271 a.u.

M06 SCF energy in DMF: -1619.332737 a.u.

M06 Free energy in DMF: -1618.894592 a.u.

C	2.85994900	-0.09186100	0.26567300
C	1.59854800	1.61986400	-0.63773800
C	2.73175700	2.33560700	-1.00795100
C	3.98508700	1.80361800	-0.70784200
C	4.04547500	0.57472000	-0.05914100
H	2.88504800	-1.05818300	0.75434100

26-s

B3LYP SCF energy in DMF: -1619.960677 a.u.

M06 SCF energy in DMF: -1619.373366 a.u.

M06 Free energy in DMF: -1618.933209 a.u.

C	2.72826400	-0.02974500	0.07924100
C	1.47509200	1.82598200	-0.50042600
C	2.61185000	2.55127000	-0.84381500
C	3.85981300	1.94891400	-0.70094700
C	3.91471400	0.63894000	-0.23343200
H	2.74538900	-1.05538900	0.42721200
H	2.51970300	3.56448200	-1.21539200
H	4.76452200	2.48932100	-0.95626300
C	0.12145700	2.39493600	-0.60012200
N	-0.93830600	1.74265300	-0.27514600

C	-1.46045600	3.86713200	-1.14350900
C	-2.07334000	2.69917500	-0.33524600
H	-1.70866400	3.82080700	-2.20721900
H	-2.89575900	2.23695900	-0.88741300
O	-0.01157700	3.65483000	-1.02697000
H	-1.67477900	4.86320800	-0.75988000
N	1.53119600	0.55159000	-0.03822100
C	-2.59954100	3.08755900	1.08698600
C	-3.04317500	1.82172200	1.84082800
H	-2.20509800	1.13793300	2.01150900
H	-3.45630000	2.09572700	2.81818900
H	-3.81916100	1.27952900	1.29100000
C	-3.82236100	4.00744500	0.90184500
H	-4.23878900	4.27951900	1.87780000
H	-3.56737300	4.93870100	0.38470900
H	-4.61220500	3.50868300	0.32824100
C	-1.52331400	3.81294600	1.91643700
H	-1.20148800	4.75255200	1.45536900
H	-1.92363400	4.05949900	2.90575700
H	-0.63865600	3.18540400	2.07072900
C	5.23377700	-0.05421800	-0.01160900
F	6.19347600	0.42888700	-0.82518500
F	5.66815600	0.10736000	1.25886500
F	5.14251300	-1.38351500	-0.22967500
Pd	-0.42701100	-0.42541300	0.13177800
C	-2.01587100	-2.07669300	-0.27888300
C	-1.67476800	-1.70939000	-1.60925800
C	-3.26745700	-1.65047900	0.23265500
C	-2.57186600	-0.96459100	-2.39514500
H	-0.77423300	-2.10568800	-2.06838100
C	-4.15134600	-0.92634900	-0.55744400
H	-3.54376300	-1.93259700	1.24495800
C	-3.80449800	-0.58354700	-1.87503300
H	-2.30611200	-0.71461400	-3.41811600
H	-5.11733000	-0.63233700	-0.15788200
H	-4.50593400	-0.02791000	-2.49091300
C	0.18665700	-2.26804400	0.74565300
C	-1.11422000	-3.03890200	0.51439600
H	0.99708000	-2.57736300	0.07653500
H	-1.60436600	-3.22196900	1.47785600
C	-0.94366600	-4.40001600	-0.18525900
C	0.62690000	-2.15385400	2.19431000
H	-0.17681800	-1.76355300	2.82931300
H	0.88866500	-3.14896400	2.58476400
H	1.50694100	-1.51553300	2.31968600
C	-0.10524900	-5.38044400	0.63227700
H	0.91305300	-5.00856300	0.78550700
H	-0.56430300	-5.56284700	1.61010500
H	-0.02822600	-6.33949700	0.10638800
O	-2.26509800	-4.90626300	-0.39444300
H	-2.18019700	-5.74574100	-0.86936200
H	-0.44815500	-4.23207800	-1.15477300

27-s

B3LYP SCF energy in DMF: -1619.948363 a.u.

M06 SCF energy in DMF: -1619.355701 a.u.

M06 Free energy in DMF: -1618.916878 a.u.

C	2.79551000	-0.01177900	-0.06331400
C	1.37131200	1.74526200	-0.50813000
C	2.42487200	2.60950500	-0.78555200
C	3.72728100	2.12242900	-0.68342400
C	3.91180000	0.79459400	-0.31178300
H	2.91803300	-1.05178100	0.21351500
H	2.23187300	3.63602600	-1.07239600
H	4.57389400	2.76707000	-0.89212500
C	-0.03316700	2.18223200	-0.54257600
N	-1.01838900	1.41636400	-0.20474400
C	-1.78010100	3.49318100	-0.98322200
C	-2.24712800	2.26024800	-0.17950800
H	-2.04508500	3.43583100	-2.04202600
H	-3.04493900	1.73403500	-0.70724700

O	-0.31093400	3.42913600	-0.90600400
H	-2.08217300	4.45629100	-0.57768500
N	1.54770400	0.44945100	-0.15853800
C	-2.73921500	2.58039300	1.27213600
C	-3.04083600	1.27621500	2.03030300
H	-2.14079200	0.66901400	2.16571000
H	-3.43783000	1.51054800	3.02434400
H	-3.78649200	0.67108300	1.50613500
C	-4.04739800	3.38803200	1.15065000
H	-4.44702400	3.59973000	2.14815800
H	-3.90266200	4.34955800	0.64659500
H	-4.80979700	2.82810300	0.59677400
C	-1.69780200	3.39169200	2.06607400
H	-1.48670100	4.36452000	1.61040300
H	-2.07463500	3.58391700	3.07632400
H	-0.75227200	2.84796900	2.17126700
C	5.29442100	0.22503300	-0.12624500
F	6.19363000	0.82898600	-0.92784800
F	5.72467700	0.38254500	1.14567000
F	5.32907200	-1.09757300	-0.39457100
Pd	-0.48100500	-0.66064700	-0.19492000
C	-2.35476800	-1.23671500	-0.60302000
C	-2.82258200	-0.94677500	-1.89252700
C	-3.21551700	-1.84210700	0.32060300
C	-4.13831800	-1.26342900	-2.25358800
H	-2.17075300	-0.47504600	-2.62353500
C	-4.53226800	-2.15279100	-0.04520400
H	-2.88036800	-2.07266600	1.32736700
C	-4.99626300	-1.86684400	-1.33083800
H	-4.48702500	-1.03514300	-3.25779800
H	-5.19133000	-2.62028300	0.68226200
H	-6.01674600	-2.11237000	-1.61149000
C	0.45531000	-2.61576700	-0.82446900
C	-0.04923500	-2.75665500	0.45849500
H	1.49491200	-2.30973200	-0.93431400
C	-0.15179800	-3.22465400	-2.05672400
H	-0.10690400	-2.54448900	-2.91301800
H	0.44187300	-4.10994100	-2.32328300
H	-1.18483200	-3.54029500	-1.90076600
H	-0.99948000	-3.27346800	0.57530100
C	0.79907900	-2.70741600	1.71684400
H	1.61601600	-1.98521900	1.58591600
C	-0.00452900	-2.33663600	2.96053500
H	0.63250600	-2.38296300	3.85160400
H	-0.39763100	-1.31760600	2.88531500
H	-0.84231400	-3.02803200	3.10148000
O	1.34057700	-4.03405100	1.82804200
H	1.76420800	-4.09543000	2.69787400

TS15-s

B3LYP SCF energy in DMF: -1619.919589 a.u.

M06 SCF energy in DMF: -1619.329024 a.u.

M06 Free energy in DMF: -1618.889746 a.u.

C	2.83349100	-0.22223000	0.07277100
C	1.61234600	1.67727200	-0.42797900
C	2.76230500	2.42804800	-0.64281100
C	4.00230800	1.81209100	-0.47703200
C	4.03435000	0.47196600	-0.10609700
H	2.83112600	-1.27157300	0.34176100
H	2.68980300	3.47077600	-0.92687700
H	4.91901600	2.36915600	-0.63352100
C	0.26015400	2.25283000	-0.51074500
N	-0.79363200	1.60775700	-0.14571700
C	-1.33107600	3.71092000	-1.05452500
C	-1.92697900	2.57258700	-0.19506500
H	-1.59361600	3.62448700	-2.11225500
H	-2.77074600	2.10063600	-0.70460600
O	0.12090600	3.50456400	-0.95241500
H	-1.54024800	4.72046600	-0.70527500
N	1.64532200	0.36426500	-0.08914300
C	-2.40037800	3.01710300	1.22971000

C	-2.84304800	1.78970200	2.04415000
H	-2.01789900	1.08800000	2.20132100
H	-3.20482000	2.10692400	3.02873800
H	-3.65754600	1.25632800	1.54557800
C	-3.61553900	3.94930300	1.05034000
H	-3.99866900	4.25752900	2.02915100
H	-3.36622100	4.86034800	0.49608700
H	-4.42845100	3.44302300	0.51702200
C	-1.28669700	3.75347200	1.99839300
H	-0.95064100	4.66005000	1.48467500
H	-1.65794900	4.05938400	2.98242700
H	-0.41574100	3.11024700	2.16537500
C	5.33416000	-0.24884700	0.13749000
F	6.37953400	0.39906900	-0.41118200
F	5.58738900	-0.37456700	1.45939300
F	5.30976600	-1.49775300	-0.37719300
Pd	-0.30795800	-0.59558400	-0.14727400
C	-2.19295400	-1.39708300	-0.63875700
C	-2.31347600	-1.43814700	-2.04399700
C	-3.33836800	-1.14871500	0.13252400
C	-3.53809200	-1.16872100	-2.65734600
H	-1.45443400	-1.68309700	-2.66097500
C	-4.56680900	-0.89885100	-0.48779900
H	-3.28901000	-1.13762700	1.21539200
C	-4.66995700	-0.90115400	-1.88068800
H	-3.61007600	-1.18580400	-3.74154200
H	-5.44344300	-0.70358400	0.12396700
H	-5.62705300	-0.71141700	-2.35806800
C	0.36565900	-2.56583300	-0.17872500
C	-0.99872900	-2.90043600	0.10578100
H	-1.48942900	-3.52365900	-0.63544500
C	-1.43300400	-3.20061200	1.54992500
H	-1.87843200	-2.30827900	2.00070600
C	-2.45253700	-4.33854700	1.58110100
H	-3.34799100	-4.07749000	1.00749400
H	-2.02086500	-5.25211600	1.15815700
H	-2.76005900	-4.54611700	2.61168000
O	-0.25595900	-3.54395000	2.29366800
H	-0.52711200	-3.62638100	3.21985700
H	1.02888700	-2.56665000	0.68543000
C	1.00768800	-3.00115600	-1.47774000
H	1.87911100	-2.38777700	-1.72660600
H	1.36052300	-4.03774600	-1.38038100
H	0.30754300	-2.97076800	-2.31712500

28-s

B3LYP SCF energy in DMF: -1619.955899 a.u.

M06 SCF energy in DMF: -1619.369064 a.u.

M06 Free energy in DMF: -1618.928288 a.u.

C	2.64287400	0.25402800	0.17349400
C	1.22829300	1.97291700	-0.45588400
C	2.28277400	2.87451400	-0.55696000
C	3.57159400	2.43354000	-0.26266700
C	3.74828200	1.10682200	0.11884600
H	2.75723600	-0.78762600	0.44763200
H	2.09550600	3.90101900	-0.84703000
H	4.41394200	3.11313000	-0.32771900
C	-0.17450400	2.38022900	-0.63895600
N	-1.17064800	1.65135500	-0.27278200
C	-1.87442700	3.62924800	-1.34346400
C	-2.38676200	2.50024200	-0.42285500
H	-2.07638100	3.43535100	-2.40067100
H	-3.16602600	1.91751900	-0.91996100
O	-0.41698200	3.58413900	-1.16793700
H	-2.20365200	4.63371000	-1.08389300
N	1.40857600	0.67312500	-0.11758200
C	-2.94649300	2.99163700	0.95476500
C	-3.28257700	1.78424100	1.84548300
H	-2.39440600	1.18518800	2.06840600
H	-3.70223600	2.12834100	2.79752300
H	-4.02385700	1.13534600	1.37106100

C	-4.24497500	3.77685800	0.68037600
H	-4.69414500	4.10111100	1.62531700
H	-4.07041600	4.67414200	0.07724100
H	-4.98107800	3.15640400	0.15612100
C	-1.94120800	3.89401200	1.69584300
H	-1.68698500	4.79575500	1.12896100
H	-2.37403200	4.22243500	2.64698300
H	-1.01264200	3.36163400	1.93010200
C	5.10347000	0.57521800	0.50568000
F	6.09937000	1.27843400	-0.06818200
F	5.29298500	0.63147900	1.84295300
F	5.25114000	-0.71690400	0.14118400
Pd	-0.36534300	-0.54851400	-0.29524900
C	-1.74354300	-2.44113600	-0.22859000
C	-2.19709700	-1.79400500	-1.40877600
C	-2.53858600	-2.32164800	0.94244800
C	-3.43765100	-1.12670600	-1.43497400
H	-1.66051800	-1.94852800	-2.34073100
C	-3.76636000	-1.67581100	0.89791800
H	-2.21210900	-2.78080300	1.86889700
C	-4.22701500	-1.08964300	-0.29432500
H	-3.78166400	-0.67639500	-2.36120500
H	-4.37952800	-1.63125300	1.79298900
H	-5.19915300	-0.60651600	-0.31824300
C	0.65303000	-2.30859700	-0.47261000
C	-0.48675800	-3.32259800	-0.34603900
H	-0.57582400	-3.89141700	-1.28052400
C	-0.26765200	-4.34510600	0.77895000
H	-0.24611500	-3.81879500	1.74611600
C	-1.32563700	-5.44699800	0.81775000
H	-2.32935400	-5.05276700	1.00066300
H	-1.33596400	-5.99533900	-0.13056000
H	-1.09981900	-6.15755100	1.62156500
O	1.02546000	-4.90895700	0.51962000
H	1.20347100	-5.55021500	1.22284900
H	1.29734100	-2.30900800	0.41270400
C	1.44025300	-2.37981500	-1.76807600
H	2.20602100	-1.60259300	-1.84379300
H	1.94899600	-3.35354800	-1.82279600
H	0.78846200	-2.30566400	-2.64532400

29-s

B3LYP SCF energy in DMF: -1619.945242 a.u.

M06 SCF energy in DMF: -1619.351815 a.u.

M06 Free energy in DMF: -1618.912833 a.u.

C	2.31582600	-0.84797900	-0.12950100
C	0.48270000	-2.08054100	0.56651000
C	1.27756800	-3.16263400	0.92620600
C	2.65497000	-3.07301100	0.73144100
C	3.17591100	-1.90283800	0.18768100
H	2.69061200	0.07950500	-0.54283900
H	0.82740100	-4.05684000	1.33943700
H	3.30149200	-3.90327400	0.99315800
C	-0.98515300	-2.10940900	0.67100100
N	-1.74024900	-1.18444300	0.18510300
C	-2.98536500	-2.80514600	1.35621700
C	-3.14797200	-1.64964900	0.34206600
H	-3.17925600	-2.49601600	2.38660200
H	-3.74167100	-0.83999200	0.77457800
O	-1.55905300	-3.15036600	1.27263700
H	-3.55188700	-3.70642400	1.13018700
N	0.99571400	-0.93375800	0.05666100
C	-3.80842600	-2.06521900	-1.01332300
C	-3.81305200	-0.87168100	-1.98326500
H	-2.79758500	-0.57283800	-2.26014100
H	-4.34193700	-1.14062200	-2.90425500
H	-4.32696400	-0.00694200	-1.54832400
C	-5.26934200	-2.46082900	-0.71867600
H	-5.77981900	-2.72573200	-1.65080900
H	-5.34297000	-3.32558800	-0.05065300
H	-5.81967600	-1.63134300	-0.25962600

C	-3.06839400	-3.24445300	-1.67108600
H	-3.07856300	-4.14536700	-1.04888100
H	-3.55343800	-3.50210000	-2.61863800
H	-2.02576300	-2.99427700	-1.89689500
C	4.66067300	-1.73301000	-0.01037500
F	5.26714400	-2.91171300	-0.25359500
F	4.93577400	-0.90907900	-1.04277500
F	5.24547600	-1.20276600	1.08722800
Pd	-0.48091600	0.65175700	-0.16784000
C	0.96264000	2.00812800	-0.41826300
C	1.61402400	2.60719800	0.66753100
C	1.43980900	2.23357700	-1.71747400
C	2.72776800	3.43012500	0.45218600
H	1.26994200	2.43839300	1.68382400
C	2.55524200	3.05464700	-1.92629900
H	0.95184000	1.77388200	-2.57329600
C	3.19995700	3.65639800	-0.84262000
H	3.22491600	3.89002500	1.30278200
H	2.91571600	3.22067500	-2.93854600
H	4.06461900	4.29357100	-1.00623600
C	-2.09496300	2.02808400	0.54790800
C	-2.05652300	2.20251200	-0.82561500
H	-2.73818500	1.24034300	0.93808400
C	-1.73243000	3.09025800	1.56711300
H	-0.85115900	3.64871100	1.23009400
C	-1.46420700	2.49847300	2.94846600
H	-0.61551500	1.80711400	2.93048200
H	-2.34531900	1.95509300	3.30790500
H	-1.23358500	3.29391700	3.66617600
O	-2.87746900	3.96036800	1.59504100
H	-2.71935100	4.61010300	2.29693800
H	-2.62560000	1.49853300	-1.42757600
C	-1.65013900	3.45296800	-1.54762300
H	-1.15155300	3.22692200	-2.49382500
H	-2.56968000	4.00131600	-1.79482600
H	-1.01326100	4.11205300	-0.95694200

30-s

B3LYP SCF energy in DMF: -1619.957322 a.u.

M06 SCF energy in DMF: -1619.36996 a.u.

M06 Free energy in DMF: -1618.925869 a.u.

C	2.68802400	0.07770000	0.02417000
C	1.27511600	1.83811200	-0.44349900
C	2.33455100	2.69931100	-0.71029900
C	3.63399600	2.20673600	-0.59520500
C	3.80963000	0.87944000	-0.21699800
H	2.79397300	-0.96033400	0.31527400
H	2.14876900	3.72732300	-0.99699100
H	4.48537600	2.84857200	-0.79222200
C	-0.12876700	2.27493000	-0.48972700
N	-1.11684300	1.49405900	-0.20263900
C	-1.87310100	3.60309700	-0.88621400
C	-2.34482900	2.33555700	-0.13956000
H	-2.13208100	3.58947500	-1.94801800
H	-3.14396600	1.83808500	-0.69237300
O	-0.40551700	3.53903100	-0.80004700
H	-2.18134700	4.54679300	-0.44136900
N	1.44426100	0.54380600	-0.08480800
C	-2.84352500	2.59206200	1.32346100
C	-3.16889800	1.26007800	2.02365000
H	-2.28550400	0.62094500	2.11316300
H	-3.54317600	1.45746300	3.03428700
H	-3.94537600	0.70383500	1.48780100
C	-4.14073700	3.42138700	1.23242300
H	-4.55194000	3.57816400	2.23537400
H	-3.97875300	4.40963600	0.78904900
H	-4.90167800	2.90444500	0.63625800
C	-1.79728800	3.35313000	2.15947100
H	-1.56460800	4.33830500	1.74214000
H	-2.18213200	3.51445200	3.17211300
H	-0.86262600	2.78909600	2.25338800

C	5.18428400	0.27483800	-0.11078600
F	6.12033500	1.20285000	0.17138900
F	5.23905300	-0.66858700	0.85354900
F	5.55216200	-0.32201500	-1.26751700
Pd	-0.58269400	-0.56601600	-0.12336100
C	-0.79766200	-2.71173100	0.74628200
C	0.06313500	-2.88395900	-0.37096700
C	-0.23199600	-2.79618000	2.04721700
C	1.43130600	-3.18868200	-0.17629100
H	-0.34680000	-2.97053400	-1.37198500
C	1.10849600	-3.09680300	2.22084700
H	-0.87988500	-2.66136500	2.90914900
C	1.94568600	-3.30259400	1.10445100
H	2.06559700	-3.35622300	-1.04180400
H	1.51608100	-3.18813100	3.22357800
H	2.99164700	-3.55454400	1.25328900
C	-2.45394300	-1.35477100	-0.40366100
C	-2.31288000	-2.55737700	0.54897600
H	-3.14783600	-0.60271700	-0.02510700
C	-2.78242900	-1.63194600	-1.87417800
H	-2.23713200	-2.52079800	-2.22042000
C	-2.47910900	-0.47994200	-2.83304400
H	-1.40405700	-0.27906200	-2.88921300
H	-2.99141600	0.43582500	-2.52094200
H	-2.82441800	-0.73656300	-3.84209200
O	-4.19586500	-1.91704300	-1.88297000
H	-4.41432200	-2.24146200	-2.76974700
H	-2.72000200	-2.25455800	1.51966300
C	-2.98379900	-3.88331600	0.15480100
H	-2.80041900	-4.63197400	0.93436100
H	-4.06307000	-3.75448300	0.04260700
H	-2.59135000	-4.27857700	-0.78706400

31-s

B3LYP SCF energy in DMF: -1619.949299 a.u.

M06 SCF energy in DMF: -1619.353235 a.u.

M06 Free energy in DMF: -1618.914692 a.u.

C	-2.36646300	-0.74208500	0.21289500
C	-0.65105100	-2.16195100	-0.42699100
C	-1.50923900	-3.25114200	-0.51000500
C	-2.85679800	-3.06513000	-0.19934700
C	-3.28452000	-1.79653600	0.17506600
H	-2.66998800	0.26278600	0.47975800
H	-1.13213000	-4.22377400	-0.80146300
H	-3.55160800	-3.89573800	-0.24696900
C	0.79905500	-2.27347700	-0.65995400
N	1.62954100	-1.33481700	-0.35665900
C	2.69663100	-3.12503500	-1.45280900
C	2.99823400	-1.87531000	-0.59398700
H	2.79240100	-2.93608300	-2.52512000
H	3.56958100	-1.14005100	-1.16722400
O	1.27578000	-3.39904500	-1.19044300
H	3.25541400	-4.01923700	-1.18402800
N	-1.07752700	-0.92051100	-0.08346300
C	3.78006700	-2.17567400	0.72821400
C	3.94327000	-0.88817800	1.55204000
H	2.97749700	-0.48872000	1.87532400
H	4.53483600	-1.09304200	2.45120100
H	4.47075000	-0.11459800	0.98269400
C	5.18207000	-2.68473300	0.33688800
H	5.78059000	-2.85570400	1.23799700
H	5.14488300	-3.63025000	-0.21408500
H	5.71227300	-1.95245000	-0.28312200
C	3.06328500	-3.23301300	1.58857700
H	2.95421700	-4.19132300	1.06999900
H	3.64289400	-3.42286100	2.49826600
H	2.06889700	-2.89559900	1.90100600
C	-4.71560100	-1.52032900	0.55899600
F	-5.52713300	-2.54933400	0.25149500
F	-4.83444400	-1.29320800	1.88598300
F	-5.18916100	-0.42226100	-0.06968900

Pd	0.46655200	0.59632000	-0.22930000
C	-0.90125400	2.05140200	-0.23609400
C	-1.64832700	2.28115000	-1.40009100
C	-1.23071200	2.73819500	0.94041000
C	-2.71106800	3.19313500	-1.38747500
H	-1.41308500	1.75507700	-2.32156900
C	-2.29806200	3.64657100	0.94722800
H	-0.64480800	2.59286300	1.84284400
C	-3.03943500	3.87673000	-0.21393800
H	-3.28152700	3.36355900	-2.29732000
H	-2.54249100	4.17649200	1.86485000
H	-3.86515600	4.58298800	-0.20496600
C	2.21771800	1.99539200	0.00202100
C	2.00709800	1.83753800	-1.35847400
H	2.85435600	1.27030800	0.50201600
C	2.05904700	3.27429300	0.78553800
H	1.21300600	3.85929000	0.40746300
C	3.33560400	4.11826100	0.67724600
H	4.20784600	3.55608700	1.02682400
H	3.51182300	4.43309900	-0.35626000
H	3.23702200	5.02149200	1.29073200
O	1.82035200	2.88479400	2.14478900
H	1.73528300	3.69775400	2.66481800
C	1.54327200	2.89340000	-2.31904600
H	2.42968100	3.30524900	-2.82107100
H	0.90826500	2.46696600	-3.10113700
H	1.01164800	3.71580800	-1.83880600
H	2.47278300	0.97258900	-1.83030700

TS17-s

B3LYP SCF energy in DMF: -1619.918393 a.u.

M06 SCF energy in DMF: -1619.328482 a.u.

M06 Free energy in DMF: -1618.888434 a.u.

C	-2.47055300	-0.49233200	0.03126200
C	-0.85976300	-2.00651900	-0.63155300
C	-1.80510900	-2.99130900	-0.89577200
C	-3.14960300	-2.69714500	-0.67021700
C	-3.48194300	-1.43480600	-0.18995100
H	-2.70123700	0.50309000	0.39103800
H	-1.49718100	-3.96491900	-1.25720500
H	-3.91500600	-3.44176500	-0.85620800
C	0.58751400	-2.24547100	-0.71859300
N	1.45985700	-1.35169900	-0.39233300
C	2.49180800	-3.32677100	-1.10494900
C	2.76467300	-2.06164400	-0.27039400
H	2.77024700	-3.20785100	-2.15609800
H	3.54130200	-1.44234700	-0.71409600
O	1.02559800	-3.45770400	-1.05979100
H	2.91358300	-4.25056600	-0.71330600
N	-1.18546500	-0.76981000	-0.18603100
C	3.14774200	-2.34723800	1.22519600
C	3.15735600	-1.04254200	2.04324600
H	2.15791000	-0.59949500	2.10535300
H	3.49298500	-1.25223100	3.06523500
H	3.82893600	-0.30189400	1.60406200
C	4.57006600	-2.94286100	1.22512900
H	4.88995200	-3.15521300	2.25103100
H	4.62706500	-3.88172400	0.66374800
H	5.29253400	-2.24502000	0.78642600
C	2.17509800	-3.33609100	1.89751900
H	2.16014500	-4.31484600	1.40734900
H	2.48067800	-3.49984000	2.93677000
H	1.15050100	-2.94808600	1.92171500
C	-4.91287100	-1.04213800	0.06535000
F	-5.72193300	-2.11556800	0.15640500
F	-5.03364700	-0.33954500	1.21273300
F	-5.39590600	-0.25861600	-0.92612600
Pd	0.58126300	0.64528500	-0.30268800
C	-0.56794900	2.32881200	0.09166400
C	-1.68394300	2.67210200	-0.69077500
C	-0.59409400	2.57778700	1.47650600

C	-2.81939000	3.22337400	-0.09126500
H	-1.66561400	2.51768400	-1.76635300
C	-1.74121500	3.10694200	2.07324400
H	0.27988300	2.36547800	2.08621400
C	-2.85278200	3.43635400	1.29054500
H	-3.67637300	3.48724900	-0.70519800
H	-1.75833000	3.27989100	3.14599600
H	-3.73498400	3.86939200	1.75332100
C	2.10776400	1.94157700	-1.01253800
C	1.12469500	2.97982700	-0.92095300
H	2.18750700	1.48595400	-2.00377300
C	3.45730100	2.00990100	-0.31646400
H	3.32483900	2.16691000	0.76395300
C	4.35199000	3.12413900	-0.88080300
H	4.44723400	3.02737400	-1.96748300
H	3.97592800	4.12178500	-0.64821000
H	5.35308300	3.04324700	-0.43963900
O	4.09310100	0.74814300	-0.55877900
H	4.98625000	0.80025100	-0.18752800
C	1.34583700	4.26279700	-0.15159900
H	2.00291200	4.89915900	-0.75701100
H	0.41049800	4.80498600	-0.00476300
H	1.82380900	4.10322100	0.81700100
H	0.55012500	3.11717400	-1.83172800

32-s

B3LYP SCF energy in DMF: -1619.953772 a.u.

M06 SCF energy in DMF: -1619.363148 a.u.

M06 Free energy in DMF: -1618.923099 a.u.

C	-2.62776400	-0.22503800	0.43369700
C	-1.20738200	-1.79761700	-0.47630100
C	-2.23819300	-2.71241000	-0.66144400
C	-3.52530500	-2.35096700	-0.26244200
C	-3.71729700	-1.09380300	0.29941600
H	-2.75152200	0.76614800	0.85268600
H	-2.03963100	-3.68349300	-1.09855100
H	-4.35398800	-3.03853400	-0.38593100
C	0.19209200	-2.10759300	-0.81005200
N	1.19474500	-1.39780900	-0.40864900
C	1.86266100	-3.09923400	-1.89944100
C	2.43520900	-2.09027100	-0.87587700
H	1.93266400	-2.74384300	-2.93068900
H	3.07245300	-1.35629900	-1.37620000
O	0.43533300	-3.17576200	-1.56777000
H	2.26433800	-4.10774000	-1.82993300
N	-1.39852800	-0.56472400	0.04705200
C	3.26443600	-2.74704600	0.27540100
C	3.80612600	-1.66039100	1.21697200
H	3.01316300	-1.07244100	1.68337200
H	4.39947800	-2.12329800	2.01432000
H	4.46431100	-0.97027500	0.67737000
C	4.47014400	-3.46927000	-0.36222200
H	5.12936300	-3.85021600	0.42512700
H	4.17773200	-4.32365900	-0.98096400
H	5.05873700	-2.78632100	-0.98607900
C	2.42097900	-3.75240500	1.08013100
H	2.01997500	-4.55687500	0.45369100
H	3.04132900	-4.22188500	1.85118900
H	1.58276100	-3.26256300	1.58779600
C	-5.06901500	-0.62827600	0.77173800
F	-6.03853900	-1.52170000	0.49959300
F	-5.07709000	-0.41336300	2.10643800
F	-5.41628800	0.54135600	0.18753400
Pd	0.52535500	0.63629300	0.07491400
C	0.45059400	2.72465000	-0.95215400
C	-0.29819000	2.66637500	-2.15831700
C	-0.25813600	2.91448000	0.26774400
C	-1.67237400	2.83832300	-2.15134800
H	0.23133500	2.51942600	-3.09589200
C	-1.66240500	3.09081500	0.25449600
H	0.27413400	3.11920300	1.18972600

C	-2.36153000	3.05416500	-0.93999500
H	-2.22302900	2.81820400	-3.08759600
H	-2.18051400	3.27513800	1.19127400
H	-3.43795200	3.19775000	-0.94834800
C	2.33739200	1.59468400	0.06055400
C	1.98546600	2.68498600	-0.97149500
H	3.04528700	0.85993100	-0.33083600
C	2.72443100	2.03991000	1.47595300
H	2.27137700	3.01454000	1.69666700
C	4.24050000	2.17690200	1.64350900
H	4.73964700	1.21947100	1.46565500
H	4.65158400	2.91674600	0.95028700
H	4.48036800	2.50885200	2.66145800
O	2.20032500	1.07139200	2.40626600
H	2.49273000	1.33511800	3.29238900
C	2.61625200	4.07898200	-0.81927800
H	3.70720100	4.02590400	-0.89376900
H	2.25812200	4.73179700	-1.62348700
H	2.35772500	4.55234200	0.13217800
H	2.27083900	2.30375100	-1.95730800

33-s

B3LYP SCF energy in DMF: -1619.949982 a.u.

M06 SCF energy in DMF: -1619.354537 a.u.

M06 Free energy in DMF: -1618.91477 a.u.

C	-2.83022800	0.00232600	0.36059500
C	-1.51668100	-1.63353800	-0.60231200
C	-2.62262700	-2.37307700	-1.00491700
C	-3.89196200	-1.88930400	-0.68958000
C	-3.99444100	-0.69009200	0.00819100
H	-2.88066400	0.94480500	0.89509400
H	-2.49551400	-3.30494600	-1.54250800
H	-4.77846100	-2.44251700	-0.97865400
C	-0.13571000	-2.09258300	-0.82059400
N	0.89171000	-1.49551800	-0.30890900
C	1.54023600	-3.27060000	-1.69317500
C	2.07648500	-2.36345500	-0.56648400
H	1.77730300	-2.89335200	-2.69116600
H	2.89852800	-1.74109400	-0.92533800
O	0.07658800	-3.18715100	-1.54227900
H	1.81471800	-4.32051800	-1.61835300
N	-1.61487900	-0.45912500	0.06429700
C	2.55484500	-3.13479700	0.70960700
C	2.92772300	-2.14184600	1.82335900
H	2.06191200	-1.55867300	2.15173100
H	3.30927700	-2.68864000	2.69292400
H	3.70569400	-1.44554200	1.49713800
C	3.81503700	-3.93424800	0.32017200
H	4.21285200	-4.45369900	1.19842900
H	3.60870700	-4.69351800	-0.44179600
H	4.60125400	-3.27464000	-0.06453700
C	1.47435100	-4.09655800	1.24007200
H	1.20295800	-4.86628700	0.51048700
H	1.84960400	-4.61320300	2.12991000
H	0.56364600	-3.56408100	1.53623000
C	-5.33958800	-0.10162100	0.34527800
F	-5.31612400	0.55231200	1.52583700
F	-5.73576400	0.78866000	-0.59206400
F	-6.29331300	-1.05056800	0.42139100
Pd	0.42641900	0.53243900	0.21542500
C	2.32570100	1.13273300	0.03028700
C	2.82953400	1.31581600	-1.26603600
C	3.18477100	1.27935000	1.12535900
C	4.17658000	1.64771800	-1.45920500
H	2.17471200	1.22560900	-2.12710900
C	4.53164900	1.61247900	0.92704900
H	2.82189800	1.13466000	2.13797400
C	5.03126900	1.79666300	-0.36397000
H	4.55252700	1.79100800	-2.46944600
H	5.18682800	1.72348000	1.78768400
H	6.07590300	2.05444700	-0.51544000

C	-0.43980200	2.59891600	0.01546400
C	-0.23289600	2.39195900	1.37038800
H	-1.38788300	2.27500100	-0.41218700
C	0.27359800	3.60496700	-0.85325300
H	1.32433500	3.69360500	-0.55482400
C	-0.39940300	4.97821500	-0.73305800
H	0.08576800	5.69011000	-1.41101800
H	-1.46022900	4.91768800	-0.99833100
H	-0.31349700	5.37186500	0.28474000
O	0.18044100	3.10972300	-2.19459500
H	0.65837600	3.73112000	-2.76325500
C	0.73793600	3.13097000	2.24389100
H	0.18852500	3.94034900	2.74454000
H	1.13530900	2.48647200	3.03323800
H	1.56793400	3.57561400	1.69434900
H	-1.02312200	1.87860400	1.91800600

34-s

B3LYP SCF energy in DMF: -1619.955649 a.u.

M06 SCF energy in DMF: -1619.366168 a.u.

M06 Free energy in DMF: -1618.924218 a.u.

C	-2.50494000	-0.50198600	0.38052200
C	-0.90554000	-1.93122200	-0.48484100
C	-1.84688300	-2.92343600	-0.73577400
C	-3.17712200	-2.68226000	-0.39705600
C	-3.50355300	-1.45895900	0.17978700
H	-2.73789700	0.46125100	0.81259500
H	-1.54192300	-3.86469100	-1.17646600
H	-3.93592200	-3.43626700	-0.57233300
C	0.53167900	-2.12762300	-0.72899900
N	1.42822800	-1.30392000	-0.30891200
C	2.37100700	-3.04543500	-1.57804400
C	2.74601900	-1.95227400	-0.55387400
H	2.51405200	-2.72198100	-2.61280600
H	3.42457300	-1.21862800	-0.99559200
O	0.92592000	-3.22600300	-1.37889200
H	2.84515100	-4.01331000	-1.42666400
N	-1.23152200	-0.73049600	0.05392300
C	3.40023200	-2.49538000	0.76162800
C	3.55940600	-1.35342200	1.77923900
H	2.59148800	-0.93643100	2.07422900
H	4.05363300	-1.72646500	2.68335500
H	4.17180500	-0.54277400	1.37526500
C	4.79924200	-3.03305700	0.39938400
H	5.30735800	-3.39448700	1.29991400
H	4.75558300	-3.86721800	-0.30908500
H	5.42242400	-2.24825900	-0.04487400
C	2.56280800	-3.61841100	1.40295000
H	2.44962300	-4.48694300	0.74623900
H	3.05664700	-3.96631400	2.31668500
H	1.56403100	-3.26998900	1.68867900
C	-4.92621300	-1.11248700	0.53140200
F	-4.99676800	-0.40004000	1.67663500
F	-5.50225500	-0.36018900	-0.43432100
F	-5.68784400	-2.21311200	0.68593300
Pd	0.37543800	0.70265600	0.02609200
C	1.67351600	2.61526900	0.34126800
C	1.81639200	2.32429500	-1.04213600
C	2.80298000	2.43707000	1.18299900
C	3.05696700	1.88270700	-1.55467400
H	1.03461100	2.59051400	-1.74554200
C	4.02189500	2.03973800	0.66007200
H	2.70787400	2.66265300	2.24185300
C	4.15094800	1.75469700	-0.71417600
H	3.15076100	1.68213900	-2.61785600
H	4.88545200	1.94859200	1.31215200
H	5.11239400	1.44407000	-1.11243300
C	-0.75399700	2.38702400	0.36923300
C	0.39474200	3.27710500	0.88080600
H	-1.41706000	2.07513400	1.18405800
C	-1.57029100	2.87312600	-0.83172100

H	-0.93001900	3.45954700	-1.50455200
C	-2.74711000	3.75383000	-0.39170700
H	-3.31133300	4.09817700	-1.26749900
H	-3.42533700	3.18695900	0.25539900
H	-2.41125700	4.64018900	0.15225900
O	-2.06738600	1.72758000	-1.54575300
H	-2.66385100	2.06141400	-2.23271600
C	0.36998600	4.78573900	0.57703900
H	-0.48466900	5.27318700	1.05600000
H	1.28092700	5.24793600	0.97419000
H	0.33254400	4.99456800	-0.49600400
H	0.43177400	3.16570500	1.96919200

35-s

B3LYP SCF energy in DMF: -1619.945695 a.u.

M06 SCF energy in DMF: -1619.3532 a.u.

M06 Free energy in DMF: -1618.913813 a.u.

C	2.86198800	-0.15896300	0.05876100
C	1.59476800	1.70074000	-0.45318800
C	2.72131400	2.47117000	-0.71842000
C	3.97639400	1.88239100	-0.57062200
C	4.04512100	0.55145400	-0.17039000
H	2.88868600	-1.20295400	0.35106900
H	2.62090200	3.50357300	-1.03083400
H	4.87745300	2.45268000	-0.76745100
C	0.22985000	2.24608000	-0.53183700
N	-0.82027100	1.57000200	-0.19469100
C	-1.40102100	3.66895800	-1.05989300
C	-1.97843800	2.50843300	-0.22163600
H	-1.64242300	3.58654600	-2.12273800
H	-2.80795600	2.02687700	-0.74330300
O	0.05761100	3.49802700	-0.93934300
H	-1.63822600	4.66878300	-0.70259000
N	1.65923500	0.40095800	-0.07880700
C	-2.46139800	2.92040900	1.20938000
C	-2.87294200	1.67355100	2.01013600
H	-2.02522600	1.00227400	2.17795300
H	-3.25923500	1.97474000	2.99029600
H	-3.65975100	1.11109500	1.49877900
C	-3.70040900	3.82254800	1.03765700
H	-4.08945900	4.11231400	2.01962200
H	-3.47542500	4.74449600	0.49117500
H	-4.50055500	3.29958200	0.50130400
C	-1.36845100	3.67704900	1.98832600
H	-1.06300700	4.60384600	1.49196900
H	-1.74640700	3.95157600	2.97889200
H	-0.47666500	3.05919000	2.14164100
C	5.37438300	-0.11917500	0.06183600
F	6.33322000	0.39089800	-0.73632200
F	5.78948300	0.04185400	1.33825500
F	5.31179900	-1.44739100	-0.16892000
Pd	-0.42871200	-0.53368300	-0.15926100
C	-2.33243500	-0.99827700	-0.56034900
C	-2.76230000	-0.76967700	-1.87588100
C	-3.25262600	-1.45343600	0.39057500
C	-4.09421500	-1.00832800	-2.23667000
H	-2.06658100	-0.40868300	-2.62916200
C	-4.58486100	-1.69142400	0.02452300
H	-2.95325600	-1.62027300	1.41982300
C	-5.00840100	-1.47298000	-1.28784800
H	-4.41117800	-0.83056500	-3.26144700
H	-5.28814800	-2.04679500	0.77374200
H	-6.04130600	-1.66014200	-1.56818900
C	0.25996400	-2.58040400	0.45145700
C	0.31008900	-2.55221900	-0.93352600
H	1.13704700	-2.23590800	0.99883800
C	-0.64116100	-3.48584800	1.26757100
C	-0.73489800	-3.03968000	2.72451600
H	0.25981700	-3.03254400	3.18417600
H	-1.15950800	-2.03423400	2.80943300
H	-1.37328100	-3.72317400	3.29564300

H	-1.64388300	-3.52004400	0.82675000
O	-0.02632800	-4.78348400	1.16597500
H	-0.54108900	-5.38129000	1.72940000
C	-0.54888300	-3.35327900	-1.86628800
H	-0.78116700	-2.79092700	-2.77479800
H	0.02716400	-4.23628600	-2.17470600
H	-1.47877700	-3.69681100	-1.41219800
H	1.21005300	-2.14339300	-1.39191600

TS19-s

B3LYP SCF energy in DMF: -1619.920347 a.u.

M06 SCF energy in DMF: -1619.332555 a.u.

M06 Free energy in DMF: -1618.892934 a.u.

C	-2.79300300	-0.01599700	-0.04166500
C	-1.40808500	-1.80857000	-0.48606200
C	-2.48490100	-2.64652700	-0.75637200
C	-3.77504700	-2.13201500	-0.64655700
C	-3.92683900	-0.79812800	-0.28043500
H	-2.88979900	1.02886300	0.22151100
H	-2.31572600	-3.67654700	-1.04568100
H	-4.63749400	-2.75766200	-0.84795500
C	-0.01493400	-2.27662600	-0.54453100
N	0.98503600	-1.53264200	-0.21819600
C	1.69051300	-3.61643100	-1.04316600
C	2.19401300	-2.40187500	-0.23204300
H	1.93615800	-3.54660300	-2.10632000
H	2.99431500	-1.88343100	-0.76568900
O	0.22700100	-3.52979400	-0.93278900
H	1.98825300	-4.59024100	-0.65966500
N	-1.55435900	-0.50681800	-0.13465200
C	2.70683200	-2.74924400	1.20619200
C	3.03462900	-1.45731500	1.97346600
H	2.14506600	-0.83777300	2.12193300
H	3.43977900	-1.70473600	2.96114900
H	3.78311300	-0.85871000	1.44593700
C	4.00218300	-3.57159900	1.05506600
H	4.41340900	-3.80547200	2.04303900
H	3.83668000	-4.52231100	0.53713900
H	4.76454200	-3.01334300	0.49929200
C	1.66818900	-3.55759000	2.00680800
H	1.44217000	-4.52444100	1.54561400
H	2.05553000	-3.76173300	3.01079800
H	0.72910100	-3.00612300	2.12762900
C	-5.29517100	-0.19799700	-0.08826900
F	-6.21119200	-0.78139000	-0.88669600
F	-5.72413500	-0.34792500	1.18533800
F	-5.30342300	1.12550900	-0.35446800
Pd	0.36613800	0.59997400	-0.15800800
C	2.20304000	1.46796900	-0.60189100
C	2.78195500	1.11517800	-1.83669500
C	3.04152600	1.79027200	0.48044200
C	4.17022700	1.05393800	-1.97270000
H	2.14843700	0.89898200	-2.69282200
C	4.42970800	1.72458400	0.34022700
H	2.61332800	2.10246100	1.42836300
C	4.99596200	1.35802300	-0.88476500
H	4.60682900	0.78043500	-2.92955600
H	5.06862500	1.96735700	1.18512100
H	6.07600800	1.32189500	-0.99566600
C	-0.35265800	2.56724000	-0.10697600
C	0.73485500	2.92232300	-0.96815100
H	-1.30823400	2.42072700	-0.61538900
C	-0.45270900	3.19253800	1.27663700
C	-1.38963200	2.46493200	2.23821100
H	-2.41249200	2.44356600	1.84879200
H	-1.05713300	1.43769500	2.42059700
H	-1.40922300	2.98531000	3.20309000
H	0.55322400	3.21504000	1.72144000
O	-0.90813900	4.53947700	1.05317100
H	-0.92514800	4.98025000	1.91633300
C	1.59901600	4.14480500	-0.76698100

H	2.49573300	4.10646400	-1.38865100
H	0.99577300	5.00511900	-1.08609700
H	1.88408600	4.30859900	0.27213400
H	0.56785700	2.68924200	-2.01749100

36-s

B3LYP SCF energy in DMF: -1619.954821 a.u.

M06 SCF energy in DMF: -1619.366334 a.u.

M06 Free energy in DMF: -1618.92571 a.u.

C	-2.56707200	-0.38327700	-0.01041900
C	-0.92750200	-1.91085900	-0.57771400
C	-1.86939400	-2.85573500	-0.97221000
C	-3.22117300	-2.53696100	-0.87099400
C	-3.57065500	-1.28435500	-0.37444100
H	-2.81874100	0.60031700	0.36435400
H	-1.54742900	-3.81864500	-1.34903200
H	-3.97941400	-3.25102700	-1.17286600
C	0.51627100	-2.19209300	-0.59800300
N	1.39922900	-1.34697000	-0.19561900
C	2.39251300	-3.31627200	-1.01631900
C	2.70203900	-2.06362800	-0.16346900
H	2.70406100	-3.20560200	-2.05840300
H	3.45850400	-1.44268200	-0.64929800
O	0.92522500	-3.39495900	-1.00903000
H	2.77007900	-4.25637800	-0.61796600
N	-1.26887200	-0.68245000	-0.11362700
C	3.18337500	-2.36611500	1.29564400
C	3.36778700	-1.04886500	2.06961800
H	2.43467800	-0.48042700	2.13666100
H	3.70430400	-1.26072700	3.09056800
H	4.12286800	-0.41293500	1.59695500
C	4.54979100	-3.07512500	1.20462400
H	4.95346100	-3.23920500	2.20953100
H	4.48146600	-4.05373600	0.71760400
H	5.27512900	-2.47044900	0.64784500
C	2.18408000	-3.25938100	2.05411900
H	2.03690900	-4.22956200	1.56828100
H	2.55997500	-3.45782900	3.06369500
H	1.20663300	-2.77621500	2.16073500
C	-5.01737300	-0.90585600	-0.19212000
F	-5.79031700	-1.42511700	-1.16762000
F	-5.50353800	-1.36340000	0.98338900
F	-5.19182100	0.43212400	-0.20035400
Pd	0.43929900	0.68295000	0.03686900
C	1.34070500	2.53613300	-1.08860900
C	1.63124800	2.20190400	-2.43784900
C	2.30038200	2.21025800	-0.09165700
C	2.84301000	1.62539600	-2.78070400
H	0.90208000	2.44531300	-3.20591600
C	3.53767800	1.63029800	-0.46299800
H	2.18379300	2.58356000	0.92170900
C	3.80629300	1.34273500	-1.79011800
H	3.06081700	1.40559000	-3.82209600
H	4.28372500	1.44126400	0.30150100
H	4.76270800	0.91364700	-2.07395800
C	-0.63520900	2.40936100	0.30235900
C	0.07821300	3.32027500	-0.71702300
H	-1.65179900	2.17571900	-0.02393500
C	-0.66488800	2.83259900	1.77190200
C	-1.03246400	1.70879600	2.74274700
H	-2.00350600	1.27241700	2.48683000
H	-0.27856600	0.91346600	2.73363500
H	-1.09406800	2.10112900	3.76515100
H	0.31457000	3.23765900	2.06263400
O	-1.64923000	3.88361200	1.84055100
H	-1.58284300	4.27722700	2.72382300
C	0.39080900	4.76684300	-0.30566700
H	0.88512400	5.28701100	-1.13433100
H	-0.52670000	5.30342700	-0.05308900
H	1.05681900	4.81339700	0.56130700
H	-0.54254900	3.35636900	-1.61825700

TS20-s

B3LYP SCF energy in DMF: -1619.917663 a.u.

M06 SCF energy in DMF: -1619.33047 a.u.

M06 Free energy in DMF: -1618.893276 a.u.

C	-2.10730200	-1.17197100	0.23485800
C	-0.21462400	-2.28148500	-0.49236300
C	-0.91550100	-3.46371400	-0.70549700
C	-2.28052300	-3.48532600	-0.42097600
C	-2.87852700	-2.32634400	0.06604100
H	-2.54553800	-0.25042600	0.59919300
H	-0.40683700	-4.34484400	-1.07716100
H	-2.85848600	-4.39049500	-0.57010500
C	1.23581300	-2.15936900	-0.70958200
N	1.92436800	-1.14573000	-0.30254800
C	3.22057600	-2.62464700	-1.60237100
C	3.35325000	-1.44546700	-0.61300700
H	3.25862400	-2.30717900	-2.64780100
H	3.79138100	-0.57448500	-1.10730200
O	1.86625300	-3.13818800	-1.35933600
N	3.91576300	-3.44613200	-1.44134600
H	-0.80364300	-1.14933700	-0.04511200
C	4.21031100	-1.76452000	0.65458800
C	4.18822300	-0.56241500	1.61064900
H	3.17963700	-0.36712800	1.98586500
H	4.83498400	-0.75613700	2.47345600
H	4.55696100	0.34207500	1.11509400
C	5.66319000	-1.99520800	0.19178700
H	6.30752500	-2.16657600	1.06068100
H	5.76074600	-2.86692400	-0.46400900
H	6.05118500	-1.12238800	-0.34617400
C	3.69604400	-3.01015500	1.40007600
H	3.73448200	-3.91469800	0.78407500
H	4.31920500	-3.19490900	2.28173300
H	2.66680000	-2.87766000	1.75139700
C	-4.35493000	-2.26861900	0.35621700
F	-4.86614800	-3.48965300	0.60884000
F	-4.62094300	-1.48420300	1.42255400
F	-5.04254000	-1.75614000	-0.68990100
Pd	0.56658700	0.59400000	-0.01741300
C	-0.95755800	1.97072900	-0.03732500
C	-1.84823800	1.94161600	-1.12600600
C	-1.42038200	2.37871300	1.22593600
C	-3.19221200	2.27284800	-0.94025000
H	-1.49446900	1.65910500	-2.11352600
C	-2.76876600	2.70534000	1.40497700
H	-0.73623900	2.43742800	2.06748800
C	-3.65475300	2.65416300	0.32431400
H	-3.87600800	2.24125000	-1.78430700
H	-3.12292000	3.00671200	2.38727500
H	-4.69914300	2.91806600	0.46455200
C	1.93008800	2.21831200	-0.03805300
C	0.87974000	2.93168600	-0.67456600
H	2.66126400	1.76298000	-0.70845300
C	2.43896400	2.63197100	1.32345600
H	1.62098600	2.87931600	2.00695100
H	3.06289600	3.52877300	1.22258000
H	3.04396700	1.85043200	1.78233700
C	0.52899100	4.36112800	-0.23556800
H	0.32200700	4.38440000	0.84051200
H	0.77379700	2.77256600	-1.74571700
C	-0.61517000	5.01827200	-0.99898100
H	-0.46065100	4.93278400	-2.07996000
H	-1.58633200	4.59211600	-0.74523900
H	-0.64815800	6.08413700	-0.74454800
O	1.76013700	5.05717500	-0.51015400
H	1.59984300	5.99413400	-0.32058500

37-s

B3LYP SCF energy in DMF: -1619.95735 a.u.

M06 SCF energy in DMF: -1619.370437 a.u.

M06 Free energy in DMF: -1618.928849 a.u.

C	2.64353800	0.05987800	0.41918000
C	1.41390000	1.72938300	-0.58666200
C	2.55559800	2.38690600	-1.03396800
C	3.80024200	1.83523300	-0.72951600
C	3.84156500	0.65912600	0.01214300
H	2.64519600	-0.85948600	0.99180200
H	2.47532900	3.30544600	-1.60246100
H	4.71244700	2.31820500	-1.06132400
C	0.05819200	2.25346800	-0.81774600
N	-1.00008200	1.75121600	-0.26894200
C	-1.54282000	3.45552600	-1.79299200
C	-2.13854100	2.65155500	-0.61757500
H	-1.79209500	3.02948200	-2.76835800
H	-2.98026500	2.04067000	-0.95268900
O	-0.09092100	3.30722300	-1.61789700
H	-1.76356500	4.52090000	-1.78839700
N	1.45259100	0.57594900	0.11916100
C	-2.61667900	3.53129200	0.58477900
C	-3.08967000	2.63270700	1.73806200
H	-2.28094800	2.00125900	2.11783600
H	-3.45062900	3.24960900	2.56836700
H	-3.91623000	1.98812800	1.42204000
C	-3.81457000	4.37313200	0.10035200
H	-4.21735300	4.96073100	0.93226300
H	-3.53833200	5.07641500	-0.69202100
H	-4.62081300	3.73548600	-0.28023300
C	-1.50081300	4.46196700	1.09619700
H	-1.15122000	5.15923600	0.32769600
H	-1.87722900	5.06306000	1.93076800
H	-0.63779900	3.89766200	1.46650200
C	5.14386100	-0.02361000	0.33543600
F	6.19155600	0.81882300	0.24912400
F	5.13727600	-0.54379400	1.58187500
F	5.38207100	-1.04928000	-0.51507600
Pd	-0.66739300	-0.31774900	0.26913600
C	-0.79665200	-2.56357000	-0.28494700
C	0.10163100	-2.85911400	-1.34738700
C	-0.29757500	-2.61535600	1.04498500
C	1.40749400	-3.24159100	-1.09024000
H	-0.26555500	-2.81875200	-2.36896600
C	1.03877500	-3.00420400	1.29031500
H	-0.97049800	-2.52375200	1.88961100
C	1.87887500	-3.32382600	0.23529700
H	2.06864400	-3.49222700	-1.91476600
H	1.39086200	-3.07276600	2.31543100
H	2.90098700	-3.63741000	0.42641300
C	-2.60222500	-0.98895800	0.14009100
C	-2.28587700	-2.31849900	-0.56493100
H	-3.09059600	-0.27574600	-0.52878900
C	-3.29728200	-1.03974500	1.49026900
H	-2.82351500	-1.72132600	2.20178000
H	-4.32853300	-1.39155100	1.34716300
H	-3.34585200	-0.05321100	1.95389400
C	-3.18979400	-3.51618400	-0.20774600
H	-3.14924400	-3.68516200	0.87867600
H	-2.38432300	-2.16604100	-1.64517200
C	-2.78736200	-4.80578100	-0.92028400
H	-2.79412100	-4.67036000	-2.00743300
H	-1.79243700	-5.14610800	-0.61606700
H	-3.49518600	-5.60550100	-0.67186300
O	-4.51211700	-3.11633800	-0.58933300
H	-5.11128900	-3.83777200	-0.34762800

TS21-s

B3LYP SCF energy in DMF: -1619.923745 a.u.

M06 SCF energy in DMF: -1619.33506 a.u.

M06 Free energy in DMF: -1618.895598 a.u.

C	-2.26781300	-0.88389500	0.13489700
C	-0.51522900	-2.24398500	-0.51447400

C	-1.36380000	-3.31346600	-0.78098000
C	-2.73030800	-3.14469600	-0.56178500
C	-3.18462900	-1.91526300	-0.09230000
H	-2.58839000	0.08952700	0.48702100
H	-0.96730000	-4.25269500	-1.14714300
H	-3.42214600	-3.95642900	-0.75655000
C	0.94676900	-2.32605400	-0.66239700
N	1.73667400	-1.36307300	-0.32558400
C	2.91466800	-3.14659100	-1.30485400
C	3.13028500	-1.87160900	-0.45659700
H	3.08532600	-2.97781100	-2.37123400
H	3.72106200	-1.13742100	-1.01033900
O	1.48561800	-3.44707100	-1.13982600
H	3.47019800	-4.02289300	-0.97743100
N	-0.96020300	-1.04539700	-0.07125700
C	3.82969900	-2.11578400	0.92187200
C	3.92146200	-0.79695800	1.70922900
H	2.93220600	-0.39915200	1.95518900
H	4.45762500	-0.96162600	2.65039300
H	4.47186000	-0.03491500	1.14608800
C	5.26220800	-2.61206100	0.63805700
H	5.80543500	-2.74122000	1.58029900
H	5.27740000	-3.57618100	0.11884900
H	5.81874300	-1.89141000	0.02751300
C	3.07642900	-3.15747400	1.76989600
H	3.02300500	-4.13576600	1.28044500
H	3.59473500	-3.30175200	2.72386800
H	2.05577100	-2.83254500	1.99974000
C	-4.64278900	-1.69703000	0.21352300
F	-5.00451000	-0.40813600	0.04095700
F	-5.43413800	-2.45326800	-0.57419600
F	-4.93202900	-2.02070200	1.49454400
Pd	0.64770300	0.50409200	-0.03623700
C	-0.64574900	2.10028200	0.15560200
C	-1.32342400	2.44048500	-1.02798700
C	-1.28523400	2.28212800	1.39315200
C	-2.64312400	2.89473300	-0.97430300
H	-0.82685700	2.34661800	-1.99003300
C	-2.60451900	2.74153500	1.44165700
H	-0.75700800	2.06500300	2.31779000
C	-3.28651500	3.04350200	0.25896400
H	-3.16746100	3.13783900	-1.89498600
H	-3.09541800	2.86953600	2.40299600
H	-4.31075300	3.40384200	0.29792600
C	2.23017600	1.86502000	-0.25491800
C	1.36880200	2.86009700	0.29000800
H	2.91561400	1.42122700	0.46588300
C	2.73118700	1.88906400	-1.68361400
H	1.97249800	2.24038200	-2.38909200
H	1.35968800	2.91938100	1.37612000
C	1.15965800	4.21630600	-0.36471500
H	0.88991800	4.09084900	-1.42119500
C	2.47596900	5.00859000	-0.26907200
H	3.28926900	4.53411600	-0.82339500
H	2.32334600	6.00783300	-0.69306500
H	2.77977000	5.12317800	0.77642400
O	0.13675900	4.90555200	0.34465600
H	0.03606800	5.77159400	-0.07596900
H	3.60359400	2.54966100	-1.77730700
H	3.05457600	0.89215200	-1.99756200

38-s

B3LYP SCF energy in DMF: -1619.959567 a.u.

M06 SCF energy in DMF: -1619.372367 a.u.

M06 Free energy in DMF: -1618.931163 a.u.

C	2.68840900	-0.31730100	0.13580500
C	1.70770000	1.68112100	-0.46051600
C	2.93854400	2.29462900	-0.67438400
C	4.09544900	1.54671000	-0.46247700
C	3.96551100	0.22505700	-0.04537800
H	2.55685400	-1.34467200	0.45293200

H	2.98984600	3.32892900	-0.99228000
H	5.07327200	1.99052800	-0.61465600
C	0.43382000	2.40422100	-0.60130200
N	-0.71060000	1.87725900	-0.31631400
C	-0.96250200	4.03851000	-1.18759600
C	-1.73103900	2.95980800	-0.39161800
H	-1.16925300	4.00105200	-2.26038200
H	-2.58978900	2.59750400	-0.96167600
O	0.45061900	3.67134600	-1.00895900
H	-1.07975300	5.05724100	-0.82409300
N	1.57874700	0.39227600	-0.06997100
C	-2.23357800	3.43016500	1.01529200
C	-2.89659600	2.26354200	1.76867800
H	-2.19738300	1.44095400	1.94638800
H	-3.25831100	2.61084600	2.74288600
H	-3.75922700	1.87344600	1.21797800
C	-3.29633000	4.52507600	0.78845100
H	-3.70938200	4.84682900	1.75033100
H	-2.88683900	5.41353300	0.29665900
H	-4.12561700	4.15198000	0.17642500
C	-1.08294600	3.99009400	1.87326400
H	-0.58996000	4.84863400	1.40527700
H	-1.47438900	4.32894000	2.83842400
H	-0.32255000	3.22900700	2.08118400
C	5.17946900	-0.64271200	0.15389400
F	6.23653100	0.07205500	0.59105200
F	4.95159500	-1.62705200	1.04880600
F	5.55546500	-1.23847100	-1.00104500
Pd	-0.65565600	-0.24475100	-0.18659600
C	-1.28970000	-2.40631600	0.32087900
C	-0.47899000	-2.64208000	-0.81940200
C	-0.75426800	-2.72349100	1.59839900
C	0.79149400	-3.23959300	-0.68169400
H	-0.88641500	-2.50952100	-1.81578500
C	0.49588000	-3.30978100	1.72085300
H	-1.36165300	-2.54073200	2.48043700
C	1.26830800	-3.58218100	0.57541900
H	1.38091500	-3.44696900	-1.56992000
H	0.87465100	-3.57460200	2.70378000
H	2.23850300	-4.05948000	0.67966600
C	-2.64185200	-0.57921100	-0.54206100
C	-2.74551000	-1.93454900	0.17355200
H	-3.17160400	0.20677200	-0.00458300
C	-2.90924600	-0.47849900	-2.03700200
H	-2.37317800	-1.22278000	-2.63235400
H	-3.11463600	-1.75533700	1.18926400
C	-3.66326600	-3.00260100	-0.45531400
H	-3.39661500	-3.12601700	-1.51550200
C	-5.14205400	-2.63498100	-0.34085400
H	-5.37270300	-1.69360600	-0.84869500
H	-5.76408500	-3.41588300	-0.79405700
H	-5.42750100	-2.53941000	0.71267400
O	-3.39446500	-4.21822200	0.25222100
H	-3.94764500	-4.90780000	-0.14266200
H	-3.98101900	-0.60881000	-2.24500100
H	-2.63320100	0.51361400	-2.40998600

TS22-s

B3LYP SCF energy in DMF: -1619.920248 a.u.

M06 SCF energy in DMF: -1619.332365 a.u.

M06 Free energy in DMF: -1618.893836 a.u.

C	2.89817900	-0.40835000	0.20133800
C	1.87739000	1.51787600	-0.56126000
C	3.09785200	2.11997600	-0.84813300
C	4.26887900	1.41281000	-0.58132100
C	4.16353300	0.13567000	-0.03907000
H	2.79420700	-1.40557900	0.61104200
H	3.12979400	3.12085400	-1.26087500
H	5.23787200	1.85487700	-0.78448600
C	0.59261000	2.21313800	-0.73859900
N	-0.52594100	1.72897000	-0.32056300

C	-0.83513400	3.74776100	-1.48705200
C	-1.55305500	2.78993300	-0.51039400
H	-1.09374200	3.55758700	-2.53229800
H	-2.43447700	2.34576900	-0.97936200
O	0.58695100	3.41061100	-1.32805800
H	-0.94616800	4.80792200	-1.26727900
N	1.77417200	0.26479400	-0.05534500
C	-1.99636100	3.44721100	0.83907000
C	-2.57205500	2.37222400	1.77584500
H	-1.81767800	1.62832200	2.04815400
H	-2.93323400	2.83742500	2.70003300
H	-3.41549600	1.85088000	1.31295600
C	-3.10673500	4.46892600	0.52216900
H	-3.47692900	4.91772500	1.45035000
H	-2.75259100	5.28547900	-0.11597900
H	-3.95542100	3.99132300	0.01890200
C	-0.82433400	4.15516000	1.54485900
H	-0.41457700	4.97905400	0.95130100
H	-1.16829300	4.58094100	2.49364300
H	-0.01031500	3.45944300	1.77658300
C	5.38757400	-0.69170200	0.25139800
F	5.70230800	-1.49573300	-0.78940300
F	6.46434100	0.08067400	0.49707400
F	5.20266700	-1.49047900	1.32422500
Pd	-0.30616200	-0.47734700	-0.01009800
C	-2.28909800	-1.03993900	-0.14221600
C	-2.98642700	-0.65347500	-1.30053500
C	-2.98852100	-1.18304400	1.06787500
C	-4.34905300	-0.35652500	-1.23348500
H	-2.46634500	-0.58202200	-2.25204400
C	-4.35448800	-0.89573700	1.12735200
H	-2.47328900	-1.52263800	1.96212200
C	-5.03509600	-0.47834100	-0.02041900
H	-4.87820400	-0.04539900	-2.13058000
H	-4.88666100	-0.99953300	2.06945900
H	-6.09857800	-0.26040500	0.02668900
C	0.15138700	-2.52477600	0.11707300
C	-1.07906800	-2.78195900	-0.55307600
H	-1.05226600	-2.67370500	-1.63552100
C	-2.05227400	-3.86309600	-0.11213400
H	-2.26780600	-3.77200100	0.95930500
C	-1.39499000	-5.22937200	-0.38084300
H	-1.14929200	-5.33582000	-1.44230900
H	-0.48717400	-5.37396300	0.21030500
H	-2.10003700	-6.02405100	-0.11099300
O	-3.23978600	-3.73958600	-0.88432200
H	-3.84294400	-4.43742000	-0.59057500
C	0.42359900	-2.97485300	1.53574600
H	0.74706200	-4.02433500	1.55624400
H	1.22874200	-2.38578400	1.98532900
H	-0.45966600	-2.88536400	2.17420800
H	1.02230100	-2.50340500	-0.54160900

39-s

B3LYP SCF energy in DMF: -1619.957035 a.u.

M06 SCF energy in DMF: -1619.370486 a.u.

M06 Free energy in DMF: -1618.930389 a.u.

C	2.71773400	0.05112700	0.19673800
C	1.40661800	1.78646400	-0.59440200
C	2.52220200	2.52755500	-0.97229700
C	3.78806500	1.99507900	-0.74144000
C	3.88297700	0.74328200	-0.13896100
H	2.76736300	-0.92673900	0.65942300
H	2.39903500	3.50163200	-1.42965000
C	4.67733700	2.55008900	-1.01954900
H	0.03730700	2.31107800	-0.72339700
N	-0.99391900	1.71421300	-0.23669600
C	-1.58779600	3.66807200	-1.40876700
C	-2.13698300	2.65808600	-0.37627900
H	-1.88970800	3.43155900	-2.43280300
H	-2.99674500	2.11864200	-0.78107700

O	-0.13232200	3.48766400	-1.33412000	C	-2.42723900	2.55842700	1.91702600
H	-1.79776500	4.71433600	-1.19484800	H	-1.64993800	1.84138500	2.19784300
N	1.50176400	0.55773200	-0.02933400	H	-2.69998600	3.12559500	2.81410800
C	-2.55822300	3.29253000	0.99208000	H	-3.30968500	1.99750300	1.59608800
C	-2.97319200	2.18585800	1.97657800	C	-3.08344400	4.50167800	0.48533700
H	-2.15357500	1.48858700	2.17606700	H	-3.37561200	5.05573900	1.38399100
H	-3.27459300	2.63038500	2.93173900	H	-2.79258500	5.23741500	-0.27156500
H	-3.82255200	1.61322700	1.59318700	H	-3.96897200	3.97035500	0.11772200
C	-3.77733300	4.20039800	0.73513800	C	-0.72219400	4.30006100	1.34550800
H	-4.14004700	4.61563800	1.68165900	H	-0.35355500	5.04050100	0.62800900
H	-3.54054100	5.04516700	0.07922000	H	-0.99759300	4.84311000	2.25604200
H	-4.60112900	3.63922700	0.27884800	H	0.10643400	3.63171500	1.60498100
C	-1.41801700	4.11854400	1.61643100	C	5.37612900	-0.60788900	0.38111700
H	-1.10809400	4.95478000	0.98088200	F	6.45866300	-0.19875900	-0.30841800
H	-1.75132700	4.54409600	2.56914900	F	5.64833400	-0.43482800	1.69398800
H	-0.53731100	3.50167700	1.82661300	F	5.24007400	-1.93694600	0.18139500
C	5.22648200	0.10403400	0.09554000	Pd	-0.31826300	-0.51098400	0.12455700
F	5.67234300	-0.52296200	-1.01628900	C	-2.31410400	-1.04448200	0.01038100
F	6.15894200	1.01771600	0.43333800	C	-2.81291700	-1.03265300	-1.30610400
F	5.17997000	-0.81735500	1.07976300	C	-3.18915200	-0.79025600	1.07921300
Pd	-0.39394500	-0.47283600	0.15295200	C	-4.15188300	-0.71308700	-1.54691800
C	-1.81721900	-2.16948800	-0.51219000	H	-2.16041500	-1.26660200	-2.14265300
C	-2.25713900	-1.80969900	-1.81453400	C	-4.53026800	-0.48295700	0.83271500
C	-2.55415600	-1.68742800	0.59954900	H	-2.82983500	-0.83619100	2.10315200
C	-3.41139300	-1.06296200	-1.99494900	C	-5.01325800	-0.43987500	-0.47859100
H	-1.69704500	-2.16941500	-2.67316200	H	-4.52417800	-0.69105600	-2.56769400
C	-3.73564000	-0.94419300	0.40104900	H	-5.19767700	-0.28488500	1.66713800
H	-2.30194000	-2.01470000	1.60310600	H	-6.05766100	-0.20821500	-0.66727800
C	-4.16355800	-0.63969000	-0.88320500	C	0.19377500	-2.54984900	0.24699500
H	-3.74726600	-0.82187800	-2.99941600	C	-1.17137300	-2.79040600	0.55772600
H	-4.31726100	-0.63303500	1.26250500	H	-1.42695600	-2.72003800	1.61199700
H	-5.08237300	-0.08040500	-1.03366900	C	-1.97426600	-3.85322500	-0.20335700
C	0.40365500	-2.33189800	0.44719500	C	-3.40743200	-4.04977500	0.28077400
C	-0.64539000	-3.14531500	-0.32618000	H	-3.42866900	-4.21838800	1.36277100
H	-0.24959800	-3.34550300	-1.32766700	H	-4.05292700	-3.20380300	0.04129100
C	-1.07719500	-4.50326800	0.26201200	H	-3.83227700	-4.93429100	-0.20834700
H	-1.37539500	-4.36478100	1.31163800	H	-1.96772200	-3.62981900	-1.27732500
C	0.03368500	-5.55011500	0.18220900	O	-1.21054100	-5.04714100	0.05070400
H	0.31119700	-5.72731600	-0.86278900	H	-1.70181000	-5.78290100	-0.34514500
H	0.92975100	-5.24348500	0.73009100	C	0.84699600	-3.05611100	-1.01948300
H	-0.30741400	-6.49979800	0.61083800	H	1.78693300	-2.53419800	-1.21774600
O	-2.21109000	-4.91903300	-0.50806600	H	1.07113300	-4.12424100	-0.91536500
H	-2.51890400	-5.75800300	-0.13542900	H	0.19959200	-2.94105400	-1.89380000
C	0.59351300	-2.53843600	1.94206300	H	0.84869300	-2.48202000	1.11889900
H	1.05666000	-3.51460200	2.14533500				
H	1.26759500	-1.77823600	2.35248700				
H	-0.34314000	-2.49909000	2.50530300				
H	1.36332000	-2.32852900	-0.07529800				

40-s

B3LYP SCF energy in DMF: -1619.958319 a.u.

M06 SCF energy in DMF: -1619.371169 a.u.

M06 Free energy in DMF: -1618.930186 a.u.

TS23-s

B3LYP SCF energy in DMF: -1619.918602 a.u.

M06 SCF energy in DMF: -1619.331361 a.u.

M06 Free energy in DMF: -1618.892363 a.u.

C	2.88189900	-0.39565700	0.28271900	C	2.73158400	-0.20748500	0.21560200
C	1.82171300	1.45419600	-0.60893700	C	1.62952800	1.67823100	-0.55157300
C	3.02746800	2.04335000	-0.97094100	C	2.82652600	2.33618500	-0.81254900
C	4.21248900	1.37222500	-0.67263000	C	4.02496000	1.68409800	-0.52836600
C	4.13547900	0.14289200	-0.02621600	C	3.97246700	0.40027900	0.00557000
H	2.79627600	-1.36082600	0.76801600	H	2.66469100	-1.21366700	0.61119100
H	3.03916300	3.00684200	-1.46566300	H	2.81898200	3.34037000	-1.21812400
H	5.17118900	1.80373900	-0.93703900	H	4.97506800	2.17191100	-0.71515700
C	0.52462800	2.12451200	-0.79044600	C	0.31971700	2.32980000	-0.71602500
N	-0.56406600	1.67953300	-0.26280000	N	-0.77603000	1.81301200	-0.28168900
C	-0.95845200	3.57023600	-1.60207100	C	-1.15593900	3.84319000	-1.41345900
C	-1.60486300	2.72158800	-0.48530800	C	-1.82835000	2.85294100	-0.43610200
H	-1.27626200	3.26457000	-2.60269300	H	-1.43720900	3.66488800	-2.45495000
H	-2.51857300	2.24007500	-0.84205300	H	-2.71121900	2.39756100	-0.89146900
O	0.47489500	3.25840700	-1.49168000	O	0.27559500	3.53408000	-1.29415900
H	-1.06732400	4.64764200	-1.49343400	H	-1.28436100	4.89689400	-1.17309100
N	1.74522100	0.24115600	-0.00801000	N	1.58246000	0.41220200	-0.06598700
C	-1.94234300	3.51996600	0.81931100	C	-2.25317800	3.47640300	0.93573400
				C	-2.76961500	2.36932000	1.87120100
				H	-1.99503100	1.62701900	2.08769500
				H	-3.09260200	2.80480200	2.82350800
				H	-3.62764800	1.84969300	1.43467300

C	-3.40078900	4.46980100	0.66653100
H	-3.75571200	4.89688400	1.61076900
H	-3.09011400	5.30367400	0.02778500
H	-4.25054000	3.97378100	0.18322300
C	-1.08292200	4.20772500	1.62064800
H	-0.70844500	5.04820200	1.02710500
H	-1.41542600	4.61497100	2.58161000
H	-0.24591600	3.53154700	1.82679300
C	5.22795300	-0.33265000	0.40044800
F	6.30297300	0.12125900	-0.27330200
F	5.49058500	-0.18485300	1.71832600
F	5.12643900	-1.65872000	0.16617000
Pd	-0.39552000	-0.44986700	-0.04942800
C	-2.19676300	-1.93505300	0.06292700
C	-2.26982600	-1.49904500	-1.28737500
C	-3.19368200	-1.47927900	0.96544600
C	-3.32194700	-0.66288200	-1.71256000
H	-1.60333400	-1.91399600	-2.03514200
C	-4.23739000	-0.67828000	0.52852800
H	-3.15237500	-1.80587200	2.00071200
C	-4.30414400	-0.26735600	-0.81558600
H	-3.37259600	-0.36009300	-2.75421800
H	-5.01052500	-0.37114000	1.22630200
H	-5.12909300	0.35501700	-1.14990700
C	0.19886900	-2.39844100	0.12789100
C	-1.16919700	-2.99153600	0.49813300
H	-1.22976800	-3.05938500	1.58974100
C	-1.47203500	-4.40315000	-0.04573800
C	-2.86981800	-4.90056000	0.31618400
H	-3.01797000	-4.89358300	1.40167700
H	-3.65141800	-4.29081800	-0.14767500
H	-3.00353700	-5.92900800	-0.03960500
H	-1.36947600	-4.39226800	-1.14115400
O	-0.46811900	-5.24993200	0.52854700
H	-0.60216800	-6.13924300	0.16928700
C	0.91265300	-2.92057200	-1.10819900
H	1.84163100	-2.37429300	-1.29696000
H	1.17513400	-3.97530600	-0.95162800
H	0.30594900	-2.86937900	-2.01685000
H	0.87216000	-2.37422600	0.99157200

41-s

B3LYP SCF energy in DMF: -1619.950547 a.u.

M06 SCF energy in DMF: -1619.353712 a.u.

M06 Free energy in DMF: -1618.914439 a.u.

C	2.30530500	-0.86749700	-0.13150300
C	0.46269300	-2.08125500	0.57260800
C	1.25012100	-3.16367900	0.94756500
C	2.62851800	-3.08435400	0.75615100
C	3.15826700	-1.92322600	0.20119600
H	2.68611900	0.05353200	-0.55388800
H	0.79334000	-4.05003200	1.37034000
H	3.26924700	-3.91529400	1.02974700
C	-1.00545400	-2.09811400	0.67687300
N	-1.75309500	-1.17191000	0.18216100
C	-3.01075400	-2.76728600	1.37364500
C	-3.16465400	-1.62076500	0.34768400
H	-3.19871500	-2.44486900	2.40105300
H	-3.74781800	-0.79971300	0.77345900
O	-1.58805400	-3.12750000	1.29025600
H	-3.58636200	-3.66551400	1.15874700
N	0.98405500	-0.94407800	0.05019700
C	-3.83219600	-2.04375600	-1.00200900
C	-3.83260300	-0.85879500	-1.98241100
H	-2.81640700	-0.56309200	-2.26004200
H	-4.36039600	-1.13483300	-2.90195500
H	-4.34636700	0.01021600	-1.55587000
C	-5.29474500	-2.42788100	-0.70074900
H	-5.80929400	-2.69580100	-1.62980300
H	-5.37220600	-3.28760300	-0.02674800
H	-5.83866400	-1.59179300	-0.24604500

C	-3.10125200	-3.23321600	-1.65152600
H	-3.11449900	-4.12815000	-1.02080100
H	-3.59107400	-3.49679100	-2.59497200
H	-2.05800700	-2.99105900	-1.88306000
C	4.64488500	-1.76565900	0.00729500
F	5.24095700	-2.94865700	-0.24194100
F	4.93015900	-0.93824400	-1.01947400
F	5.23252500	-1.24828500	1.10943000
Pd	-0.48191100	0.64792900	-0.19248500
C	0.96005500	1.99975000	-0.46202700
C	1.57589800	2.64734900	0.61685400
C	1.46430300	2.18299200	-1.75758500
C	2.68763000	3.47171600	0.39744900
H	1.19130100	2.52008200	1.62483500
C	2.57626500	3.00827900	-1.96974100
H	1.00067900	1.68754800	-2.60722600
C	3.19031600	3.65353300	-0.89317000
H	3.15906500	3.96958100	1.24142500
H	2.95887600	3.14261000	-2.97859300
H	4.05340800	4.29225700	-1.05939100
C	-2.04875300	2.05668800	0.59384800
C	-2.06824300	2.19862700	-0.78408000
H	-2.66212000	1.27172500	1.03537100
C	-1.62598800	3.10707000	1.58884400
C	-2.83332000	3.96668200	1.98351100
H	-2.53588800	4.69936900	2.74278000
H	-3.21975400	4.51728400	1.11998000
H	-3.63718000	3.34764000	2.39551100
C	-1.67948400	3.42564200	-1.55836900
H	-1.23299900	3.16293400	-2.52127700
H	-2.59752000	3.98851200	-1.77703500
H	-0.99853600	4.08663700	-1.02094100
H	-2.68092800	1.49357100	-1.33952000
H	-0.85403900	3.75524900	1.15926600
O	-1.09972000	2.40536800	2.72308400
H	-0.87352100	3.06949900	3.39146500

TS24-s

B3LYP SCF energy in DMF: -1619.927899 a.u.

M06 SCF energy in DMF: -1619.337261 a.u.

M06 Free energy in DMF: -1618.898118 a.u.

C	-2.40589700	-0.69498700	0.10678200
C	-0.64924700	-2.06990900	-0.49833200
C	-1.50219700	-3.11837400	-0.82493000
C	-2.87462800	-2.93098600	-0.66317800
C	-3.32863600	-1.70513100	-0.18594900
H	-2.72645400	0.27249700	0.47621600
H	-1.10435700	-4.05735700	-1.19032500
H	-3.57001800	-3.72800200	-0.90106300
C	0.81599200	-2.17121800	-0.58599000
N	1.60166100	-1.22796800	-0.19288500
C	2.79958700	-2.99762200	-1.16972800
C	2.99481800	-1.74500200	-0.28387900
H	3.01403800	-2.80637400	-2.22439300
H	3.59797400	-0.99499400	-0.79870100
O	1.36119400	-3.28696100	-1.07013000
H	3.33143300	-3.88845000	-0.84152100
N	-1.09332700	-0.87443500	-0.04387100
C	3.63562200	-2.03212500	1.11469900
C	3.70984500	-0.73407200	1.93764300
H	2.71619800	-0.32274900	2.13985700
H	4.19220300	-0.93002400	2.90174900
H	4.30272400	0.02952300	1.42208600
C	5.07389800	-2.53589600	0.87726100
H	5.57922600	-2.68879300	1.83704200
H	5.10215800	-3.48927800	0.33917000
H	5.65951800	-1.80798800	0.30371600
C	2.83839900	-3.08566800	1.90631200
H	2.79056000	-4.04997000	1.38884200
H	3.31799500	-3.26291900	2.87506800
H	1.81389800	-2.75281900	2.10629900

C	-4.79959700	-1.42564100	-0.02709200
F	-5.51238600	-2.55954900	0.12424200
F	-5.04375000	-0.64222800	1.04525700
F	-5.29956500	-0.78165900	-1.10646500
Pd	0.53775300	0.64075900	0.09962000
C	-0.72879300	2.25901300	0.38425500
C	-1.34991500	2.70649800	-0.79746200
C	-1.42254000	2.35924500	1.60420600
C	-2.65802600	3.19427900	-0.76323200
H	-0.81435900	2.67566500	-1.74251900
C	-2.72582200	2.86337000	1.63482400
H	-0.94359700	2.05078700	2.52972700
C	-3.34676700	3.27705600	0.45181600
H	-3.13568100	3.52066800	-1.68328500
H	-3.25277400	2.93667800	2.58241500
H	-4.35832600	3.67216500	0.47755500
C	2.10811300	2.03199100	0.02421200
C	1.22445700	2.94238700	0.68687700
H	2.81805700	1.52124900	0.67432300
C	2.63635500	2.31552000	-1.37084800
C	3.88858000	3.19988100	-1.32478000
H	4.26485300	3.37228300	-2.34053000
H	3.67635600	4.17652700	-0.88037300
H	4.67868700	2.71548700	-0.74121500
C	1.00381900	4.37033600	0.23803900
H	0.15558900	4.82282200	0.75515500
H	1.90597400	4.93354300	0.51420600
H	0.86212300	4.47163600	-0.83873500
H	1.21048700	2.83261000	1.76853300
H	1.86046300	2.82530300	-1.95931400
O	2.94576500	1.05623200	-1.98526400
H	3.38119000	1.25126800	-2.82851700

42-s

B3LYP SCF energy in DMF: -1619.959486 a.u.

M06 SCF energy in DMF: -1619.369062 a.u.

M06 Free energy in DMF: -1618.926116 a.u.

C	-2.69420400	-0.16011200	0.04562600
C	-1.21241000	-1.86041600	-0.42932200
C	-2.23702400	-2.76660700	-0.68388500
C	-3.55484000	-2.32900500	-0.55810400
C	-3.78347100	-1.00870000	-0.18297800
H	-2.84057400	0.87395400	0.33270000
H	-2.01041400	-3.78675900	-0.96898400
H	-4.38012000	-3.00694000	-0.74518200
C	0.20834700	-2.23747700	-0.48864600
N	1.16186800	-1.43836500	-0.14550000
C	2.00383800	-3.45601200	-0.98995000
C	2.42861900	-2.21959300	-0.16616600
H	2.24740700	-3.36019800	-2.05136300
H	3.18088200	-1.63945200	-0.70345600
O	0.53627100	-3.46562100	-0.88634000
H	2.36058000	-4.41298900	-0.61513400
N	-1.43310000	-0.57365900	-0.07394600
C	2.96761700	-2.55334300	1.26663400
C	3.25307200	-1.25955300	2.05033700
H	2.35128300	-0.65353100	2.17939800
H	3.63521200	-1.50801100	3.04671500
H	4.01276400	-0.64937500	1.55037700
C	4.29546200	-3.31986000	1.09935200
H	4.73747600	-3.51812600	2.08176800
H	4.16427700	-4.28579300	0.60036700
H	5.01929400	-2.73616200	0.51873200
C	1.96794900	-3.40950000	2.06713000
H	1.76971100	-4.37603200	1.59265400
H	2.37435500	-3.61654400	3.06293900
H	1.01216900	-2.89238700	2.20720500
C	-5.18121200	-0.46029000	-0.07419100
F	-6.07897800	-1.42501600	0.20923500
F	-5.27343500	0.48140500	0.88928800
F	-5.57466800	0.12076700	-1.23081900

Pd	0.56025100	0.60565500	-0.07333400
C	0.60379000	2.79268500	0.65896700
C	-0.16458300	2.89194000	-0.53111100
C	-0.07231900	2.90434900	1.90460700
C	-1.55184100	3.15552700	-0.46486200
H	0.32648000	2.94002300	-1.49755100
C	-1.43130600	3.16642400	1.95395500
H	0.50418600	2.82437300	2.82233300
C	-2.17502700	3.30386100	0.76388700
H	-2.11623200	3.26397900	-1.38634000
H	-1.92559100	3.28051600	2.91445500
H	-3.23694100	3.52677400	0.81396900
C	2.42220300	1.45508900	-0.24118200
C	2.13744000	2.71560000	0.59683800
H	3.09094500	0.76273200	0.27110700
C	2.84755800	1.59510200	-1.70246400
C	4.35312300	1.85805600	-1.84138400
H	4.62862900	1.90344800	-2.90272400
H	4.64969600	2.80522900	-1.38484800
H	4.92620100	1.05130500	-1.37163200
C	2.76035600	4.05620300	0.17217400
H	2.39546700	4.85053600	0.83361000
H	3.85070400	4.02936600	0.25751300
H	2.50026000	4.33088900	-0.85436300
H	2.47357000	2.50725900	1.61774800
H	2.30231700	2.41844500	-2.18446300
O	2.51916000	0.36031500	-2.36659000
H	2.87655900	0.41934900	-3.26550800

43-s

B3LYP SCF energy in DMF: -1619.94453 a.u.

M06 SCF energy in DMF: -1619.351746 a.u.

M06 Free energy in DMF: -1618.914304 a.u.

C	-2.41445400	-0.65966100	0.18484600
C	-0.74973800	-2.14235900	-0.44279300
C	-1.65868300	-3.18008400	-0.60592700
C	-3.00764900	-2.93385200	-0.34790500
C	-3.38415200	-1.66024300	0.06229700
H	-2.67747000	0.34639400	0.48850500
H	-1.31866800	-4.15962200	-0.91941200
H	-3.74140400	-3.72379400	-0.45922000
C	0.70009000	-2.32345300	-0.62404400
N	1.55965700	-1.41019800	-0.32625300
C	2.59078700	-3.28766000	-1.29749400
C	2.91108100	-2.01649500	-0.47757800
H	2.74215600	-3.14783800	-2.37083900
H	3.54030900	-1.33368000	-1.05512800
O	1.14819100	-3.48839700	-1.08961200
H	3.09544200	-4.19399400	-0.96889100
N	-1.12488200	-0.89374700	-0.06481000
C	3.61502400	-2.28492900	0.89428200
C	3.78687400	-0.96530100	1.66590700
H	2.82381300	-0.50608500	1.90862300
H	4.31492000	-1.15015400	2.60791500
H	4.38150200	-0.24467000	1.09342100
C	5.01360900	-2.86199500	0.59761400
H	5.55866300	-3.01827100	1.53474100
H	4.96687500	-3.82712500	0.08220100
H	5.60333400	-2.17605800	-0.02167200
C	2.81729800	-3.27515200	1.76339700
H	2.70511000	-4.25517800	1.28787800
H	3.33952000	-3.43551800	2.71257200
H	1.81871100	-2.89324800	2.00263800
C	-4.82254600	-1.31148200	0.34490700
F	-5.59406900	-2.40931900	0.45536800
F	-4.94209600	-0.60852700	1.49193500
F	-5.34532700	-0.54693200	-0.63982000
Pd	0.50214500	0.55738000	-0.17106800
C	-0.77106800	2.08521900	0.00501100
C	-1.48213000	2.60688900	-1.08284600
C	-1.08051900	2.52379100	1.30138800

C	-2.48192100	3.56655100	-0.87626400
H	-1.27255400	2.27374100	-2.09478500
C	-2.08125100	3.48313600	1.50240800
H	-0.55206000	2.12206300	2.16197400
C	-2.78211000	4.00883300	0.41409600
H	-3.02659200	3.96298200	-1.72974000
H	-2.30958700	3.81485900	2.51235100
H	-3.55816600	4.75291300	0.57072700
C	1.98305800	1.57754600	-1.57785700
C	2.32237000	1.86603200	-0.26313100
H	2.34990100	0.63838000	-1.99066000
C	1.48072600	2.54821200	-2.60091100
H	1.04577000	3.44958600	-2.16947200
H	2.98904800	1.17055700	0.24059900
C	2.31342500	3.26419800	0.32699200
H	1.38084500	3.77922000	0.06720700
H	2.33669100	2.84632800	-3.22206900
H	0.75486300	2.07759500	-3.27090000
C	2.48938400	3.25555000	1.84332100
H	1.66841500	2.73042100	2.33983800
H	3.43049800	2.76497700	2.11521600
H	2.51191500	4.28079800	2.22984100
O	3.42129400	3.92812600	-0.30966600
H	3.48861900	4.80797000	0.09170700

TS25-s

B3LYP SCF energy in DMF: -1619.913168 a.u.

M06 SCF energy in DMF: -1619.325121 a.u.

M06 Free energy in DMF: -1618.88707 a.u.

C	-2.27657600	-0.81137000	0.36992500
C	-0.52855500	-2.10556300	-0.41416300
C	-1.33349300	-3.23398500	-0.52845400
C	-2.67315100	-3.13013900	-0.15668900
C	-3.14589000	-1.90487600	0.30628700
H	-2.61321900	0.16202400	0.70861600
H	-0.92167200	-4.16911100	-0.88821600
H	-3.32982800	-3.99028400	-0.22194700
C	0.91064200	-2.11276200	-0.72381300
N	1.73069700	-1.20407800	-0.30986300
C	2.76271900	-2.72054400	-1.79320500
C	3.09589200	-1.65595600	-0.72693400
H	2.75508900	-2.31647400	-2.80931100
H	3.62305600	-0.80936700	-1.17458700
O	1.38350300	-3.10861200	-1.47477600
H	3.37127300	-3.62204200	-1.76033000
N	-0.99435100	-0.91247200	0.01515000
C	3.95838500	-2.20085800	0.46042200
C	4.14212800	-1.10436300	1.51843800
H	3.18848200	-0.80115900	1.95774500
H	4.78351600	-1.46750600	2.32920000
H	4.62174600	-0.21980100	1.08769500
C	5.34659700	-2.57220300	-0.10013500
H	5.99799200	-2.91103800	0.71267200
H	5.30188700	-3.37957300	-0.83848000
H	5.82718100	-1.70873600	-0.57475400
C	3.31588200	-3.43508300	1.12122500
H	3.20804300	-4.27599900	0.42836400
H	3.94542900	-3.77779700	1.94945600
H	2.32922300	-3.20444800	1.53788800
C	-4.59176300	-1.71699000	0.68245900
F	-5.18588800	-2.88603300	0.99221300
F	-4.72585100	-0.89422700	1.74498500
F	-5.29832200	-1.16693600	-0.33156600
Pd	0.50462000	0.70522100	-0.09915400
C	-0.91560100	2.16847700	-0.44684200
C	-1.75454400	2.00041700	-1.56581000
C	-1.42862300	2.77874800	0.71274400
C	-3.08671000	2.41301600	-1.51346800
H	-1.36437300	1.55531800	-2.47692900
C	-2.76910500	3.17186400	0.76461600
H	-0.78781500	2.94938800	1.57239900

C	-3.59733200	2.99472500	-0.34764200
H	-3.72523800	2.28244400	-2.38300100
H	-3.16166200	3.62710300	1.66993400
H	-4.63411300	3.31664200	-0.31013700
C	1.88051300	2.28985300	-0.28725800
C	0.91187900	2.90534500	-1.14540000
H	2.68119800	1.74166700	-0.78999700
C	2.29633800	3.03167400	0.97572900
H	1.40402300	3.50394200	1.41047200
C	2.95431900	2.17443800	2.04824200
H	3.20617200	2.79438800	2.91722400
H	2.28351100	1.37903800	2.38846500
H	3.87589100	1.72385800	1.67270100
O	3.20284800	4.05569300	0.52307100
H	3.43179900	4.59342500	1.29640500
C	0.55583000	4.37482500	-1.09975500
H	1.39367000	4.91257600	-1.56245900
H	-0.34548200	4.57954700	-1.68110100
H	0.42928600	4.76412300	-0.08953500
H	0.87903800	2.49951200	-2.15453800

44-s

B3LYP SCF energy in DMF: -1619.949369 a.u.

M06 SCF energy in DMF: -1619.361635 a.u.

M06 Free energy in DMF: -1618.920175 a.u.

C	2.60871000	0.21127100	0.55177800
C	1.21788900	1.74177300	-0.47373400
C	2.27286100	2.60125300	-0.76125800
C	3.55582900	2.23415900	-0.35457800
C	3.72072100	1.02924000	0.32081100
H	2.70842600	-0.73996800	1.06062600
H	2.09630100	3.53543900	-1.28053400
H	4.40258600	2.88103100	-0.55370100
C	-0.18121100	2.06190300	-0.80292900
N	-1.18807600	1.41471300	-0.31437500
C	-1.86108300	2.97994200	-1.94281500
C	-2.42240900	2.09548900	-0.80707800
H	-1.95748600	2.51846700	-2.92903200
H	-3.09925800	1.33618400	-1.20704400
O	-0.42383200	3.06358900	-1.64731700
H	-2.24624000	3.99720100	-1.97277400
N	1.38357100	0.55511800	0.15477700
C	-3.18526200	2.88311200	0.30640100
C	-3.55558400	1.93003500	1.45234400
H	-2.66298900	1.55837700	1.96166600
H	-4.17026900	2.45271400	2.19361600
H	-4.12974500	1.07186700	1.08798100
C	-4.48368700	3.43344000	-0.31742700
H	-5.06210400	3.97236600	0.44061500
H	-4.29127500	4.13056100	-1.13982600
H	-5.11197400	2.62241100	-0.70377000
C	-2.34339900	4.04267000	0.87082800
H	-2.09201200	4.78777000	0.10881900
H	-2.90691300	4.56077000	1.65440500
H	-1.41183300	3.68493100	1.32337600
C	5.07635900	0.55687000	0.77407500
F	5.97750700	1.55745400	0.80002300
F	5.02205300	0.02090400	2.01305600
F	5.56488600	-0.40220700	-0.04558700
Pd	-0.54452100	-0.62987100	0.19910400
C	-0.46283200	-2.60758100	-1.03084900
C	0.31094600	-2.45541500	-2.21202500
C	0.21917000	-2.91136800	0.18249300
C	1.68419000	-2.63392800	-2.19078400
H	-0.19782200	-2.22401300	-3.14409400
C	1.62421300	-3.08691300	0.18424700
H	-0.33302200	-3.20356200	1.06892700
C	2.34863400	-2.95053700	-0.98757900
H	2.25408800	-2.53777700	-3.11075900
H	2.12242600	-3.35191400	1.11240000
H	3.42507300	-3.09413100	-0.98599600

C	-2.35670700	-1.58088000	0.08501800
C	-1.99610400	-2.53392700	-1.07240600
H	-3.06650800	-0.80485100	-0.21257700
C	-2.82104200	-2.22147700	1.39981400
H	-2.34839400	-3.20584800	1.51426200
C	-2.53432100	-1.41983500	2.66970200
H	-2.87499100	-1.98304500	3.54761500
H	-1.46035900	-1.23325100	2.78962800
H	-3.05596600	-0.46100200	2.65919600
O	-4.23922100	-2.41109700	1.23274800
H	-4.54874200	-2.92317500	1.99553000
C	-2.66007900	-3.92039100	-1.10189100
H	-3.74944600	-3.82683900	-1.12182700
H	-2.34236600	-4.46122500	-2.00067500
H	-2.38717900	-4.52730100	-0.23347100
H	-2.25289300	-2.02567800	-2.00802200

45-s

B3LYP SCF energy in DMF: -1619.945762 a.u.

M06 SCF energy in DMF: -1619.353255 a.u.

M06 Free energy in DMF: -1618.913041 a.u.

C	-2.84253800	0.02701900	0.29338900
C	-1.53398300	-1.64371800	-0.61147200
C	-2.64215700	-2.37493000	-1.02225100
C	-3.91186700	-1.86754600	-0.74368900
C	-4.00984600	-0.65318600	-0.07394000
H	-2.89410400	0.98236600	0.80513000
H	-2.51747900	-3.31618600	-1.54392600
H	-4.79970900	-2.41021600	-1.04741800
C	-0.15579700	-2.12308200	-0.80084800
N	0.87403600	-1.51294800	-0.30986400
C	1.51567800	-3.35934900	-1.60108400
C	2.05354700	-2.40037100	-0.51804500
H	1.76776000	-3.04020000	-2.61551700
H	2.88131100	-1.80219600	-0.90388600
O	0.05154600	-3.25039900	-1.47087700
H	1.77442100	-4.40722700	-1.46585800
N	-1.62784100	-0.45545400	0.03266100
C	2.52103000	-3.10997400	0.79708100
C	2.90107200	-2.06542800	1.86054500
H	2.03978900	-1.46141900	2.16232800
H	3.28086600	-2.57137300	2.75523800
H	3.68250900	-1.38991700	1.50009400
C	3.77471000	-3.93968000	0.45339300
H	4.16424900	-4.41765100	1.35847200
H	3.56455300	-4.73538800	-0.26950000
H	4.56853500	-3.30739900	0.03941800
C	1.42952500	-4.03225700	1.37134200
H	1.15923900	-4.84115200	0.68486400
H	1.79247900	-4.50006900	2.29273400
H	0.52006100	-3.47727500	1.62709500
C	-5.34404000	-0.05462400	0.28828000
F	-5.61984900	-0.22126400	1.60085500
F	-5.36734800	1.27479400	0.04847700
F	-6.35216600	-0.61315800	-0.40812000
Pd	0.42859600	0.52199900	0.17407200
C	2.33320300	1.09079400	-0.05770500
C	2.82834300	1.13302300	-1.37023500
C	3.20294700	1.35074800	1.00727100
C	4.16951900	1.45665900	-1.61120000
H	2.17842000	0.91644000	-2.21391700
C	4.54505500	1.67136600	0.76182500
H	2.85577700	1.30012500	2.03367900
C	5.03089700	1.73043400	-0.54587700
H	4.53575000	1.49166000	-2.63432400
H	5.20737000	1.87094800	1.60069900
H	6.07126900	1.98139400	-0.73327200
C	-0.40243300	2.60431900	0.06000800
C	-0.23447200	2.33342400	1.40933100
H	-1.34874900	2.32088900	-0.39929400
C	0.34394700	3.68647400	-0.69783100

H	1.40781400	3.66967000	-0.43222100
C	0.19084800	3.53960400	-2.20920300
H	0.61293400	2.59441500	-2.56213400
H	-0.86782400	3.57458700	-2.48968300
H	0.71152300	4.35278000	-2.72758100
O	-0.25012900	4.91461700	-0.23934000
H	0.14454200	5.62923200	-0.76212200
C	0.72293700	3.01433400	2.33890900
H	0.16312100	3.78995900	2.87961000
H	1.10721600	2.32103200	3.09290100
H	1.55769200	3.49536200	1.82953400
H	-1.03392500	1.79226400	1.91481500

TS26-s

B3LYP SCF energy in DMF: -1619.91966 a.u.

M06 SCF energy in DMF: -1619.332334 a.u.

M06 Free energy in DMF: -1618.892312 a.u.

C	2.71826900	-0.17779000	-0.38078400
C	1.30227400	-1.69862700	0.62979700
C	2.35727100	-2.52774100	0.99360000
C	3.65176000	-2.15341500	0.63473200
C	3.82900400	-0.96977900	-0.07460500
H	2.83339700	0.76018300	-0.90959000
H	2.16947700	-3.44865100	1.53227700
C	4.49842600	-2.77682000	0.89911400
H	-0.10720600	-2.05604600	0.85392800
N	-1.07610300	-1.43069600	0.27645200
C	-1.86295800	-3.07594800	1.76206700
C	-2.31766800	-2.19751300	0.57546800
H	-2.10187000	-2.63351300	2.73282600
H	-3.09937300	-1.49965400	0.88515100
O	-0.39668600	-3.08969300	1.64519800
H	-2.20144100	-4.10966300	1.73429300
N	1.48030100	-0.52460200	-0.02368500
C	-2.83998200	-3.00642800	-0.65983700
C	-3.11932800	-2.05566300	-1.83528500
H	-2.20963400	-1.54945000	-2.17239200
H	-3.52028400	-2.62157400	-2.68368800
H	-3.85469700	-1.29344200	-1.56334300
C	-4.16492600	-3.67952000	-0.24892200
H	-4.58159200	-4.23409800	-1.09664400
H	-4.03669000	-4.39049200	0.57451300
H	-4.90703600	-2.93477400	0.06117200
C	-1.83060600	-4.07835000	-1.11456000
H	-1.62506100	-4.82184000	-0.33733000
H	-2.23421200	-4.61744000	-1.97835100
H	-0.87852600	-3.63440400	-1.42612600
C	5.18941800	-0.53421400	-0.55128400
F	5.39836700	-0.88905800	-1.83920800
F	5.32945800	0.80828600	-0.48561700
F	6.17841600	-1.08470000	0.17943700
Pd	-0.36350500	0.64818500	-0.19575200
C	-2.20180600	1.61143900	-0.19701900
C	-2.65468200	1.89603500	1.10654200
C	-3.14284200	1.39995800	-1.21904100
C	-4.02212600	1.91176900	1.38905400
H	-1.94160000	2.11409800	1.89698900
C	-4.51057000	1.44372200	-0.93596700
H	-2.81178100	1.21485100	-2.23674100
C	-4.95211100	1.69207500	0.36720200
H	-4.36113500	2.11531600	2.40137100
H	-5.23022800	1.28585400	-1.73474900
H	-6.01613300	1.72847000	0.58334400
C	0.46292300	2.56760000	-0.41322300
C	-0.79318700	2.97597800	-0.96194800
H	1.23016600	2.32928600	-1.15464900
C	0.97900600	3.24356500	0.85074700
H	0.14290900	3.33825200	1.55988400
C	2.12663800	2.52494200	1.55474800
H	1.81124500	1.54799700	1.93264400
H	2.98228800	2.38844900	0.88575000

H	2.45943900	3.12007900	2.41341700
O	1.39771600	4.55363100	0.42393100
H	1.67385300	5.03576100	1.21820200
C	-1.51411500	4.24009000	-0.55596700
H	-0.96754600	5.07123400	-1.01994000
H	-2.53897700	4.24891100	-0.93185700
H	-1.52280700	4.41127600	0.52062800
H	-0.92783200	2.72730700	-2.01215800

46-s

B3LYP SCF energy in DMF: -1619.952271 a.u.

M06 SCF energy in DMF: -1619.36482 a.u.

M06 Free energy in DMF: -1618.924039 a.u.

C	-2.51796300	-0.47865200	0.39344500
C	-0.95490600	-1.89547800	-0.55339900
C	-1.90871700	-2.87890900	-0.78740600
C	-3.22731500	-2.64027800	-0.39994200
C	-3.52753300	-1.42864600	0.21158700
H	-2.73567200	0.47846100	0.85119100
H	-1.62243200	-3.81492800	-1.25131200
H	-3.99480800	-3.38709500	-0.56662800
C	0.47722300	-2.10627700	-0.81483400
N	1.38946300	-1.32211900	-0.35365200
C	2.29939600	-3.03038600	-1.69195700
C	2.69331400	-1.99300600	-0.61824200
H	2.45610700	-2.66445300	-2.71039000
H	3.39449500	-1.25911700	-1.02245800
O	0.84887100	-3.18484900	-1.50863700
H	2.74858700	-4.01540000	-1.58129800
N	-1.25986300	-0.69720000	0.00660900
C	3.32156200	-2.60862600	0.67803400
C	3.51320200	-1.51178900	1.73845600
H	2.55965400	-1.06566600	2.03701600
H	3.98074700	-1.93551700	2.63430700
H	4.16343900	-0.71403000	1.36981300
C	4.70456400	-3.17773700	0.30291100
H	5.19812300	-3.58119600	1.19361700
H	4.63825700	-3.98922400	-0.42972200
H	5.35358800	-2.39960800	-0.11541400
C	2.44361500	-3.72736200	1.27042000
H	2.30267900	-4.56349600	0.57778400
H	2.92085500	-4.13093600	2.17002300
H	1.45648300	-3.35639300	1.56791000
C	-4.91741000	-1.09595300	0.68734700
F	-4.98091400	-1.05156600	2.03657600
F	-5.31009900	0.11760100	0.23751300
F	-5.82329600	-1.99862400	0.26846600
Pd	0.36960800	0.71213100	-0.01991300
C	1.67106500	2.59814600	0.47606000
C	1.96502800	2.31769900	-0.88540100
C	2.68932700	2.37782900	1.44017700
C	3.24815700	1.85533900	-1.25837600
H	1.28017000	2.61754500	-1.67168900
C	3.95152800	1.96004800	1.05517000
H	2.47714600	2.59072900	2.48446900
C	4.23458100	1.69366700	-0.29999400
H	3.46098900	1.66767500	-2.30668400
H	4.73108700	1.83880600	1.80148900
H	5.22986300	1.36949800	-0.58946300
C	-0.74780800	2.42008400	0.21695200
C	0.35161600	3.27836800	0.87069200
H	-1.52151400	2.13665800	0.93739500
C	-1.41282400	2.97691700	-1.04817800
H	-0.65513400	3.48086100	-1.66397800
C	-2.14346000	1.96955500	-1.93641900
H	-1.45997700	1.21553200	-2.33972900
H	-2.94709000	1.46494900	-1.39215800
H	-2.59540400	2.49685900	-2.78543200
O	-2.34731800	3.96069900	-0.56025100
H	-2.67325500	4.44982400	-1.33096100
C	0.38003300	4.78686600	0.56847100

H	-0.55431000	5.26279600	0.87491400
H	1.20680700	5.25180200	1.11792000
H	0.53182300	4.98831700	-0.49607500
H	0.25823400	3.16192800	1.95549100

47-s

B3LYP SCF energy in DMF: -1619.951368 a.u.

M06 SCF energy in DMF: -1619.355791 a.u.

M06 Free energy in DMF: -1618.916931 a.u.

C	2.87392200	-0.17534500	0.04701000
C	1.62334100	1.70700800	-0.41719100
C	2.75638700	2.47554000	-0.65591900
C	4.00778200	1.87345300	-0.52167700
C	4.06413300	0.53181500	-0.16206100
H	2.89231700	-1.22768400	0.30981600
H	2.66491600	3.51707000	-0.93950100
H	4.91344000	2.44244400	-0.69809200
C	0.26242500	2.26173700	-0.49506300
N	-0.79527300	1.57758700	-0.20203700
C	-1.35510900	3.71093000	-0.99249700
C	-1.94933100	2.52098100	-0.20876400
H	-1.58046000	3.67101000	-2.06135300
H	-2.77274300	2.06380800	-0.76111200
O	0.10076600	3.52978900	-0.85593700
H	-1.59515500	4.69663300	-0.59984100
N	1.67644200	0.39664800	-0.07593300
C	-2.45254200	2.87896200	1.23026000
C	-2.87718400	1.60392500	1.97802500
H	-2.03228300	0.92691600	2.13632400
H	-3.28010100	1.87058100	2.96152200
H	-3.65506200	1.05962400	1.43430900
C	-3.68713100	3.79024700	1.07530100
H	-4.09327700	4.03795200	2.06188000
H	-3.45074000	4.73456100	0.57371900
H	-4.47847200	3.29275900	0.50284100
C	-1.37028400	3.60271700	2.05388300
H	-1.06385000	4.55256900	1.60377100
H	-1.75920100	3.82934800	3.05231000
H	-0.47769300	2.98153900	2.18767700
C	5.37696500	-0.17991900	0.03549100
F	6.40422700	0.49597500	-0.51288900
F	5.65558900	-0.34287900	1.34781100
F	5.35568900	-1.41278500	-0.51670900
Pd	-0.41455100	-0.52611400	-0.18652300
C	-2.30870000	-0.98164000	-0.63885400
C	-2.70886600	-0.71148700	-1.95603600
C	-3.24555700	-1.47750700	0.27516200
C	-4.03051000	-0.94662800	-2.35555500
H	-1.99837200	-0.32072300	-2.68047500
C	-4.56731700	-1.70937000	-0.13015700
H	-2.95591000	-1.68661000	1.29990800
C	-4.96302700	-1.44708900	-1.44348600
H	-4.32519900	-0.73686000	-3.38096600
H	-5.28548800	-2.09581000	0.58914100
H	-5.98831700	-1.62962400	-1.75348100
C	0.19399700	-2.57419400	0.53396800
C	0.32526800	-2.57799100	-0.84612100
H	1.03597400	-2.22167300	1.12998800
C	-0.49389000	-3.37505400	-1.82083100
H	-1.46447000	-3.67975100	-1.42804100
H	-0.64629400	-2.82083800	-2.75138800
H	0.07040000	-4.28163500	-2.07878300
C	-0.77897800	-3.39659700	1.33924700
C	-0.15279800	-4.75296300	1.68576400
H	-0.84016200	-5.33060300	2.31507100
H	0.04235200	-5.33643300	0.78032600
H	0.78815300	-4.62210000	2.23030900
O	-1.06235600	-2.64313800	2.52608400
H	-1.63327000	-3.19169500	3.08495300
H	-1.70178900	-3.56641200	0.77343900
H	1.26715200	-2.21197400	-1.25292200

TS27-s

B3LYP SCF energy in DMF: -1619.925939 a.u.

M06 SCF energy in DMF: -1619.335578 a.u.

M06 Free energy in DMF: -1618.896796 a.u.

C	-2.73772000	-0.14424700	0.06273900
C	-1.30436200	-1.86510600	-0.51592100
C	-2.35761200	-2.73939500	-0.76046300
C	-3.66078700	-2.27932600	-0.57718800
C	-3.84768400	-0.96754100	-0.15159400
H	-2.84016000	0.87907200	0.40505000
H	-2.16178800	-3.75424400	-1.08440200
H	-4.50609800	-2.93265200	-0.76231100
C	0.10564400	-2.27057000	-0.62530900
N	1.07852300	-1.50716800	-0.26214400
C	1.85580800	-3.50234400	-1.23654800
C	2.32506400	-2.31460300	-0.36609100
H	2.07775500	-3.36073600	-2.29777000
H	3.08156500	-1.72572000	-0.89100600
O	0.39224200	-3.48492400	-1.09828800
H	2.20176800	-4.48314300	-0.91597100
N	-1.48900900	-0.58076300	-0.12423600
C	2.90244200	-2.71448900	1.03162500
C	3.20272000	-1.44802400	1.85075800
H	2.29179100	-0.88454500	2.07289000
H	3.66704500	-1.72317200	2.80457000
H	3.89501500	-0.78595000	1.32171300
C	4.22460800	-3.47119100	0.79475700
H	4.68362700	-3.73223900	1.75448000
H	4.07887600	-4.40329300	0.23866400
H	4.94006300	-2.85470900	0.23823700
C	1.92592500	-3.60559700	1.82181400
H	1.72670800	-4.55777600	1.31918600
H	2.35362800	-3.84253300	2.80202600
H	0.96870800	-3.10246200	1.99820500
C	-5.22566500	-0.42627300	0.12163200
F	-6.16467400	-1.05844200	-0.61062600
F	-5.56837000	-0.57422300	1.42148000
F	-5.30746400	0.89249300	-0.15889600
Pd	0.35778100	0.60497300	-0.18551000
C	2.17191500	1.58893400	-0.411134100
C	2.99638600	1.23833900	-1.49688300
C	2.76407000	2.03086400	0.78664700
C	4.38600500	1.30090600	-1.37373700
H	2.55246700	0.92704400	-2.43864900
C	4.15436200	2.08378100	0.90745000
H	2.14134800	2.34621500	1.61945500
C	4.96663500	1.72421900	-0.17274800
H	5.01494500	1.02920600	-2.21733400
H	4.60241100	2.41718000	1.83968000
H	6.04768700	1.78373200	-0.08361100
C	-0.50266700	2.51165500	-0.38412600
C	0.68131800	2.88427000	-1.09792700
H	-1.34646100	2.22185700	-1.01558100
C	1.42313300	4.18374600	-0.87808800
H	1.54338200	4.44583700	0.17356300
H	2.40319300	4.16648300	-1.35871800
H	0.82654300	4.97165900	-1.35863600
C	-0.90179900	3.20829700	0.90295000
C	-1.71809700	4.47614300	0.63070800
H	-2.01713100	4.94327500	1.57704800
H	-1.13858900	5.21277600	0.06677400
H	-2.62302200	4.23539700	0.06228400
O	-1.67880800	2.27416000	1.66981900
H	-2.05750300	2.75743400	2.41953800
H	0.00030200	3.47591400	1.46923300
H	0.68665400	2.56981900	-2.13906000

48-s

B3LYP SCF energy in DMF: -1619.958073 a.u.

M06 SCF energy in DMF: -1619.368057 a.u.

M06 Free energy in DMF: -1618.926117 a.u.

C	-2.53108700	-0.51305100	0.03386900
C	-0.82599000	-1.92255300	-0.64780200
C	-1.72241400	-2.91641100	-1.02311600
C	-3.08723000	-2.68529000	-0.85288500
C	-3.49076300	-1.47264900	-0.30525800
H	-2.80631400	0.43525500	0.47963700
H	-1.35982200	-3.85231200	-1.43023600
H	-3.81229200	-3.43997000	-1.13451700
C	0.63177400	-2.11274300	-0.69956500
N	1.46427600	-1.27520000	-0.18546200
C	2.56730700	-3.04862400	-1.27194300
C	2.80599200	-1.91802900	-0.24632600
H	2.84919400	-2.76288100	-2.28906000
H	3.52899400	-1.19444500	-0.63008000
O	1.10903900	-3.22597000	-1.26279800
H	3.01420800	-4.00903800	-1.02167000
N	-1.22570500	-0.72670400	-0.14643700
C	3.29945000	-2.40670200	1.15696000
C	3.35609800	-1.22130200	2.13636600
H	2.36992100	-0.77146900	2.28828800
H	3.72279200	-1.56061200	3.11166500
H	4.03577800	-0.44265300	1.77870400
C	4.72433700	-2.96959000	0.98372500
H	5.12333900	-3.28282700	1.95459800
H	4.75171300	-3.84368900	0.32372700
H	5.40339400	-2.21485300	0.57045600
C	2.38095400	-3.49643000	1.74215700
H	2.34145200	-4.39333000	1.11530900
H	2.75683100	-3.80570600	2.72343300
H	1.35788800	-3.13212200	1.88665200
C	-4.94101200	-1.15731200	-0.04821700
F	-5.76292700	-2.08263400	-0.57822000
F	-5.20355400	-1.09280200	1.27653200
F	-5.28397600	0.04058900	-0.57241300
Pd	0.37044100	0.72612700	0.00218300
C	1.46291500	2.58058800	-0.82831300
C	2.17603800	2.21369400	-2.00171800
C	2.10733800	2.41946100	0.42685900
C	3.48563800	1.76861600	-1.92602300
H	1.69034200	2.32939300	-2.96689200
C	3.44531900	1.97158700	0.48641300
H	1.64444100	2.79618500	1.33345800
C	4.12907200	1.65694400	-0.67745800
H	4.02589700	1.52128800	-2.83540100
H	3.93853300	1.90223300	1.45044900
H	5.16390500	1.33065500	-0.63141600
C	-0.83619900	2.38859800	-0.07259000
C	0.09569400	3.27421600	-0.92280800
H	-1.70639500	2.05700000	-0.64720900
C	0.19698200	4.77627400	-0.61084400
H	0.47869100	4.96967800	0.42826000
H	0.96117900	5.22815700	-1.25360200
H	-0.74871000	5.28749000	-0.81385800
C	-1.27215400	2.85917800	1.31345300
C	-2.46991000	3.81545700	1.25435900
H	-2.77450700	4.09672500	2.27041200
H	-2.23546500	4.73703300	0.71683800
H	-3.32019500	3.33270800	0.76033800
O	-1.64103600	1.68547000	2.06398500
H	-2.05669900	1.98749600	2.88581700
H	-0.44204200	3.36446400	1.82496900
H	-0.22510800	3.17568700	-1.96456400

TS28-s

B3LYP SCF energy in DMF: -1619.918905 a.u.

M06 SCF energy in DMF: -1619.33107 a.u.

M06 Free energy in DMF: -1618.893356 a.u.

C	-2.14648400	-1.12503700	0.22140500
C	-0.27691400	-2.28375900	-0.48852400

C	-1.00539700	-3.44940600	-0.70191400	H	-2.60502500	-3.27750500	-1.49876700
C	-2.37268700	-3.43539200	-0.42897200	H	-4.80868600	-2.23831000	-0.92161500
C	-2.94577100	-2.25922500	0.04770000	C	-0.14809000	-2.23864100	-0.81862300
H	-2.56334900	-0.19131000	0.57949900	N	0.92337000	-1.76601500	-0.26959100
H	-0.51588700	-4.34449400	-1.06593500	C	1.41981800	-3.46329100	-1.81952500
H	-2.97220600	-4.32631100	-0.57973500	C	2.04313900	-2.67803900	-0.64514300
C	1.17704000	-2.19750300	-0.70069400	H	1.66874700	-3.03706800	-2.79486800
N	1.88921600	-1.20138700	-0.29185900	H	2.88632100	-2.07358800	-0.98799400
C	3.15152900	-2.71134500	-1.59134800	O	-0.02717300	-3.28666900	-1.63121800
C	3.31025000	-1.53089400	-0.60642300	H	1.61989800	-4.53277900	-1.82274200
H	3.20128300	-2.39972500	-2.63799000	N	-1.48879400	-0.50172600	0.08554400
H	3.76237000	-0.67026700	-1.10643500	C	2.53355100	-3.57353600	0.53911200
O	1.78450600	-3.19067100	-1.35131000	C	3.01858200	-2.68911500	1.69829600
H	3.82595600	-3.54880900	-1.42416500	H	2.20223100	-2.09576600	2.12017600
N	-0.84026600	-1.13611500	-0.04813800	H	3.42519500	-3.31463100	2.50058800
C	4.16881700	-1.85942400	0.65765100	H	3.81179100	-2.00752300	1.37405500
C	4.16249900	-0.65856500	1.61588500	C	3.72377300	-4.40989300	0.02790100
H	3.16110700	-0.47054500	2.01331400	H	4.12910300	-5.01897100	0.84293900
H	4.82777400	-0.85153400	2.46472100	H	3.43837400	-5.09310100	-0.77903300
H	4.51530600	0.24988100	1.11588500	H	4.53099800	-3.76805100	-0.34358900
C	5.61677700	-2.10477600	0.18734200	C	1.42254300	-4.50899300	1.05210100
H	6.26274000	-2.29153900	1.05184400	H	1.07237000	-5.20558800	0.28323700
H	5.69997800	-2.97221900	-0.47612600	H	1.80357200	-5.11111200	1.88385400
H	6.01369800	-1.23278100	-0.34547900	H	0.55939000	-3.94756900	1.42656700
C	3.64526300	-3.09998900	1.40524700	C	-5.16012200	0.15687400	0.41166000
H	3.68125500	-4.00708000	0.79289500	F	-6.22892700	-0.65993600	0.34365000
H	4.26411600	-3.28507100	2.28990100	F	-5.11510700	0.66983400	1.66059300
H	2.61547600	-2.96053900	1.75237400	F	-5.39110600	1.19273900	-0.42819400
C	-4.42446300	-2.16349100	0.31533800	Pd	0.64734700	0.31409300	0.27131700
F	-4.96024700	-3.36414900	0.61214600	C	0.93262700	2.52059800	-0.35259500
F	-4.69150800	-1.32968500	1.34290300	C	0.14913400	2.77212800	-1.51216200
F	-5.08913000	-1.68596500	-0.76179900	C	0.31049100	2.66523500	0.91645800
Pd	0.57627800	0.57285700	-0.00307100	C	-1.16366800	3.19972600	-1.40593300
C	-0.89017800	2.01657500	-0.01191600	H	0.61211300	2.66151200	-2.48858300
C	-1.80334700	2.02094100	-1.08073400	C	-1.02945500	3.10530000	1.00841900
C	-1.31780700	2.42411300	1.26411900	H	0.89621800	2.60947800	1.82655200
C	-3.13639600	2.37395300	-0.86310100	C	-1.75669500	3.37609400	-0.13967000
H	-1.47574700	1.74482300	-2.07904400	H	-1.73579500	3.41509300	-2.30388900
C	-2.65520600	2.77124800	1.47671000	H	-1.47389100	3.24786400	1.98920400
H	-0.61497300	2.46578700	2.09121200	H	-2.78277700	3.72478000	-0.06770600
C	-3.56535900	2.74571900	0.41515500	C	2.61304000	0.89561300	0.30687900
H	-3.83839000	2.36557700	-1.69292300	C	2.43194900	2.20790400	-0.47502300
H	-2.98324900	3.06684100	2.46995000	H	3.14440700	0.13811700	-0.27484800
H	-4.60245100	3.02364700	0.58171500	C	3.13406900	0.95472000	1.73595600
C	1.95979700	2.16983200	-0.01051200	H	2.66416500	1.73220700	2.34273600
C	0.94832200	2.92636500	-0.66985600	H	4.21460500	1.15878800	1.73550100
H	2.68978500	1.69746500	-0.67098600	H	2.99542400	0.00039800	2.24879500
C	2.46743900	2.55888200	1.36056400	C	3.33191700	3.40025400	-0.08826700
H	1.67644900	2.97392600	1.99147800	H	3.25572900	3.57246000	0.99521600
H	3.25558900	3.31994000	1.27650200	C	2.61719000	2.00338600	-1.53524800
H	2.90484600	1.70596600	1.88063000	H	4.79393300	3.16843500	-0.46701100
C	0.62501800	4.36784200	-0.30380600	H	5.40165800	4.03738800	-0.18800100
H	0.46709900	4.46310100	0.77695000	H	5.21555100	2.29458700	0.03887400
H	0.84330800	2.74685200	-1.73831900	H	4.88613300	3.02033700	-1.54870100
C	1.82142700	5.24210400	-0.72001400	O	2.80542300	4.53202200	-0.79067200
H	1.58979600	6.29132400	-0.50291900	H	3.33787200	5.29962400	-0.53614400
H	2.73219800	4.98260000	-0.17452900				
H	2.01121800	5.14796700	-1.79410900				
O	-0.53479000	4.76682700	-1.02298700				
H	-0.70130500	5.69394900	-0.79963800				

TS29-s

B3LYP SCF energy in DMF: -1619.922914 a.u.

M06 SCF energy in DMF: -1619.335699 a.u.

M06 Free energy in DMF: -1618.895473 a.u.

49-s

B3LYP SCF energy in DMF: -1619.956084 a.u.

M06 SCF energy in DMF: -1619.369389 a.u.

M06 Free energy in DMF: -1618.92859 a.u.

C	-2.66198400	0.04360900	0.40401800	C	-2.22407600	-0.97396100	0.16659900
C	-1.48865500	-1.68139800	-0.57703500	C	-0.42499800	-2.26039400	-0.50563100
C	-2.65326500	-2.33675800	-0.96395800	C	-1.23284900	-3.36027500	-0.77341600
C	-3.87957100	-1.75612700	-0.63930600	C	-2.60373500	-3.24572100	-0.54584700
C	-3.88036500	-0.55366000	0.05987000	C	-3.10200600	-2.03910800	-0.06232500
H	-2.63279900	0.98266900	0.94332900	H	-2.57913200	-0.01945300	0.53789100
				H	-0.80145800	-4.28226400	-1.14377800
				H	-3.26427400	-4.08421900	-0.73665000
				C	1.03854700	-2.28694600	-0.65593600
				N	1.79177600	-1.29508900	-0.31841200

C	3.03641200	-3.03374200	-1.29544700
C	3.20371300	-1.75189500	-0.44675000
H	3.20262500	-2.85878400	-2.36150600
H	3.76827600	-0.99678100	-0.99937000
O	1.61908800	-3.38668500	-1.13285500
H	3.62322500	-3.88902800	-0.96713100
N	-0.91300400	-1.08289700	-0.05081500
C	3.90873500	-1.97160000	0.93301200
C	3.94473000	-0.65252500	1.72442300
H	2.93881700	-0.29583500	1.96584800
H	4.48155300	-0.79920200	2.66817600
H	4.46736800	0.13275100	1.16697300
C	5.36039400	-2.41067500	0.65127500
H	5.90616900	-2.52216500	1.59425600
H	5.41360300	-3.37192400	0.12919900
H	5.88978700	-1.66739300	0.04388100
C	3.19502800	-3.04427100	1.77679200
H	3.17994700	-4.02233300	1.28429200
H	3.71761600	-3.17116100	2.73091200
H	2.16240900	-2.75935400	2.00651700
C	-4.57852300	-1.84596300	0.16558900
F	-5.19545500	-3.00956000	0.45308200
F	-4.81935300	-0.99242000	1.18296100
F	-5.18431100	-1.33470700	-0.93045600
Pd	0.63426500	0.52594000	-0.01935300
C	-0.72817400	2.06132300	0.19409200
C	-1.45872400	2.35869200	-0.97080900
C	-1.33246300	2.24060000	1.45105100
C	-2.78680600	2.78314500	-0.87665300
H	-0.99763800	2.25458800	-1.94892400
C	-2.66039000	2.66902100	1.53848100
H	-0.76837800	2.05082600	2.36011200
C	-3.38932900	2.94061300	0.37604300
H	-3.34813000	2.99794300	-1.78220000
H	-3.12047100	2.79909000	2.51443800
H	-4.41817600	3.28212600	0.44559900
C	2.17563600	1.93689500	-0.25695400
C	1.25381400	2.88120700	0.27454500
H	2.87911800	1.53088200	0.46832400
C	2.67521500	1.98129700	-1.68318000
H	1.89089000	2.26629800	-2.39045300
H	1.25775900	2.96815400	1.35839300
C	0.98168300	4.20841100	-0.44600700
H	0.58959500	4.01562900	-1.45209500
H	3.48061100	2.72039800	-1.77005800
H	3.07820800	1.01100800	-1.98777200
C	0.05462100	5.16105200	0.30429200
H	-0.97217500	4.79612800	0.35622000
H	0.42291400	5.32956700	1.32207300
H	0.03284700	6.12657700	-0.21454500
O	2.29654500	4.78662300	-0.53908000
H	2.18714800	5.67019800	-0.92202900

50-s

B3LYP SCF energy in DMF: -1619.96083 a.u.

M06 SCF energy in DMF: -1619.373329 a.u.

M06 Free energy in DMF: -1618.931786 a.u.

C	-2.69434600	0.33518400	0.12989900
C	-1.72231900	-1.66894100	-0.46155400
C	-2.95581000	-2.27705300	-0.67598300
C	-4.10940600	-1.52331600	-0.46641300
C	-3.97385400	-0.20159000	-0.05117900
H	-2.55790000	1.36257700	0.44522600
H	-3.01171600	-3.31165300	-0.99216100
H	-5.08915000	-1.96284700	-0.61876700
C	-0.45158300	-2.39867900	-0.59836800
N	0.69504700	-1.87876900	-0.30831400
C	0.93743900	-4.03998500	-1.18247100
C	1.70924500	-2.96776800	-0.38126000
H	1.14795500	-4.00102100	-2.25447300
H	2.57275500	-2.60994400	-0.94690800

O	-0.47419600	-3.66508500	-1.00769100
H	1.04753800	-5.06028200	-0.82117900
N	-1.58798000	-0.38010400	-0.07339400
C	2.20264600	-3.44440500	1.02680300
C	2.86880700	-2.28366400	1.78643800
H	2.17356700	-1.45749700	1.96304200
H	3.22381500	-2.63570200	2.76142700
H	3.73633600	-1.89716900	1.24095700
C	3.26044300	-4.54452300	0.80184000
H	3.66770000	-4.87067200	1.76472100
H	2.84845300	-5.42968000	0.30620000
H	4.09431100	-4.17425000	0.19436400
C	1.04520200	-4.00046100	1.87816300
H	0.54966100	-4.85508600	1.40571700
H	1.43059300	-4.34411600	2.84406000
H	0.28788900	-3.23600100	2.08506400
C	-5.18413100	0.67168200	0.14653700
F	-6.24341500	-0.03729200	0.58764300
F	-4.95118600	1.65813500	1.03782400
F	-5.55934200	1.26498300	-1.00991800
Pd	0.65263100	0.24301800	-0.18759400
C	1.31580200	2.40925900	0.32864600
C	0.49940900	2.62816700	-0.81206400
C	0.79059200	2.75590400	1.60313300
C	-0.76957500	3.23091000	-0.67664800
H	0.90061200	2.47855800	-1.80860200
C	-0.45748700	3.34735200	1.72164100
H	1.40250500	2.58782500	2.48498600
C	-1.23801500	3.59731800	0.57646900
H	-1.36383100	3.42316700	-1.56500200
H	-0.82905600	3.63233900	2.70164000
H	-2.20703200	4.07742600	0.67802300
C	2.64380100	0.55899600	-0.52572000
C	2.76271300	1.91903700	0.17892700
H	3.15691700	-0.22832900	0.02525700
C	2.94724600	0.45742800	-2.01177800
H	2.38425200	1.16598500	-2.62662500
H	3.14489000	1.74743900	1.19109000
C	3.70417300	2.94850400	-0.47573400
H	3.38715000	3.11368100	-1.51633600
H	4.01442400	0.65984200	-2.17718600
H	2.73799000	-0.55142200	-2.38233000
C	3.72390700	4.29078700	0.25297300
H	2.75246300	4.79280500	0.20415800
H	3.99841800	4.16060200	1.30561700
H	4.45924400	4.95820100	-0.21187600
O	5.00083300	2.33759800	-0.45431100
H	5.61175000	2.94511600	-0.89652300

TS30-s

B3LYP SCF energy in DMF: -1619.921439 a.u.

M06 SCF energy in DMF: -1619.332859 a.u.

M06 Free energy in DMF: -1618.893298 a.u.

C	2.90057600	-0.44196000	0.16188500
C	1.88874900	1.50460600	-0.56066000
C	3.11133100	2.10109800	-0.85032500
C	4.27852300	1.37982300	-0.60711800
C	4.16770600	0.09349400	-0.08738900
H	2.79241600	-1.44721600	0.54961300
H	3.14729300	3.10598000	-1.25288400
H	5.24877000	1.81439800	-0.82068800
C	0.60800400	2.20944000	-0.72765900
N	-0.51243500	1.73009800	-0.30888700
C	-0.81250600	3.75203000	-1.47274600
C	-1.53509100	2.79624900	-0.49745900
H	-1.07141400	3.56430300	-2.51835700
H	-2.41789300	2.35630500	-0.96776800
O	0.60790600	3.40825100	-1.31379900
H	-0.91876600	4.81242800	-1.25192400
N	1.77975400	0.24537100	-0.07200100
C	-1.97711400	3.45504600	0.85148200

C	-2.56151900	2.38342900	1.78653800
H	-1.81292300	1.63396100	2.05946800
H	-2.92059600	2.85053400	2.71055100
H	-3.40810900	1.86854300	1.32213500
C	-3.08077800	4.48357700	0.53269200
H	-3.45170000	4.93248300	1.46051200
H	-2.71988200	5.29955100	-0.10235400
H	-3.93039600	4.01187300	0.02542700
C	-0.80231700	4.15562500	1.55991800
H	-0.38595200	4.97674600	0.96712800
H	-1.14579200	4.58377200	2.50778600
H	0.00669800	3.45474500	1.79354300
C	5.39280400	-0.71624800	0.24640200
F	6.43180000	-0.39955400	-0.55186900
F	5.79091700	-0.50643900	1.52149600
F	5.16625500	-2.04097500	0.11693100
Pd	-0.30619000	-0.47993500	-0.02232100
C	-2.29546700	-1.00824800	-0.14585000
C	-2.99312400	-0.62647400	-1.30766600
C	-2.99793100	-1.14846100	1.06390500
C	-4.35844800	-0.33977300	-1.24488400
H	-2.47091800	-0.55169400	-2.25761500
C	-4.36651200	-0.86816400	1.11891500
H	-2.48192300	-1.47730800	1.96144000
C	-5.04786800	-0.46253700	-0.03275200
H	-4.88715800	-0.03504800	-2.14425300
H	-4.89993100	-0.97186800	2.06009700
H	-6.11310000	-0.25360900	0.01001300
C	0.14756300	-2.53146000	0.09417800
C	-1.09408500	-2.76813100	-0.55767300
H	-1.07739400	-2.66872700	-1.64212900
C	-2.06551000	-3.85559900	-0.06640700
H	-2.28303600	-3.71858700	0.99420100
C	0.42351300	-3.00606100	1.50200900
H	0.61570500	-4.08670200	1.49926700
H	1.30560900	-2.51220100	1.92014800
H	-0.42059700	-2.82145100	2.17294000
H	1.01120800	-2.51943700	-0.57410600
C	-3.35626900	-3.97786900	-0.86668900
H	-4.02147900	-3.12561400	-0.72429800
H	-3.13952600	-4.06870300	-1.93854200
H	-3.88488700	-4.88090200	-0.54716700
O	-1.32457300	-5.08432100	-0.14067100
H	-1.26358500	-5.32717400	-1.07835300

51-s

B3LYP SCF energy in DMF: -1619.958816 a.u.

M06 SCF energy in DMF: -1619.371066 a.u.

M06 Free energy in DMF: -1618.928753 a.u.

C	2.71945100	-0.05531400	0.12093000
C	1.46748900	1.73604600	-0.63926300
C	2.60605000	2.43634700	-1.02336700
C	3.85466600	1.85717600	-0.80508900
C	3.90788200	0.59911300	-0.21403500
H	2.73755600	-1.04416900	0.56266800
H	2.51551800	3.41622400	-1.47577800
H	4.76138500	2.37921500	-1.08880900
C	0.11833300	2.31507500	-0.74559100
N	-0.92741500	1.75989300	-0.24123000
C	-1.46087900	3.74054700	-1.39937500
C	-2.03463700	2.74802100	-0.36275800
H	-1.79027900	3.52311400	-2.41912900
H	-2.91954400	2.24333100	-0.75852500
O	-0.01347100	3.49910800	-1.35125400
H	-1.62319600	4.79353900	-1.17700800
N	1.52166800	0.49709300	-0.08871600
C	-2.41389800	3.39180200	1.01340900
C	-2.86740100	2.29707200	1.99461600
H	-2.08030800	1.55849000	2.17569300
H	-3.13392300	2.74635500	2.95789800
H	-3.74955800	1.77165000	1.61786800

C	-3.59554300	4.35354000	0.77695400
H	-3.92520000	4.78108300	1.73007000
H	-3.33237100	5.18895600	0.11931700
H	-4.45033200	3.83046900	0.33259300
C	-1.23173900	4.16308800	1.63045800
H	-0.88924000	4.98649900	0.99483700
H	-1.53737000	4.59998800	2.58728900
H	-0.37822600	3.50620400	1.83103100
C	5.22289300	-0.06157700	0.10660600
F	6.22880600	0.44060400	-0.63552800
F	5.55748300	0.11056200	1.40526900
F	5.17602900	-1.39344200	-0.11295700
Pd	-0.40810200	-0.45528700	0.12838100
C	-1.91681300	-2.12112300	-0.50961100
C	-2.40716300	-1.79395100	-1.80252100
C	-2.58701400	-1.57861100	0.61787800
C	-3.54279200	-1.01392300	-1.95664900
H	-1.90060000	-2.20234500	-2.67257500
C	-3.75095500	-0.80032500	0.44523100
H	-2.30591200	-1.88512300	1.62024400
C	-4.22690700	-0.52412600	-0.82798000
H	-3.91781000	-0.79728200	-2.95279000
H	-4.28235300	-0.44184300	1.32037400
H	-5.13222300	0.06179600	-0.95692500
C	0.32468900	-2.34528000	0.39609300
C	-0.77605500	-3.13102600	-0.33338200
H	-0.41258900	-3.37192700	-1.33994300
C	-1.21999100	-4.46835400	0.30910600
H	-1.56834600	-4.28174400	1.33058900
C	0.56583200	-2.58425100	1.87692900
H	0.94547700	-3.60401500	2.02624600
H	1.31623000	-1.88883300	2.26856700
H	-0.33940300	-2.48059200	2.48294000
H	1.26121400	-2.37141200	-0.16641200
C	-2.33084400	-5.15928800	-0.47977700
H	-3.24554700	-4.55923600	-0.50938900
H	-2.01623300	-5.34840200	-1.51403900
H	-2.57072300	-6.12022000	-0.01404800
O	-0.09022400	-5.33451500	0.46097700
H	0.19760600	-5.58578800	-0.43048000

TS31-s

B3LYP SCF energy in DMF: -1619.91952 a.u.

M06 SCF energy in DMF: -1619.331443 a.u.

M06 Free energy in DMF: -1618.893127 a.u.

C	2.88009400	-0.42180000	0.25895100
C	1.83743700	1.45748500	-0.59005000
C	3.04823400	2.03817500	-0.94999800
C	4.22645100	1.34583900	-0.67457800
C	4.13813800	0.10488400	-0.05165200
H	2.78505300	-1.39457300	0.72724100
H	3.06849300	3.01068300	-1.42656400
H	5.18875100	1.76927900	-0.93924100
C	0.54754700	2.14636300	-0.75457400
N	-0.54670000	1.70136800	-0.23886100
C	-0.91821500	3.62908300	-1.53008900
C	-1.57386100	2.76215000	-0.43317100
H	-1.23973300	3.35067400	-2.53743900
H	-2.49533000	2.30230600	-0.79849300
O	0.51126700	3.29835200	-1.42729300
H	-1.01481200	4.70477200	-1.39611000
N	1.74962100	0.23525900	-0.01009900
C	-1.89655400	3.53302100	0.89203900
C	-2.38906200	2.55121800	1.96841500
H	-1.61961500	1.81811400	2.22879000
H	-2.65184000	3.09982700	2.87991100
H	-3.27931300	2.00947500	1.63673400
C	-3.02708500	4.53598700	0.58699400
H	-3.30667100	5.07386900	1.49941300
H	-2.73199400	5.28456700	-0.15558700
H	-3.92159000	4.02390700	0.21395600

C	-0.66523500	4.28588700	1.43211000
H	-0.29068900	5.03952500	0.73156700
H	-0.93101600	4.80943800	2.35678700
H	0.15648300	3.60181600	1.67190400
C	5.37254900	-0.66893400	0.32944200
F	6.44522300	-0.28726300	-0.39087100
F	5.68200100	-0.49205300	1.63369500
F	5.20465800	-1.99619400	0.14298400
Pd	-0.32595100	-0.49834500	0.11196000
C	-2.31307900	-1.03385800	-0.06154600
C	-2.73647800	-1.10378500	-1.40171500
C	-3.24137100	-0.70412700	0.93742900
C	-4.05182000	-0.77802900	-1.74001800
H	-2.04338700	-1.40907400	-2.18128900
C	-4.55861000	-0.38777600	0.59441800
H	-2.94139600	-0.69231800	1.98121300
C	-4.96432200	-0.41750400	-0.74256500
H	-4.36640900	-0.81629100	-2.77979400
H	-5.26879800	-0.12580500	1.37446300
H	-5.99049900	-0.17584100	-1.00554900
C	0.13211100	-2.54595200	0.24551800
C	-1.22387300	-2.78485000	0.60371000
H	-1.46092300	-2.65280800	1.65711000
C	-2.07564600	-3.85973300	-0.05168600
C	-1.51706400	-5.23472500	0.35700100
H	-0.50306600	-5.39957300	-0.01483600
H	-1.51741900	-5.34144500	1.44655900
H	-2.15758300	-6.01811400	-0.06452800
O	-3.40969500	-3.72699100	0.42222500
H	-3.92699400	-4.43502900	0.01222100
H	-2.03543700	-3.76436500	-1.14390400
C	0.75132600	-3.07594200	-1.03027400
H	1.64388400	-2.50484300	-1.30053800
H	1.06821300	-4.11941700	-0.90192700
H	0.05626100	-3.04123800	-1.87404400
H	0.81146300	-2.46978400	1.09813200

52-s

B3LYP SCF energy in DMF: -1619.9569 a.u.

M06 SCF energy in DMF: -1619.369854 a.u.

M06 Free energy in DMF: -1618.928116 a.u.

C	2.73927200	-0.20670300	0.20980700
C	1.62847100	1.68356800	-0.53375200
C	2.82231300	2.34599700	-0.79792300
C	4.02374000	1.69297300	-0.52935600
C	3.97743300	0.40398200	-0.00705000
H	2.67673200	-1.21639900	0.59697100
H	2.81018700	3.35326000	-1.19570600
H	4.97171500	2.18343100	-0.72020100
C	0.31528100	2.33040600	-0.68907700
N	-0.77663500	1.80286700	-0.25752900
C	-1.17212600	3.83757800	-1.37435900
C	-1.83608000	2.83693800	-0.40184700
H	-1.45275200	3.66287200	-2.41663100
H	-2.71721900	2.37874300	-0.85769600
O	0.26202500	3.53841000	-1.25793000
H	-1.30798500	4.88891700	-1.12806500
N	1.58709700	0.41403900	-0.05694200
C	-2.26087300	3.44974600	0.97484200
C	-2.76161500	2.33399800	1.90862800
H	-1.97706000	1.60153400	2.12288000
H	-3.08888000	2.76348400	2.86218900
H	-3.61309600	1.80348400	1.47245600
C	-3.41971400	4.43227700	0.71415600
H	-3.77252500	4.85533000	1.66098100
H	-3.12183600	5.26953500	0.07364700
H	-4.26774500	3.92807600	0.23634900
C	-1.09523200	4.19013800	1.65799900
H	-0.73171300	5.03732100	1.06720100
H	-1.42798200	4.58943900	2.62221100
H	-0.25047500	3.52171400	1.85787900

C	5.23860900	-0.33048000	0.36585800
F	6.29793500	0.10759500	-0.34264400
F	5.53719900	-0.16496200	1.67391600
F	5.12404200	-1.65907600	0.15348300
Pd	-0.38864600	-0.45302100	-0.04497000
C	-2.18856200	-1.92050700	0.01883900
C	-2.22254200	-1.50361200	-1.33873200
C	-3.20844800	-1.44855100	0.88611900
C	-3.25916100	-0.67093000	-1.80593900
H	-1.53546700	-1.92933700	-2.06114300
C	-4.23661200	-0.65081400	0.40904300
H	-3.19746600	-1.76205700	1.92601600
C	-4.26433100	-0.25898300	-0.94227300
H	-3.27973300	-0.38338000	-2.85296800
H	-5.02896100	-0.33219700	1.07971500
H	-5.07754500	0.36107600	-1.30830900
C	0.19883500	-2.40590000	0.13097400
C	-1.17788300	-2.97475600	0.50454800
H	-1.25549100	-2.99074800	1.59701700
C	-1.51221000	-4.39963900	0.01105000
C	-0.70307400	-5.46689900	0.74725200
H	0.37475700	-5.33024000	0.61654400
H	-0.92746900	-5.43738600	1.81928000
H	-0.95825600	-6.46512900	0.37226500
O	-2.91212600	-4.58355100	0.24614600
H	-3.14143100	-5.46948000	-0.07011900
H	-1.30799700	-4.46123100	-1.06808500
C	0.90524800	-2.91805800	-1.11563200
H	1.80068000	-2.32812400	-1.33443900
H	1.23982200	-3.95455000	-0.96892700
H	0.27494700	-2.90885900	-2.00884400
H	0.87849800	-2.38995600	0.98989500

55-s

B3LYP SCF energy in DMF: -1619.944967 a.u.

M06 SCF energy in DMF: -1619.352324 a.u.

M06 Free energy in DMF: -1618.914175 a.u.

C	2.37383000	-0.71036200	-0.20430000
C	0.61786900	-2.10570100	0.37029100
C	1.44269500	-3.22447100	0.39808800
C	2.79383800	-3.06463200	0.09536000
C	3.25939000	-1.79149400	-0.21814400
H	2.70953400	0.29494200	-0.42423400
H	1.03596000	-4.19761900	0.64409600
C	3.46418100	-3.91679900	0.10301000
H	-0.83335200	-2.19063800	0.60099700
N	-1.63273000	-1.19531600	0.42118100
C	-2.76447600	-3.08588300	1.25151400
C	-3.01832600	-1.73190200	0.55264700
H	-2.87641300	-3.03147400	2.33746800
H	-3.59667400	-1.06798000	1.19910900
O	-1.34719400	-3.36165800	0.97729000
H	-3.33948200	-3.92392000	0.86252400
N	1.07873900	-0.86311000	0.08536000
C	-3.76426400	-1.84259600	-0.81850300
C	-3.85898000	-0.45589000	-1.47369500
H	-2.87127400	-0.04616700	-1.70139500
H	-4.41631400	-0.52424100	-2.41485100
H	-4.38313000	0.25767700	-0.83132800
C	-5.19206600	-2.34926500	-0.53082400
H	-5.76429200	-2.40370300	-1.46316800
H	-5.19946600	-3.34981700	-0.08548700
H	-5.72311400	-1.67300200	0.14910100
C	-3.05426700	-2.80980500	-1.78376300
H	-2.99514700	-3.82933400	-1.38855900
H	-3.60999100	-2.86207200	-2.72628100
H	-2.03910000	-2.47452200	-2.02366500
C	4.69531100	-1.56744600	-0.61632100
F	5.51492900	-2.47676600	-0.05244400
F	4.85505900	-1.66369000	-1.95533600
F	5.12930200	-0.34225500	-0.25351900

Pd	-0.40764600	0.70800800	0.39221900	C	3.31470000	2.81054500	0.36485400
C	1.00937000	2.11232400	0.27534000	H	2.07300600	1.87244300	1.84452200
C	1.79386500	2.45405800	1.38572400	C	2.21848500	3.49627400	-1.67922800
C	1.31683500	2.65892200	-0.97872400	H	0.09847900	3.16188200	-1.77698300
C	2.87784400	3.32903300	1.23948900	C	3.37807700	3.39180600	-0.90523900
H	1.57407800	2.04119800	2.36687800	H	4.21144300	2.72936700	0.97323600
C	2.40264000	3.53329300	-1.11872300	H	2.25848500	3.95259700	-2.66461500
H	0.71888200	2.41082500	-1.85170800	H	4.32315300	3.76899900	-1.28531200
C	3.18453400	3.87046600	-0.01118500	C	-1.83275300	2.33960800	0.68087900
H	3.48041700	3.58398700	2.10788500	C	-0.67821900	3.00486700	1.21848000
H	2.63214200	3.94912100	-2.09675900	H	-0.49355100	3.99769700	0.81697600
H	4.02541600	4.54945400	-0.12184800	C	-0.34108300	2.87712200	2.68435900
C	-2.12312800	2.18053800	0.55271700	H	0.65344900	3.26151900	2.91828900
C	-1.51532000	2.07572700	1.79529800	H	-1.06633700	3.48825500	3.23790600
H	-0.81238900	2.85788000	2.07606600	H	-0.42228500	1.84915600	3.04647000
C	-2.02549400	1.24146500	2.93782300	H	-2.42534000	1.76841700	1.39765200
H	-1.21132400	0.77219600	3.49936700	C	-2.64232400	3.09544100	-0.35863200
H	-2.55059300	1.90664900	3.63794300	H	-1.97662300	3.59120400	-1.07394100
H	-2.72996000	0.47282300	2.61340800	C	-3.66563800	2.28966800	-1.13759800
H	-2.97287900	1.53279700	0.34728200	H	-4.20225100	2.96125200	-1.82287200
C	-2.02019600	3.40460100	-0.32682300	H	-3.15558200	1.53107200	-1.74516800
H	-2.78606800	4.11386000	0.02222300	H	-3.17252000	3.89975800	0.17491800
H	-1.05457300	3.89973500	-0.19923800	O	-4.57414500	1.68115000	-0.21460900
C	-2.28123900	3.15139700	-1.80728700	H	-5.28037300	1.26362400	-0.72761600
H	-2.04552900	4.06354500	-2.37659600				
O	-3.65695800	2.80076700	-1.96160300				
H	-3.76842300	2.42525200	-2.84583500				
H	-1.62669300	2.35043400	-2.17904800				

TS33-s

B3LYP SCF energy in DMF: -1619.914137 a.u.

M06 SCF energy in DMF: -1619.324939 a.u.

M06 Free energy in DMF: -1618.884705 a.u.

C	2.36391100	-0.75256300	-0.30271900
C	0.57730600	-1.92112900	0.58043500
C	1.36650600	-3.02805800	0.87833600
C	2.71862200	-2.98145600	0.54566900
C	3.21897500	-1.83206000	-0.06371700
H	2.72578000	0.16327900	-0.75293900
H	0.93150700	-3.90511900	1.34199600
H	3.36397500	-3.82923900	0.75021500
C	-0.88154700	-1.90229200	0.77824500
N	-1.64510800	-1.00747400	0.24081200
C	-2.86292900	-2.45671500	1.61851700
C	-3.04577500	-1.49003700	0.43546300
H	-2.97079500	-1.96515600	2.58974500
H	-3.68213600	-0.64158100	0.69336600
O	-1.45208900	-2.86731400	1.49927500
H	-3.46927600	-3.35967600	1.58886700
N	1.06864600	-0.79594700	0.01536600
C	-3.62719700	-2.17953600	-0.85067500
C	-3.58359700	-1.21518900	-2.04697800
H	-2.56137600	-0.90252400	-2.28134300
H	-3.99529000	-1.70636000	-2.93564300
H	-4.18373300	-0.32358200	-1.85465400
C	-5.09998200	-2.53098500	-0.55842300
H	-5.56192600	-2.97648300	-1.44607600
H	-5.20420900	-3.25100900	0.26038500
H	-5.67635400	-1.63647700	-0.29497300
C	-2.85612800	-3.45985500	-1.22698500
H	-2.88108500	-4.21625000	-0.43666900
H	-3.30649400	-3.90795900	-2.11927900
H	-1.80853200	-3.24901600	-1.46885000
C	4.67894000	-1.73973400	-0.41994100
F	5.12065800	-2.88247500	-0.98705600
F	4.92972700	-0.73346100	-1.28166900
F	5.44102900	-1.52683000	0.67693300
Pd	-0.45226100	0.85664100	0.11557100
C	0.93037700	2.42269900	0.08586900
C	2.10124400	2.32654500	0.85907200
C	0.99722200	3.03546200	-1.18143600

56-s

B3LYP SCF energy in DMF: -1619.947043 a.u.

M06 SCF energy in DMF: -1619.35924 a.u.

M06 Free energy in DMF: -1618.915952 a.u.

C	2.55951000	-0.50179600	-0.58005600
C	0.96109400	-1.62200900	0.64822800
C	1.89369700	-2.51386700	1.16988200
C	3.22478200	-2.37859100	0.77857400
C	3.55808200	-1.36542000	-0.11677700
H	2.78940100	0.30127600	-1.26853500
H	1.58770900	-3.29851800	1.85128000
H	3.98068300	-3.05768500	1.15803400
C	-0.48359900	-1.73961000	0.91117800
N	-1.37606900	-1.09384300	0.22931900
C	-2.35607900	-2.34617800	1.94705200
C	-2.69370100	-1.69546000	0.59477700
H	-2.51174200	-1.67391400	2.79559400
H	-4.3394600	-0.89961400	0.69688400
O	-0.90472900	-2.58538600	1.84952100
H	-2.83213100	-3.30489200	2.14196800
N	1.28755500	-0.62002500	-0.19859200
C	-3.20148600	-2.71836500	-0.48339200
C	-3.30553100	-2.04323000	-1.86064300
H	-2.33524000	-1.67619000	-2.20908000
H	-3.67608700	-2.76223300	-2.59959800
H	-4.00432500	-1.20529300	-1.83395500
C	-4.60945000	-3.17853900	-0.05387900
H	-5.01983500	-3.86983000	-0.79787400
H	-4.60265300	-3.70180200	0.90813800
H	-5.29664100	-2.32867200	0.02846000
C	-2.27682500	-3.94537700	-0.61145200
H	-2.19265900	-4.51371700	0.32005300
H	-2.68132400	-4.62647700	-1.36793300
H	-1.26844800	-3.66733700	-0.93743600
C	4.98768000	-1.15637100	-0.53886500
F	5.64065900	-2.32796800	-0.68394500
F	5.07633400	-0.49048300	-1.70890200
F	5.67105100	-0.43554800	0.38007000
Pd	-0.50490000	0.85368600	-0.25384800
C	0.12248000	2.93768300	0.51944900
C	1.16846800	2.83210800	1.47613400
C	0.47845000	2.94927500	-0.86005400
C	2.49424700	2.80027800	1.07535400
H	0.92795300	2.82168600	2.53338300
C	1.83701800	2.90685400	-1.25009700
H	-0.26437300	3.19126500	-1.61305200

C	2.83493600	2.84335900	-0.29170500
H	3.28021800	2.75506300	1.82400500
H	2.08716900	2.95652500	-2.30585900
H	3.87943100	2.83142900	-0.58883800
C	-2.11704700	2.06214300	0.18326400
C	-1.34889500	3.18748600	0.89927500
H	-1.63389400	4.15977300	0.47421800
C	-1.62430100	3.23313600	2.40272900
H	-1.06342800	4.03620200	2.89272300
H	-2.68930900	3.42066900	2.57362200
H	-1.36788000	2.28743000	2.89341400
H	-2.69008300	1.44149000	0.87768800
C	-2.97904000	2.55930400	-0.96997700
H	-2.36953700	3.05628300	-1.73369400
C	-3.86141600	1.53705100	-1.66368000
H	-4.44001400	2.04005000	-2.45173700
H	-3.24097200	0.77017200	-2.14608300
H	-3.62933800	3.34594600	-0.55178800
O	-4.73827300	0.95139900	-0.69568900
H	-5.37055900	0.39313200	-1.16968300

59-s

B3LYP SCF energy in DMF: -1619.94663 a.u.

M06 SCF energy in DMF: -1619.353432 a.u.

M06 Free energy in DMF: -1618.913188 a.u.

C	2.80356500	-0.12239800	0.01946000
C	1.43406700	1.66176200	-0.48179700
C	2.51469300	2.50544200	-0.71394200
C	3.80233800	1.99204400	-0.56320900
C	3.94463100	0.66144500	-0.18483400
H	2.89688700	-1.16237500	0.30815400
H	2.35363800	3.53721500	-1.00189800
H	4.66912700	2.62096800	-0.73216500
C	0.04180200	2.12835600	-0.56481700
N	-0.96750000	1.38509700	-0.24810000
C	-1.66605100	3.46472000	-1.07148200
C	-2.17751400	2.25611900	-0.25916000
H	-1.89861600	3.38932100	-2.13688500
H	-2.97731100	1.73981500	-0.79367100
O	-0.20077300	3.37718200	-0.94700400
H	-1.96407600	4.44093500	-0.69545600
N	1.56971800	0.36163900	-0.12627200
C	-2.68740000	2.61082800	1.17856800
C	-3.02068700	1.32648400	1.95643700
H	-2.13156800	0.70942500	2.11754100
H	-3.42986800	1.58628600	2.93916200
H	-3.76686200	0.72246900	1.43200400
C	-3.98036100	3.43620200	1.02087300
H	-4.39000600	3.67819000	2.00742200
H	-3.81254000	4.38271300	0.49625500
H	-4.74440700	2.87584800	0.46965800
C	-1.64640700	3.42046500	1.97494900
H	-1.41767200	4.38482100	1.51002400
H	-2.03388400	3.63000600	2.97770400
H	-0.70892700	2.86695400	2.09965200
C	5.30496400	0.03066300	-0.04394400
F	6.25116400	0.94144900	0.25694000
F	5.31784200	-0.91028100	0.92350500
F	5.68586200	-0.57643800	-1.19066300
Pd	-0.46696700	-0.69871200	-0.24124300
C	-2.35058100	-1.24244800	-0.66421800
C	-2.77109100	-1.01160000	-1.98335600
C	-3.26040500	-1.76876900	0.25944900
C	-4.08480100	-1.30387100	-2.37008800
H	-2.08106400	-0.60421700	-2.71832500
C	-4.57536200	-2.05784300	-0.13208300
H	-2.97042900	-1.94628300	1.28952600
C	-4.99083300	-1.82868300	-1.44501400
H	-4.39385600	-1.12057800	-3.39631800
H	-5.27209800	-2.46150100	0.59858600
H	-6.00993900	-2.05666500	-1.74483700

C	0.36538400	-2.70310000	0.38592300
C	0.04895200	-2.79657400	-0.95875200
H	1.37873800	-2.41036900	0.65046300
H	-0.88906600	-3.28324400	-1.21746400
C	1.02980500	-2.66280900	-2.09240100
H	1.30036600	-3.67064500	-2.43690200
H	0.59227800	-2.14175900	-2.95010500
H	1.94800300	-2.15146500	-1.79474100
C	-0.38971900	-3.37558900	1.50336100
H	0.15537100	-4.30453600	1.72887500
H	-1.39323300	-3.66759700	1.18252400
C	-0.48531600	-2.55736400	2.78789300
H	-1.08140500	-1.65209800	2.60558500
H	-1.00117800	-3.15255500	3.55601000
O	0.83480400	-2.21359900	3.21204800
H	0.75046700	-1.64759800	3.99214900

TS35-s

B3LYP SCF energy in DMF: -1619.9234 a.u.

M06 SCF energy in DMF: -1619.333902 a.u.

M06 Free energy in DMF: -1618.893201 a.u.

C	2.67382200	0.15653900	-0.02362700
C	1.15018300	1.81362300	-0.54676900
C	2.15695100	2.73332400	-0.81717600
C	3.48513700	2.33568600	-0.66619500
C	3.73986000	1.03250800	-0.25539500
H	2.85640100	-0.86710700	0.28963200
H	1.90590400	3.73927200	-1.13050000
H	4.29468800	3.03001100	-0.85969500
C	-0.27646400	2.16293000	-0.62091100
N	-1.21008100	1.35927500	-0.24503700
C	-2.08574900	3.33502200	-1.17308900
C	-2.48605700	2.12412600	-0.30070800
H	-2.33101900	3.19354900	-2.22917600
H	-3.23952800	1.51471000	-0.80587300
O	-0.61951000	3.37110200	-1.07313500
H	-2.45921000	4.29931800	-0.83416900
N	1.40023400	0.53702500	-0.16011500
C	-3.02965000	2.49356800	1.11943500
C	-3.26342700	1.21183400	1.93650100
H	-2.32923100	0.67241900	2.11961300
H	-3.69995600	1.46471400	2.90935900
H	-3.95496300	0.53435000	1.42647700
C	-4.38155400	3.21104400	0.93338800
H	-4.81597000	3.44885100	1.91042100
H	-4.28359500	4.15259100	0.38234300
H	-5.09606100	2.57762000	0.39494900
C	-2.05588400	3.40707000	1.88709900
H	-1.90215700	4.37007600	1.38922900
H	-2.45841700	3.62015200	2.88334000
H	-1.07856600	2.93191400	2.02706300
C	5.14267200	0.51487600	-0.08008200
F	6.04650100	1.51053000	-0.02545600
F	5.26222800	-0.20652900	1.05998200
F	5.50039600	-0.30169600	-1.09612200
Pd	-0.38908600	-0.72763100	-0.11591200
C	-2.17376200	-1.80281000	-0.41671000
C	-2.89398300	-1.44244900	-1.57065700
C	-2.88281100	-2.21738900	0.72657700
C	-4.29080800	-1.46122200	-1.56663600
H	-2.36805800	-1.14872000	-2.47416400
C	-4.27888500	-2.24022800	0.72447800
H	-2.34595100	-2.54196500	1.61302400
C	-4.98605300	-1.86254100	-0.42139800
H	-4.83476900	-1.17409300	-2.46261700
H	-4.81330900	-2.56203100	1.61429700
H	-6.07200800	-1.89168200	-0.42604400
C	0.53028800	-2.59832000	-0.04792600
C	-0.60082200	-3.07114300	-0.79480200
H	1.43547100	-2.43817300	-0.63667700
H	-1.19265100	-3.83804100	-0.30440700

C	-0.49069000	-3.25334100	-2.28897400
H	0.11223000	-4.15430800	-2.46379600
H	-1.46328600	-3.41004900	-2.75943500
H	0.01152600	-2.41359300	-2.77660900
C	0.75331200	-3.15509400	1.35126600
H	1.03897300	-4.21330100	1.24866800
H	-0.18545400	-3.14376100	1.91596600
C	1.82181500	-2.46351700	2.18578200
H	1.57145400	-1.40176800	2.32742900
H	1.86060700	-2.93131200	3.17924400
O	3.08242100	-2.60520300	1.51830300
H	3.75370600	-2.15523700	2.05232800

60-s

B3LYP SCF energy in DMF: -1619.956387 a.u.

M06 SCF energy in DMF: -1619.367124 a.u.

M06 Free energy in DMF: -1618.924059 a.u.

C	2.43322200	0.47792900	-0.08302100
C	0.68096700	1.83315000	-0.74734000
C	1.54703400	2.81915000	-1.20641600
C	2.92143600	2.61931300	-1.07973300
C	3.36299300	1.43708600	-0.49811600
H	2.76376600	-0.44886600	0.37562100
H	1.15126300	3.72832900	-1.64209800
H	3.62258000	3.37361300	-1.41789900
C	-0.77953000	2.00801500	-0.75742000
N	-1.58758100	1.16081500	-0.22382100
C	-2.74263500	2.93194700	-1.25539000
C	-2.93667800	1.78640100	-0.23556900
H	-3.06208800	2.65610800	-2.26405100
H	-3.66157100	1.05839900	-0.60735400
O	-1.28580500	3.11907100	-1.30050300
H	-3.18498600	3.88708100	-0.97730700
N	1.11676800	0.66704900	-0.20402000
C	-3.39298000	2.24630500	1.18983800
C	-3.39694700	1.04712100	2.15484700
H	-2.39860300	0.61298900	2.26994800
H	-3.73813000	1.36797500	3.14546200
H	-4.07450700	0.25994800	1.81101200
C	-4.83207400	2.78619300	1.07063500
H	-5.20500700	3.08069000	2.05759800
H	-4.89456100	3.66744300	0.42292500
H	-5.51106500	2.02486200	0.66952800
C	-2.47405500	3.34288700	1.76108700
H	-2.46810400	4.24835700	1.14548800
H	-2.82390000	3.63363300	2.75752600
H	-1.44145500	2.99283500	1.86883900
C	4.82639300	1.13784900	-0.30779300
F	5.59870800	2.21591300	-0.53426000
F	5.07942700	0.71314600	0.95361600
F	5.24507600	0.15730900	-1.13839500
Pd	-0.46590600	-0.79016900	0.13522300
C	-1.34483400	-2.82992900	-0.66224000
C	-1.69428800	-2.65540700	-2.02679300
C	-2.27785400	-2.41889000	0.32783400
C	-2.93868300	-2.15425800	-2.37893100
H	-0.99891700	-2.95953400	-2.80149200
C	-3.54807900	-1.92804500	-0.04973300
H	-2.09302400	-2.66278000	1.37086200
C	-3.87589800	-1.79872900	-1.38992600
H	-3.20058900	-2.05779800	-3.42887200
H	-4.27282300	-1.68340800	0.71942900
H	-4.85858600	-1.43914400	-1.68063400
C	0.74345400	-2.41229500	0.48089000
C	-0.06056500	-3.53179400	-0.19835100
H	1.66424000	-2.20122900	-0.06984100
H	-0.35644300	-4.27773600	0.55073100
C	0.72038400	-4.24825300	-1.29982300
H	1.58826700	-4.75494300	-0.86503700
H	0.10556500	-5.00472500	-1.79993400
H	1.09140900	-3.55037000	-2.05854300

C	0.99063200	-2.62478700	1.97107500
H	1.40060800	-3.64114400	2.09390600
H	0.04202000	-2.61749900	2.52245900
C	1.94539900	-1.65011900	2.64686800
H	1.56713000	-0.62050100	2.56619400
H	2.01324300	-1.89383200	3.71656600
O	3.23219900	-1.77046500	2.02600500
H	3.82068800	-1.11720800	2.43205500

63-s

B3LYP SCF energy in DMF: -1619.947524 a.u.

M06 SCF energy in DMF: -1619.354185 a.u.

M06 Free energy in DMF: -1618.91621 a.u.

C	2.14710100	-0.99405600	-0.19919300
C	0.18061400	-2.02120100	0.46324100
C	0.83971900	-3.20117700	0.78527700
C	2.21917700	-3.26955200	0.59137300
C	2.87605800	-2.15330600	0.08446200
H	2.63023600	-0.10484300	-0.58527200
H	0.28598300	-4.04779600	1.17206100
C	2.76221300	-4.17776100	0.82671100
H	-1.28058600	-1.87682000	0.57129000
N	-1.91220300	-0.83115100	0.16037200
C	-3.36274700	-2.37383400	1.18118500
C	-3.36668100	-1.13910600	0.25145500
H	-3.53503800	-2.11565900	2.22931200
H	-3.87602800	-0.29832500	0.72907600
O	-1.98656400	-2.88388900	1.08414300
H	-4.02931000	-3.18180600	0.88646100
N	0.82700900	-0.92819700	-0.01383300
C	-4.02602600	-1.38196200	-1.14798600
C	-3.88569700	-0.12506500	-2.02431100
H	-2.83715400	0.12947700	-2.20555400
H	-4.36099100	-0.29520100	-2.99672600
H	-4.37789600	0.73915000	-1.56492300
C	-5.52687800	-1.65330600	-0.92022800
H	-6.03493200	-1.76863000	-1.88367700
H	-5.70468100	-2.56911600	-0.34715500
H	-6.00487400	-0.82282200	-0.38785600
C	-3.38677600	-2.57744200	-1.87944600
H	-3.48371600	-3.51307300	-1.31872500
H	-3.88171400	-2.72724700	-2.84492700
H	-2.32365700	-2.40739500	-2.08255700
C	4.36933500	-2.14711300	-0.11955900
F	4.86314700	-3.39541300	-0.23121300
F	4.71341900	-1.46784100	-1.23418400
F	5.00590400	-1.55480200	0.91560800
Pd	-0.45878300	0.84087800	-0.15736400
C	1.10574500	2.01647300	-0.56582200
C	1.89774600	2.61881300	0.42154600
C	1.48960600	2.11033600	-1.91153000
C	3.06919800	3.29807700	0.06116400
H	1.60474000	2.57375600	1.46722800
C	2.66031800	2.79381900	-2.26452200
H	0.88686400	1.65155500	-2.69199200
C	3.45323700	3.38742300	-1.27895100
H	3.67815700	3.76030600	0.83448300
H	2.94806300	2.85872100	-3.31103000
H	4.36103900	3.91743500	-1.55377900
C	-2.00233900	2.45717900	-0.33807700
C	-1.39031600	2.60487000	0.89843300
H	-0.60702500	3.35234800	0.99096500
H	-2.91765000	1.86992500	-0.37065300
C	-1.78866900	3.37207900	-1.51385200
H	-0.86087400	3.94193900	-1.43346700
H	-2.62485800	4.08360200	-1.55506400
H	-1.79023900	2.82557000	-2.46202300
C	-1.98057500	2.12963200	2.20347500
H	-2.49784800	2.99569400	2.64398000
H	-2.73802500	1.35764900	2.03289500
C	-0.96721700	1.61644800	3.22220100

H	-0.47844200	0.71027300	2.83626000
H	-1.49718300	1.34401700	4.14677400
O	-0.00654000	2.64409000	3.47111200
H	0.64772800	2.28694200	4.08845500

TS37-s

B3LYP SCF energy in DMF: -1619.917722 a.u.

M06 SCF energy in DMF: -1619.329287 a.u.

M06 Free energy in DMF: -1618.889745 a.u.

C	-2.04461800	-1.26150200	0.19123900
C	-0.10202500	-2.17002100	-0.66929300
C	-0.74377900	-3.34456700	-1.04560100
C	-2.10654800	-3.46973700	-0.77346900
C	-2.76008400	-2.41888100	-0.13786400
H	-2.52504000	-0.41828500	0.67472300
H	-0.19446000	-4.14273900	-1.53020000
H	-2.64073500	-4.37222600	-1.04715600
C	1.34350200	-1.95346400	-0.84169100
N	1.97672300	-0.97311100	-0.28749200
C	3.37347900	-2.21943100	-1.71468600
C	3.42733000	-1.18618700	-0.56755800
H	3.42696600	-1.75722000	-2.70395200
H	3.85984600	-0.24440000	-0.91490200
O	2.03531000	-2.81260600	-1.58923300
H	4.09718100	-3.02937400	-1.64788400
N	-0.74483700	-1.13886000	-0.07488300
C	4.23254000	-1.66155900	0.68666400
C	4.12255500	-0.61335300	1.80517500
H	3.09387800	-0.51315300	2.16340300
H	4.74506100	-0.90707400	2.65765400
H	4.46933100	0.36736300	1.46313400
C	5.71294700	-1.78224800	0.27288300
H	6.32025100	-2.06741700	1.13863000
H	5.87171600	-2.54100600	-0.50058000
H	6.09847300	-0.82842700	-0.10579900
C	3.72603800	-3.01626200	1.21545800
H	3.83417400	-3.82135900	0.48122400
H	4.30486200	-3.30653300	2.09894300
H	2.67438900	-2.96579300	1.51864900
C	-4.23273900	-2.47367200	0.17140900
F	-4.73821600	-3.71133400	0.00881100
F	-4.48534300	-2.09235700	1.44293000
F	-4.93459600	-1.64238500	-0.63222800
Pd	0.57002800	0.65123600	0.18526700
C	-1.00167600	2.02398800	0.33950500
C	-1.95107500	2.02746200	-0.69756200
C	-1.43564400	2.24423200	1.66170300
C	-3.30713500	2.21464500	-0.41477300
H	-1.63980900	1.87934100	-1.72699800
C	-2.79382700	2.41441800	1.94030500
H	-0.71678800	2.28659200	2.47424500
C	-3.73212700	2.40583000	0.90307400
H	-4.02965900	2.21214000	-1.22656100
H	-3.11613100	2.56791000	2.96677800
H	-4.78589700	2.55600000	1.11992000
C	1.82848800	2.30428900	0.35116800
C	0.71996200	3.06482800	-0.14894700
H	0.34827700	3.83151100	0.52410900
H	2.60974500	2.07101100	-0.37527300
C	2.31819200	2.58279000	1.75762200
H	1.49224300	2.82016500	2.43423000
H	2.98836800	3.45464800	1.74163900
H	2.88286000	1.75053700	2.17892000
C	0.65942200	3.46094100	-1.61840800
H	1.68293800	3.71768800	-1.92094000
H	0.35273200	2.62941900	-2.25836500
C	-0.22456900	4.67205200	-1.88956500
H	-1.26316400	4.46764800	-1.59711300
H	-0.21990100	4.88082600	-2.97002900
O	0.30429100	5.77452400	-1.15026400
H	-0.33127300	6.50093800	-1.21647900

64-s

B3LYP SCF energy in DMF: -1619.95105 a.u.

M06 SCF energy in DMF: -1619.363668 a.u.

M06 Free energy in DMF: -1618.922545 a.u.

C	-2.67202000	0.09302100	0.39634500
C	-1.47568100	-1.52932200	-0.72073900
C	-2.62280000	-2.07236400	-1.28971500
C	-3.85397300	-1.49105500	-0.98284800
C	-3.87660300	-0.40151500	-0.12007200
H	-2.65809000	0.94908000	1.06007500
H	-2.55918200	-2.92996700	-1.94846000
H	-4.77024000	-1.88824300	-1.40401600
C	-0.14062300	-2.11659600	-0.91807800
N	0.89763700	-1.76331500	-0.23164400
C	1.45556800	-3.30855900	-1.91245500
C	1.99922100	-2.70021900	-0.60247700
H	1.81094400	-2.78446500	-2.80374900
H	2.90615400	-2.12060100	-0.79103300
O	0.00634500	-3.07719800	-1.82886800
H	1.60905900	-4.37947100	-2.02836500
N	-1.49406400	-0.45009600	0.09536100
C	2.31321400	-3.75488500	0.51040200
C	2.73085500	-3.04464600	1.80697600
H	1.92636100	-2.41824500	2.20358600
H	2.98488400	-3.78568900	2.57293100
H	3.61418100	-2.41867500	1.64568700
C	3.50063400	-4.60835200	0.02056700
H	3.78557700	-5.32771000	0.79567800
H	3.26305100	-5.17964500	-0.88303000
H	4.37535300	-3.98359100	-0.19425200
C	1.10446200	-4.66395200	0.80141000
H	0.79519600	-5.24397800	-0.07431700
H	1.36677500	-5.38048800	1.58711500
H	0.24103700	-4.09205500	1.15878400
C	-5.15921900	0.28509600	0.26729600
F	-6.24095400	-0.32991900	-0.24603800
F	-5.31085200	0.32426900	1.61012800
F	-5.17877400	1.56804800	-0.16309700
Pd	0.66291500	0.27795400	0.47451400
C	1.06076200	2.52112500	0.04057000
C	0.35128700	2.82111100	-1.15411600
C	0.34614900	2.58290300	1.26912200
C	-0.97461500	3.22774100	-1.10833700
H	0.86025200	2.76990500	-2.11020500
C	-1.00086200	3.00321100	1.29919100
H	0.88201400	2.47966600	2.20760600
C	-1.65327600	3.33220400	0.12022300
H	-1.48893600	3.48205400	-2.03081700
H	-1.51037800	3.08686000	2.25475800
H	-2.68690400	3.66479100	0.14059300
C	2.64166200	0.77899200	0.58750700
C	2.57575400	2.23494800	0.10248400
H	2.99546300	2.89541900	0.86999700
H	3.11691800	0.11586000	-0.14268800
C	3.21044700	0.60081100	1.98391300
H	2.71960400	1.25095600	2.71527200
H	4.27614100	0.88069800	1.97404700
H	3.14685400	-0.42716200	2.34333900
C	3.36518000	2.48299300	-1.19072400
H	4.36381900	2.04816800	-1.05906100
H	2.90877800	1.95667300	-2.03774300
C	3.54375700	3.95492300	-1.55249500
H	2.56929100	4.44759300	-1.68036500
H	4.07265800	4.02547300	-2.51569500
O	4.29548400	4.58397700	-0.51284100
H	4.30921100	5.53326900	-0.69827900

65-s

B3LYP SCF energy in DMF: -1619.945669 a.u.

M06 SCF energy in DMF: -1619.352571 a.u.

M06 Free energy in DMF: -1618.9125 a.u.

C	2.79863100	-0.06193400	0.44036300
C	1.45734400	1.48410600	-0.61984200
C	2.54945900	2.22939300	-1.05031200
C	3.82681200	1.79912900	-0.69467000
C	3.94917400	0.64203200	0.06823500
H	2.87416000	-0.97636800	1.01609400
H	2.40430500	3.12618600	-1.64026300
H	4.70261500	2.35697100	-1.00703100
C	0.07048300	1.90597800	-0.86981600
N	-0.94695100	1.33444700	-0.31214900
C	-1.62075100	2.99397500	-1.82370100
C	-2.14289900	2.16741400	-0.63084100
H	-1.85297400	2.53936600	-2.79028600
H	-2.95843300	1.51011500	-0.93859200
O	-0.15646500	2.94279400	-1.66876700
H	-1.90994400	4.04236400	-1.82746400
N	1.57408800	0.34515200	0.10298600
C	-2.62837500	3.02837000	0.58372700
C	-2.98350800	2.11918300	1.77171600
H	-2.11141900	1.56629600	2.13376200
H	-3.36265600	2.72635500	2.60130100
H	-3.75962300	1.39708100	1.50320400
C	-3.90327100	3.77474400	0.14043700
H	-4.29900500	4.36418400	0.97440500
H	-3.71732800	4.46540100	-0.68869500
H	-4.68381300	3.07228300	-0.17346900
C	-1.56086400	4.04465400	1.03440500
H	-1.29939700	4.75893100	0.24675000
H	-1.94256000	4.62414200	1.88173100
H	-0.64250200	3.54970400	1.36973300
C	5.29842100	0.16329200	0.53729500
F	6.27652300	0.50935600	-0.32302100
F	5.61737000	0.69542000	1.73833500
F	5.33217800	-1.17886100	0.67740200
Pd	-0.46611200	-0.67444900	0.30504400
C	-2.37888400	-1.26401000	0.21585700
C	-2.93179800	-1.54926900	-1.04131100
C	-3.19635700	-1.31517000	1.35080700
C	-4.28944200	-1.87486600	-1.15744600
H	-2.31104100	-1.54393300	-1.93258800
C	-4.55309900	-1.64494700	1.22957900
H	-2.79500100	-1.09425800	2.33504300
C	-5.10361500	-1.92360800	-0.02324600
H	-4.70406500	-2.09639600	-2.13793000
H	-5.17590300	-1.67816500	2.12023700
H	-6.15566800	-2.17938600	-0.11434000
C	0.29514300	-2.48737400	1.41563500
C	0.07740100	-2.86312000	0.09814900
H	1.29685300	-2.15727700	1.68959500
H	-0.85258600	-3.37905800	-0.12659800
C	1.16275100	-3.03070800	-0.93964000
C	-0.55487500	-2.90565800	2.58247900
H	-1.53483900	-3.27424400	2.27611400
H	-0.03288200	-3.71937000	3.10495900
H	-0.68256200	-2.09644900	3.30852600
C	0.77987200	-2.62719200	-2.35988900
H	0.55589200	-1.55058900	-2.39338300
H	2.07370600	-2.49866300	-0.65198800
H	1.41292500	-4.10253100	-0.94897600
H	1.63802700	-2.81135800	-3.02359600
O	-0.35060800	-3.39739700	-2.76480200
H	-0.60762800	-3.09675900	-3.64785000

TS38-s

B3LYP SCF energy in DMF: -1619.919251 a.u.

M06 SCF energy in DMF: -1619.331079 a.u.

M06 Free energy in DMF: -1618.891387 a.u.

C	2.89157300	-0.43754700	0.23546800
C	1.85763400	1.42824200	-0.65370900

C	3.07198500	1.98385000	-1.04430300
C	4.24522000	1.28682500	-0.76481800
C	4.14975100	0.06214800	-0.10847600
H	2.79410200	-1.395526100	0.72996400
H	3.09585200	2.94042700	-1.55193500
H	5.20869900	1.69178400	-1.05483700
C	0.57198000	2.11529300	-0.85425400
N	-0.53611900	1.67526700	-0.36675600
C	-0.86891300	3.58440200	-1.70245800
C	-1.56598000	2.71822400	-0.62900200
H	-1.15419600	3.30728100	-2.72096800
H	-2.45711300	2.23553300	-1.03812300
O	0.55538700	3.25465600	-1.54970600
H	-0.97055900	4.66022800	-1.57173500
N	1.76378500	0.22775200	-0.03207400
C	-1.98159600	3.49445900	0.66430100
C	-2.53194600	2.50964200	1.70858100
H	-1.76779300	1.79838400	2.03541900
H	-2.87778800	3.05822100	2.59199300
H	-3.38097400	1.94366800	1.31378100
C	-3.10374600	4.47951300	0.27914900
H	-3.44735600	5.02125600	1.16701700
H	-2.77332800	5.22536800	-0.45136300
H	-3.96564300	3.95127700	-0.14491100
C	-0.79648000	4.26585100	1.27579200
H	-0.38756300	5.01821400	0.59305600
H	-1.12538500	4.79321200	2.17775200
H	0.01629900	3.59292000	1.57082600
C	5.38917500	-0.70771000	0.26524800
F	6.33524000	-0.61651200	-0.69167300
F	5.93653000	-0.23760000	1.40825800
F	5.12819700	-2.01746400	0.45939700
Pd	-0.29029600	-0.49598100	0.17351800
C	-2.30133200	-1.10390100	0.15752800
C	-3.00576900	-0.79710400	-1.02006300
C	-2.98985800	-1.09548000	1.38594300
C	-4.35713200	-0.44261100	-0.96265600
H	-2.50579100	-0.83577000	-1.98352300
C	-4.34150800	-0.75083800	1.43775500
H	-2.47358700	-1.37550200	2.30019900
C	-5.02808100	-0.42306200	0.26382000
H	-4.88805300	-0.19836800	-1.87894000
H	-4.86033800	-0.74714000	2.39259200
H	-6.08294100	-0.16638600	0.30291300
C	0.17124500	-2.47890100	0.56927000
C	-1.11964600	-2.81972000	0.05197200
H	1.00653000	-2.66626600	-0.10969200
H	-1.80649800	-3.25616400	0.76909000
C	-1.25577900	-3.39129900	-1.35086600
C	0.47514300	-2.70328500	2.03695200
H	-0.38395400	-2.46038300	2.66956300
H	0.72368800	-3.76074900	2.20711700
H	1.33182400	-2.11238600	2.37525100
C	-2.58991300	-4.07754600	-1.61589400
H	-3.41787900	-3.36159800	-1.53540700
H	-1.06446400	-2.63813900	-2.12013800
H	-0.46553500	-4.14694100	-1.45630300
H	-2.58859400	-4.46787400	-2.64476900
O	-2.73622900	-5.13441800	-0.66531500
H	-3.64082100	-5.46927500	-0.73924500

66-s

B3LYP SCF energy in DMF: -1619.956108 a.u.

M06 SCF energy in DMF: -1619.368336 a.u.

M06 Free energy in DMF: -1618.927618 a.u.

C	2.73057300	-0.65533700	0.12359500
C	1.94331300	1.44472200	-0.44424900
C	3.21937600	1.89071800	-0.77478500
C	4.29310000	1.01451300	-0.63442100
C	4.04077400	-0.27709700	-0.18072900
H	2.50694200	-1.65893200	0.46275400

H	3.36584300	2.90117400	-1.13616700
H	5.29984600	1.33157800	-0.88247900
C	0.75747000	2.31026300	-0.54964500
N	-0.42876300	1.91095500	-0.25476700
C	-0.43629900	4.11610300	-1.07974200
C	-1.31732600	3.09934200	-0.31513600
H	-0.66700400	4.15451300	-2.14760800
H	-2.20641200	2.84519100	-0.89826600
O	0.92330200	3.57501200	-0.95014800
H	-0.42599500	5.12486300	-0.67024100
N	1.70073100	0.18758800	0.00586300
C	-1.78633100	3.56529000	1.10277100
C	-2.55202700	2.42407200	1.79578500
H	-1.91527100	1.54779600	1.95646000
H	-2.91680700	2.75805800	2.77372200
H	-3.41935500	2.11038500	1.20595700
C	-2.74345600	4.75893500	0.91456800
H	-3.13418300	5.08285800	1.88525900
H	-2.24662700	5.62195600	0.45863100
H	-3.59763500	4.48919900	0.28272500
C	-0.59735300	3.98809000	1.98576800
H	-0.03486400	4.82245500	1.55371800
H	-0.96140900	4.31698400	2.96514800
H	0.09703100	3.15819100	2.15835100
C	5.16585200	-1.25589400	0.03176500
F	6.19404300	-1.02167000	-0.80821300
F	5.65494700	-1.17953000	1.29004100
F	4.76411000	-2.53072000	-0.15858700
Pd	-0.41967300	-0.32703200	0.11002700
C	-2.33887100	-1.55855200	-0.38419600
C	-1.86879300	-1.28342900	-1.69795000
C	-3.48129300	-0.85705200	0.07686700
C	-2.53452100	-0.35155100	-2.51303800
H	-1.06455000	-1.87839500	-2.12041200
C	-4.14161400	0.04957600	-0.74375900
H	-3.85763600	-1.06649900	1.07443900
C	-3.66792800	0.30364400	-2.04134200
H	-2.17509900	-0.16952500	-3.52165600
H	-5.03131400	0.55692600	-0.38289900
H	-4.19448900	1.00622600	-2.68099300
C	-0.25577700	-2.27979400	0.66303200
C	-1.71026000	-2.69695800	0.43906300
H	0.43939900	-2.75631900	-0.03787900
H	-2.22557300	-2.71373000	1.40412100
C	-1.86851200	-4.08718600	-0.20987400
C	0.21662900	-2.35670400	2.10273800
H	-0.43785200	-1.78694600	2.77274100
H	0.19135200	-3.40348800	2.44404600
H	1.24240200	-2.00059400	2.23750700
C	-3.31324200	-4.55564800	-0.32696500
H	-3.89511000	-3.84420800	-0.93301000
H	-1.41835800	-4.08682100	-1.20981600
H	-1.30902200	-4.81501800	0.39154900
H	-3.33684300	-5.52272400	-0.85279700
O	-3.86175500	-4.67506800	0.98614100
H	-4.80141100	-4.88413700	0.89032400

67-s

B3LYP SCF energy in DMF: -1619.94801 a.u.

M06 SCF energy in DMF: -1619.35484 a.u.

M06 Free energy in DMF: -1618.914113 a.u.

C	2.86667800	-0.24002200	-0.01457200
C	1.56590600	1.59742300	-0.51187600
C	2.67749400	2.39244400	-0.76810600
C	3.94371900	1.82755300	-0.62576100
C	4.03653900	0.49565300	-0.23500200
H	2.91805600	-1.28252700	0.27405200
H	2.55615400	3.42599200	-1.06904900
H	4.83387700	2.41645300	-0.81694000
C	0.19388500	2.12418200	-0.58176700
N	-0.84551500	1.42324100	-0.26782800

C	-1.45578700	3.54357300	-1.05981300
C	-2.01757800	2.34396100	-0.26640800
H	-1.70021800	3.50078600	-2.12426500
H	-2.83749300	1.86989200	-0.80949000
O	0.00450100	3.38697500	-0.94952800
H	-1.70567000	4.52478400	-0.66198000
N	1.65194800	0.29430100	-0.15126600
C	-2.51449700	2.69421700	1.17665400
C	-2.91535500	1.41241800	1.92655700
H	-2.05940400	0.74861300	2.08101900
H	-3.31771600	1.67270600	2.91203200
H	-3.68722000	0.85587000	1.38651800
C	-3.76423100	3.58666700	1.03345900
H	-4.16657700	3.82462700	2.02401100
H	-3.54671200	4.53624500	0.53338900
H	-4.55211800	3.07855700	0.46558900
C	-1.43643500	3.43412100	1.99129300
H	-1.14967900	4.38913400	1.53907200
H	-1.81907800	3.65380500	2.99371100
H	-0.53221800	2.82782700	2.11530000
C	5.37827200	-0.14858500	-0.00095100
F	6.32977100	0.38496600	-0.79263500
F	5.78549500	0.01475100	1.27789600
F	5.34458300	-1.47691100	-0.23819500
Pd	-0.43430200	-0.67949800	-0.26079800
C	-2.32939000	-1.13154300	-0.72579000
C	-2.74739800	-0.81323300	-2.02602300
C	-3.24955100	-1.67678500	0.17881300
C	-4.07290900	-1.04172800	-2.41707600
H	-2.04901300	-0.38737300	-2.74229500
C	-4.57555900	-1.89784400	-0.21746100
H	-2.94410500	-1.93681900	1.18844300
C	-4.99054400	-1.58314400	-1.51338600
H	-4.38259500	-0.79335100	-3.42935400
H	-5.28124400	-2.31999700	0.49409200
H	-6.01870800	-1.75976100	-1.81721800
C	0.39397100	-2.69675400	-0.82273700
C	-0.18417000	-2.82130000	0.43101800
H	1.46026900	-2.47919500	-0.87184600
C	-0.19033200	-3.25232900	-2.09366300
H	-0.05120100	-2.57176300	-2.93967600
H	0.34495600	-4.17949900	-2.34041400
H	-1.25186300	-3.48737000	-1.99565800
H	-1.18623300	-3.23846600	0.47604200
C	0.56751100	-2.83544800	1.73965900
H	0.71711400	-3.89379500	2.00220300
C	-0.15221100	-2.15389800	2.89987300
H	0.45320800	-2.26512500	3.81146200
H	1.56201900	-2.39320100	1.63223300
H	-0.25180000	-1.07876400	2.69090500
O	-1.43469400	-2.76129300	3.06709900
H	-1.88716500	-2.29248800	3.78272200

TS39-s

B3LYP SCF energy in DMF: -1619.917929 a.u.

M06 SCF energy in DMF: -1619.329125 a.u.

M06 Free energy in DMF: -1618.88962 a.u.

C	2.87610300	-0.52612300	0.16824800
C	1.89521700	1.47478500	-0.44857400
C	3.12863000	2.08026600	-0.66011100
C	4.28474000	1.33604600	-0.42783500
C	4.15304400	0.01902500	0.00060000
H	2.74647900	-1.55610800	0.47892000
H	3.18265900	3.11050400	-0.98987800
H	5.26318100	1.77777100	-0.57864200
C	0.62007600	2.19765400	-0.58408700
N	-0.49798800	1.71809100	-0.15832100
C	-0.79796900	3.76427600	-1.27797500
C	-1.50876100	2.80307600	-0.30033300
H	-1.07383400	3.58592200	-2.32092700
H	-2.41234500	2.38633100	-0.75191500

O	0.62300800	3.40997500	-1.14307000
H	-0.89493300	4.82330500	-1.04735200
N	1.76774300	0.18384900	-0.05471300
C	-1.89687100	3.44919500	1.07277200
C	-2.45035400	2.37511600	2.02474400
H	-1.70154100	1.61045500	2.25310200
H	-2.75449800	2.83819600	2.97020900
H	-3.32721000	1.87986800	1.59819800
C	-3.00631900	4.48610400	0.80492800
H	-3.33656600	4.93281700	1.74897300
H	-2.66681800	5.30290600	0.15909800
H	-3.87880400	4.02192900	0.33079600
C	-0.69340900	4.13958200	1.74355000
H	-0.29190700	4.96145400	1.14192900
H	-1.00271100	4.56462100	2.70451900
H	0.11898700	3.43351500	1.94818300
C	5.35663300	-0.82911300	0.31796200
F	6.47440700	-0.35278800	-0.26380700
F	5.58746800	-0.88016200	1.64920800
F	5.18817900	-2.10289400	-0.09937200
Pd	-0.29664500	-0.53054500	-0.09588000
C	-2.29411100	-1.05448000	-0.42984500
C	-2.62650700	-1.01117300	-1.79938300
C	-3.27240400	-0.72318400	0.51899300
C	-3.89235000	-0.58676700	-2.20651300
H	-1.89896800	-1.31594100	-2.54631700
C	-4.54459100	-0.31154100	0.10640200
H	-3.05017100	-0.77862000	1.57957000
C	-4.85579300	-0.23763600	-1.25343000
H	-4.13154300	-0.54541500	-3.26585300
H	-5.29220600	-0.05359900	0.85161700
H	-5.84689700	0.07535600	-1.56942200
C	0.14173500	-2.55733200	-0.20819600
C	-1.24166800	-2.80541300	0.05566300
H	0.80882200	-2.69161100	0.64734300
C	0.73591700	-2.94251700	-1.54803000
H	1.67944700	-2.42479400	-1.74366800
H	0.94853000	-4.02106000	-1.55894000
H	0.04762600	-2.73403600	-2.37294100
H	-1.79464400	-3.26838400	-0.75554100
C	-1.69079200	-3.24607600	1.44100800
H	-0.94402800	-3.96569200	1.80152100
C	-3.04630800	-3.94137300	1.45589900
H	-3.29865600	-4.20527800	2.49397500
H	-1.68710400	-2.42020600	2.15735300
H	-3.83222400	-3.27082600	1.08452800
O	-2.94510700	-5.10874100	0.63771000
H	-3.83774300	-5.46356000	0.52315400

68-s

B3LYP SCF energy in DMF: -1619.951997 a.u.

M06 SCF energy in DMF: -1619.364571 a.u.

M06 Free energy in DMF: -1618.92429 a.u.

C	2.67259700	-0.61119600	0.17328000
C	1.88595800	1.45310900	-0.51328700
C	3.17540700	1.95426200	-0.66071300
C	4.25439400	1.12656300	-0.35754100
C	3.99424900	-0.16847100	0.08122800
H	2.44948900	-1.62251900	0.48902200
H	3.32829700	2.97427300	-0.99123900
H	5.27141300	1.48948000	-0.45564700
C	0.69173400	2.29603000	-0.68463200
N	-0.48154800	1.93397800	-0.29746600
C	-0.51579200	4.04164600	-1.35004600
C	-1.35337900	3.13580200	-0.421113000
H	-0.79459300	3.94070100	-2.40255300
H	-2.29011000	2.84663300	-0.90373500
O	0.84809000	3.51452500	-1.21158400
H	-0.48852100	5.09487300	-1.07693900
N	1.63677600	0.17761200	-0.12724600
C	-1.69480000	3.77051600	0.96917200

C	-2.38679700	2.72885800	1.86388200
H	-1.73593200	1.87282800	2.06614400
H	-2.65443400	3.18156700	2.82524900
H	-3.30649900	2.35794800	1.40319200
C	-2.67274900	4.93696000	0.72429500
H	-2.97405200	5.38044000	1.67945600
H	-2.22872800	5.73490300	0.11963100
H	-3.58003500	4.59248700	0.21484200
C	-0.43738600	4.28992900	1.69145800
H	0.08126600	5.07211700	1.12727900
H	-0.72184200	4.72372500	2.65628000
H	0.27588000	3.48430400	1.89810300
C	5.10990100	-1.08737600	0.50534700
F	6.25670200	-0.81641300	-0.14830700
F	5.36679300	-0.96759600	1.82752800
F	4.80400900	-2.38256200	0.27920600
Pd	-0.44129700	-0.39175000	-0.24764300
C	-2.40440700	-1.68391400	-0.18547600
C	-2.54299400	-0.99759600	-1.42178300
C	-3.18917900	-1.24130800	0.91057900
C	-3.47903000	0.04512900	-1.56769500
H	-2.03484200	-1.37941000	-2.30296200
C	-4.12333200	-0.22738600	0.74826100
H	-3.09870300	-1.73549900	1.87150200
C	-4.27885900	0.41219700	-0.49407800
H	-3.59263800	0.53000500	-2.53271800
H	-4.74597600	0.06663500	1.58794400
H	-5.02575100	1.19189400	-0.61076200
C	-0.09361400	-2.40312800	-0.29429200
C	-1.51900100	-2.94693400	-0.16282500
H	0.48870900	-2.56287500	0.62147500
C	0.64845200	-2.84167800	-1.54429400
H	1.64750100	-2.40382400	-1.62585500
H	0.77252800	-3.93573000	-1.52937500
H	0.09023600	-2.59473400	-2.45369500
H	-1.77185400	-3.52379700	-1.05949700
C	-1.70036400	-3.88069000	1.04335500
H	-0.88762800	-4.61696000	1.01801800
C	-3.02129500	-4.64371500	1.05783000
H	-3.08021300	-5.24061800	1.98128900
H	-1.59155900	-3.33132700	1.98620200
H	-3.87300800	-3.94853000	1.06669300
O	-3.06495000	-5.48505700	-0.09597200
H	-3.94631100	-5.88186900	-0.13354300

TS40-s

B3LYP SCF energy in DMF: -1619.94236 a.u.

M06 SCF energy in DMF: -1619.351323 a.u.

M06 Free energy in DMF: -1618.908865 a.u.

C	-2.91352500	0.34475400	-0.24051300
C	-1.76337100	-1.64772600	-0.00942500
C	-2.93645200	-2.37885000	0.14292200
C	-4.15149300	-1.69381200	0.10629100
C	-4.13857400	-0.31587500	-0.08796700
H	-2.86536500	1.41647000	-0.40228200
H	-2.90464300	-3.45207800	0.28651000
H	-5.08710400	-2.22875900	0.22322000
C	-0.42401300	-2.25824200	0.04337500
N	0.67111500	-1.57419300	-0.03750200
C	1.11073600	-3.87507800	0.05310100
C	1.80299600	-2.50739000	0.24136400
H	1.24398500	-4.28224200	-0.95264100
H	2.57500400	-2.34844000	-0.51408600
O	-0.32145300	-3.57496400	0.20729500
H	1.36381400	-4.62995800	0.79456400
N	-1.75246300	-0.30768000	-0.19844200
C	2.44645400	-2.29504800	1.65180300
C	3.02513500	-0.87416700	1.75723300
H	2.24459800	-0.11301000	1.68243500
H	3.52488500	-0.74724700	2.72418600
H	3.76655300	-0.68657400	0.97355500

C	3.60474300	-3.30441400	1.79071700
H	4.12337700	-3.14608400	2.74243700
H	3.25963000	-4.34354900	1.77777200
H	4.33887000	-3.18207500	0.98579700
C	1.42824000	-2.51096400	2.78659200
H	1.01015600	-3.52308200	2.78701000
H	1.91793600	-2.36431800	3.75534000
H	0.60094800	-1.79490100	2.72916000
C	-5.41431400	0.48437300	-0.10197500
F	-6.48684800	-0.28659300	-0.36761300
F	-5.63570700	1.08388100	1.08967200
F	-5.37354600	1.46315300	-1.03183700
Pd	0.32008000	0.41549600	-0.68155900
C	1.61504200	2.89266600	0.28289000
C	0.35316600	3.35334000	0.69408200
C	2.63915300	2.81068600	1.24176800
C	0.11340400	3.70543100	2.02682400
H	-0.44409200	3.45088200	-0.03973300
C	2.40326700	3.16647900	2.57038300
H	3.62719900	2.46815400	0.94667100
C	1.13814000	3.61132900	2.96958200
H	-0.87035500	4.06057000	2.32182800
H	3.20893100	3.09934600	3.29665300
H	0.95807000	3.88951900	4.00420600
C	2.13838400	1.01957800	-1.34509000
C	1.86111800	2.51956800	-1.17913400
H	2.92883600	0.65966500	-0.68402700
H	0.92464600	2.73637700	-1.72634100
C	2.94957400	3.42112500	-1.81624700
C	2.33379600	0.56464900	-2.78683300
H	1.47423400	0.87018100	-3.39982800
H	2.71873700	4.47364200	-1.62268000
H	3.93492400	3.20171600	-1.39220000
C	2.56606600	-0.92597200	-3.00444400
H	1.70291000	-1.50686500	-2.64994000
H	3.00116100	3.27989100	-2.89865500
H	2.67070000	-1.11130400	-4.08327000
H	3.20435500	1.09393400	-3.20295100
O	3.75802400	-1.31558000	-2.31352900
H	3.93917300	-2.23779500	-2.54532500

69-s

B3LYP SCF energy in DMF: -1619.951994 a.u.

M06 SCF energy in DMF: -1619.361761 a.u.

M06 Free energy in DMF: -1618.921769 a.u.

C	-2.85827200	0.60501400	-0.12401400
C	-2.05647600	-1.56255500	-0.06253800
C	-3.33600600	-2.09951100	0.02801500
C	-4.42034300	-1.22313400	0.05121600
C	-4.17560800	0.14593800	-0.02165200
H	-2.63420000	1.66307300	-0.19437300
H	-3.48181800	-3.17157900	0.07964600
H	-5.43301000	-1.60448600	0.12201300
C	-0.83462400	-2.38299700	-0.04692700
N	0.34926200	-1.86992600	-0.11476300
C	0.43551700	-4.21379200	-0.05340000
C	1.32441200	-2.96550500	0.14994100
H	0.51970500	-4.63226700	-1.05961400
H	2.11187200	-2.92292100	-0.60373600
O	-0.93710000	-3.70243700	0.08538300
H	0.56206900	-5.00183700	0.68638900
N	-1.81982600	-0.23266600	-0.14091000
C	2.00194100	-2.85836600	1.55636900
C	2.76841500	-1.52766500	1.66619400
H	2.08976400	-0.66941400	1.65979900
H	3.33246800	-1.50069300	2.60540800
H	3.47549100	-1.41138200	0.83883600
C	3.01633800	-4.01480400	1.67225300
H	3.54231700	-3.95186400	2.63085900
H	2.54020300	-4.99982300	1.62577400
H	3.76782000	-3.96560800	0.87565800

C	0.97379300	-2.94891000	2.69872400
H	0.43674500	-3.90360300	2.70514700
H	1.48525500	-2.85903900	3.66315200
H	0.23577000	-2.14063500	2.64596100
C	-5.30668000	1.13721000	0.06015400
F	-6.43138300	0.65769700	-0.50835000
F	-5.60707900	1.43496200	1.34434900
F	-5.00036100	2.29918000	-0.55406800
Pd	0.32292800	0.20829200	-0.56414000
C	1.98364400	2.90648200	0.22173000
C	1.05025500	3.42348100	1.13068400
C	3.34742100	3.15272200	0.44065300
C	1.46880500	4.16102300	2.24069600
H	-0.01068000	3.24481700	0.97156800
C	3.76640100	3.89136700	1.54918900
H	4.08428800	2.76889000	-0.25981400
C	2.82897000	4.39651100	2.45387600
H	0.73146500	4.54943900	2.93786000
H	4.82653900	4.07124400	1.70531200
H	3.15599800	4.96880000	3.31737500
C	2.17936800	0.80378200	-1.20198700
C	1.54580200	2.14775600	-1.02392700
H	2.91209400	0.54519700	-0.43951500
H	0.37169900	1.95177600	-0.84629400
C	1.46697300	3.06964500	-2.25953300
C	2.57772600	0.33857500	-2.59105800
H	1.77902000	0.52120000	-3.31786000
H	0.86663300	3.95485000	-2.03275600
H	2.47512900	3.39905500	-2.53116300
C	2.96725800	-1.13011800	-2.69775600
H	2.08947700	-1.76282400	-2.50220200
H	1.02205600	2.56326300	-3.11847600
H	3.29747300	-1.33406400	-3.72655100
H	3.43576700	0.94987700	-2.91430000
O	4.01678000	-1.40853800	-1.76779700
H	4.27361700	-2.33437800	-1.88342500

TS41-s

B3LYP SCF energy in DMF: -1619.943672 a.u.

M06 SCF energy in DMF: -1619.351094 a.u.

M06 Free energy in DMF: -1618.914703 a.u.

C	-2.87000300	0.38272400	-0.14190600
C	-1.85950700	-1.69532900	0.02449300
C	-3.07997900	-2.33894700	0.19439700
C	-4.24215800	-1.56939700	0.20172800
C	-4.13197600	-0.19125900	0.03382500
H	-2.74966100	1.44899000	-0.28543000
H	-3.11932200	-3.41427800	0.31845900
H	-5.21036500	-2.04020500	0.33294100
C	-0.56866000	-2.40204500	0.03812700
N	0.55925200	-1.78649700	-0.06551300
C	0.84745100	-4.12104200	0.02172700
C	1.63201000	-2.79456000	0.16014500
H	0.93791500	-4.56336900	-0.97365600
H	2.37242700	-2.69740200	-0.63619200
O	-0.55841400	-3.72535400	0.18998400
H	1.06427200	-4.87193800	0.77907300
N	-1.75515100	-0.35526700	-0.14549800
C	2.37329400	-2.60565900	1.52448500
C	3.03266800	-1.21548000	1.56834900
H	2.28679000	-0.41519000	1.57291500
H	3.63376600	-1.11654800	2.47927900
H	3.69340500	-1.06604400	0.70814000
C	3.48345200	-3.67320500	1.60686400
H	4.05484600	-3.54306000	2.53219400
H	3.08728400	-4.69425200	1.61036800
H	4.18332100	-3.58583400	0.76749400
C	1.41664400	-2.75298800	2.72112000
H	0.94885400	-3.74247500	2.76413600
H	1.96972400	-2.61719800	3.65684300
H	0.62312100	-1.99787300	2.69890000

C	-5.35129500	0.69208600	0.08448400
F	-6.42784700	0.08466800	-0.45437600
F	-5.67343400	1.01374900	1.35724400
F	-5.15840800	1.84997700	-0.58067000
Pd	0.24057700	0.32756800	-0.60896500
C	1.75435200	2.94058500	0.23907700
C	0.74868500	3.67790200	0.88764700
C	3.04051400	2.92144000	0.80144100
C	1.01388800	4.35413500	2.07703200
H	-0.25166300	3.70728600	0.46407000
C	3.30692000	3.60466900	1.99120700
H	3.84359800	2.38951000	0.30129300
C	2.29560800	4.31778600	2.63567700
H	0.21963300	4.90862400	2.56887000
H	4.30989200	3.58133800	2.40795400
H	2.50320800	4.84669800	3.56151000
C	2.13258000	1.01516600	-1.35317700
C	1.48944500	2.25274900	-1.07767500
H	2.82085600	0.64851900	-0.59706400
H	-0.15214300	1.78909900	-0.92928100
C	1.09937400	3.19751900	-2.20886900
C	2.44390200	0.56321300	-2.76629000
H	1.60161900	0.74617900	-3.44081100
H	0.35224400	3.92524400	-1.88558700
H	1.99941600	3.75258600	-2.50365000
C	2.83686300	-0.90242500	-2.89573100
H	1.98873400	-1.54462000	-2.61741200
H	0.71987500	2.67009400	-3.08500200
H	3.08091400	-1.11190200	-3.94700000
H	3.27868700	1.17898600	-3.13650500
O	3.96635200	-1.15559100	-2.05583900
H	4.22278600	-2.08055500	-2.17937100

70-s

B3LYP SCF energy in DMF: -1619.947541 a.u.

M06 SCF energy in DMF: -1619.353171 a.u.

M06 Free energy in DMF: -1618.915031 a.u.

C	-2.95892400	-0.55344500	0.06242600
C	-1.90368200	1.50582400	-0.11943900
C	-3.10353200	2.15914300	-0.37557400
C	-4.27570000	1.40719900	-0.42140400
C	-4.19710900	0.03337600	-0.20606100
H	-2.86452400	-1.61412000	0.25337400
H	-3.11732300	3.22981200	-0.53809400
H	-5.22795200	1.88744000	-0.61929600
C	-0.60516400	2.19838900	-0.09052800
N	0.51748100	1.56992100	-0.01931900
C	0.81072500	3.90844600	0.08575600
C	1.59559900	2.59269100	-0.13011600
H	0.87598300	4.27798600	1.11240100
H	2.30541200	2.42669900	0.68437100
O	-0.59135900	3.53019700	-0.14486000
H	1.04829600	4.71164400	-0.60941200
N	-1.83386500	0.17096500	0.10629500
C	2.37346200	2.51206500	-1.48330300
C	3.00164100	1.11709500	-1.63017500
H	2.23864300	0.33632700	-1.68097800
H	3.59551200	1.06481200	-2.54961800
H	3.66847800	0.89135800	-0.79139600
C	3.50314200	3.55991200	-1.43872400
H	4.10126000	3.50421200	-2.35466100
H	3.12194400	4.58384800	-1.36021800
H	4.17347000	3.38321900	-0.58962100
C	1.45490900	2.78311600	-2.68940200
H	1.01427300	3.78538900	-2.66185600
H	2.03064100	2.70980800	-3.61844300
H	0.64106900	2.05202400	-2.75178700
C	-5.42865300	-0.83015900	-0.29720600
F	-6.51173300	-0.20097600	0.20205800
F	-5.71156400	-1.14803800	-1.57990700
F	-5.28067300	-1.98885600	0.37704600

Pd	0.08045000	-0.53715400	0.67484000
C	2.22916000	-2.54491900	-0.30842200
C	1.41280300	-3.26943600	-1.19626200
C	3.54239400	-2.23720500	-0.70122700
C	1.88675800	-3.64575900	-2.45204200
H	0.39737100	-3.52336700	-0.90609600
C	4.01959200	-2.62601800	-1.95515100
H	4.19897400	-1.70969200	-0.01638000
C	3.19266500	-3.32455500	-2.83640100
H	1.23815400	-4.19349200	-3.12997400
H	5.04061700	-2.38608300	-2.23828000
H	3.56343700	-3.62485100	-3.81230700
C	2.05725800	-0.93566200	1.61441200
C	1.74345100	-2.17672700	1.06161000
H	2.67155200	-0.27168000	1.01134700
C	1.31024500	-3.35523900	1.91231300
C	2.06082500	-0.62803000	3.09602500
H	1.23666100	-1.12602700	3.61425200
H	0.66272900	-4.03876400	1.35935200
H	2.21456000	-3.91619100	2.18663700
C	2.00668600	0.85903500	3.42631200
H	1.07178000	1.29620500	3.04571300
H	0.80382400	-3.05620200	2.83065900
H	2.01246900	0.98011300	4.51897100
H	2.99101200	-1.03841300	3.51878900
O	3.14426500	1.50076100	2.84297800
H	3.10252000	2.43849800	3.07914000
H	-0.55566300	-1.79927500	1.21971300

TS42-s

B3LYP SCF energy in DMF: -1868.472417 a.u.

M06 SCF energy in DMF: -1867.777024 a.u.

M06 Free energy in DMF: -1867.250458 a.u.

C	2.34391000	1.10926800	0.34116900
C	0.84334500	1.97046100	-1.19314900
C	1.72068100	2.99154300	-1.55214400
C	2.95876800	3.06633100	-0.91847400
C	3.27145400	2.11078900	0.04484600
H	2.56323200	0.34235500	1.07354400
H	1.43692100	3.71344100	-2.30759900
C	3.66185300	3.85123300	-1.17371300
H	-0.49629700	1.84927400	-1.80315500
N	-1.42148900	1.08140100	-1.35833700
C	-2.07894000	2.22171900	-3.34040400
C	-2.60982300	1.27982100	-2.22429900
H	-1.96638800	1.71923700	-4.30373700
H	-2.88291600	0.30849200	-2.64973200
O	-0.73973900	2.60118600	-2.88840000
H	-2.64980700	3.14030600	-3.47612800
N	1.15336400	1.03714700	-0.26436500
C	-3.85280500	1.80407500	-1.44222300
C	-4.23164200	0.78627400	-0.35107800
H	-3.46727300	0.73139700	0.42892100
H	-5.17339500	1.07984000	0.12660600
H	-4.36355000	-0.21823700	-0.76873200
C	-5.02530400	1.91957900	-2.43607500
H	-5.92914900	2.25361900	-1.91508400
H	-4.82598900	2.63915300	-3.23782800
H	-5.24654800	0.95141400	-2.90065800
C	-3.57775500	3.17004200	-0.78919100
H	-3.33830600	3.94570200	-1.52502400
H	-4.46454300	3.50789800	-0.24169900
H	-2.75069600	3.11218600	-0.07281200
C	4.57298100	2.16282400	0.79926400
F	5.54015300	2.77349600	0.08533200
F	4.44562000	2.84407000	1.96082900
F	5.01717800	0.92720800	1.11614400
Pd	-0.33638400	-0.53829200	0.19684300
C	-1.36643700	-0.84372300	2.90721500
C	-0.43127000	-0.12753900	3.68206600
C	-2.73344400	-0.61936800	3.15524500

C	-0.84614800	0.79207900	4.64390500
H	0.63151400	-0.27980400	3.51886800
C	-3.14876900	0.30015600	4.12164100
H	-3.48056600	-1.18131900	2.60380800
C	-2.20893200	1.01375500	4.86716600
H	-0.10363200	1.33639300	5.22124800
H	-4.21084100	0.44875800	4.29722200
H	-2.53239100	1.72697200	5.61998500
C	-1.70648700	-2.10587300	0.74898800
C	-0.90831500	-1.84724500	1.88321500
H	-2.65340800	-1.57540200	0.67597400
C	0.11307200	-2.84955200	2.39042600
C	-1.68084100	-3.39126200	-0.05396400
H	-0.66486300	-3.78202300	-0.16346500
H	0.95978300	-2.36161100	2.87926800
H	-0.36535000	-3.49471900	3.14088900
C	-2.28581500	-3.25252000	-1.44645700
H	-1.72479200	-2.50044100	-2.02182500
H	0.50525100	-3.48602000	1.59762100
H	-2.19791900	-4.21302400	-1.97669400
H	-2.25387800	-4.15825000	0.49043400
O	-3.65817400	-2.87366900	-1.31797400
H	-4.00081200	-2.71054900	-2.20783200
H	0.89722100	-1.55455600	0.07032500
N	3.08184400	-3.42154400	-1.90808600
C	4.16460700	-3.94529100	-1.07858200
H	4.03427300	-3.60811600	-0.05178200
H	4.15514200	-5.03918000	-1.11071000
H	5.12479600	-3.58863200	-1.46376700
C	3.10987600	-3.77371200	-3.32591700
H	2.25722100	-3.32609000	-3.83847500
H	4.03576700	-3.40807400	-3.78044700
H	3.06732400	-4.86149000	-3.43771900
C	2.11681800	-2.66738200	-1.40511200
H	1.36261000	-2.32804400	-2.12270500
O	2.04119700	-2.34008100	-0.18688800

71-s

B3LYP SCF energy in DMF: -1619.495977 a.u.

M06 SCF energy in DMF: -1618.917841 a.u.

M06 Free energy in DMF: -1618.492243 a.u.

C	-2.57393500	0.57794800	0.16712000
C	-0.97961200	2.24294600	0.21804700
C	-1.94563300	3.24709000	0.26048200
C	-3.28801600	2.87820900	0.24896600
C	-3.60522900	1.52158700	0.19435500
H	-2.78992300	-0.48407700	0.13226600
H	-1.65228100	4.28911700	0.29868600
H	-4.06759500	3.63189800	0.28084300
C	0.46295900	2.53742200	0.18906500
N	1.36179100	1.62361500	0.09565800
C	2.31625400	3.77696000	0.32523700
C	2.67404500	2.30646900	-0.01469000
H	2.59554300	4.05493100	1.34498000
H	3.34163900	1.89140700	0.74635700
O	0.85412500	3.81988100	0.24733000
H	2.70272200	4.51973300	-0.37173600
N	-1.28395400	0.92557100	0.18570800
C	3.35711500	2.09089000	-1.40270100
C	3.56185900	0.58526800	-1.65221700
H	2.60699400	0.06332800	-1.76915800
H	4.14266000	0.43540100	-2.56982200
H	4.10306000	0.10499000	-0.82951900
C	4.73699600	2.77647600	-1.35950000
H	5.25569300	2.64086500	-2.31498000
H	4.66197100	3.85437600	-1.17838900
H	5.36818000	2.34647200	-0.57280600
C	2.51642000	2.68341700	-2.54825900
H	2.39350000	3.76838500	-2.45842800
H	3.00807400	2.49323400	-3.50864800
H	1.52037200	2.22960000	-2.59490100

C	-5.03963600	1.07598200	0.11226300
F	-5.85003900	1.86400700	0.85125200
F	-5.50101300	1.12364400	-1.15951300
F	-5.20293300	-0.19294800	0.54326100
Pd	0.54711500	-0.46017000	0.46845500
C	-0.23942700	-3.21837800	-0.26397400
C	-1.63720400	-3.29747100	-0.45470200
C	0.56790800	-3.84917000	-1.23427200
C	-2.19235000	-3.93550200	-1.56375900
H	-2.30323700	-2.83892500	0.26977400
C	0.01415200	-4.48490200	-2.34724200
H	1.64647300	-3.85644900	-1.11436200
C	-1.37044400	-4.53070600	-2.52507400
H	-3.27335600	-3.96740300	-1.67622100
H	0.67197000	-4.95951100	-3.07134400
H	-1.80134100	-5.02953900	-3.38867500
C	1.71896100	-2.14256400	0.95887200
C	0.33473800	-2.52035900	0.94039400
H	2.30872700	-2.38622600	0.07638500
C	-0.40814900	-2.80034300	2.24499500
C	2.58031400	-2.12765300	2.21302500
H	2.01762600	-1.78966000	3.08934700
H	-1.47108600	-2.55001700	2.18177600
H	-0.34793500	-3.86689700	2.51319100
C	3.82438000	-1.25218900	2.11514200
H	3.52884000	-0.20712900	1.93851300
H	0.00275700	-2.22876300	3.07988100
H	4.36916900	-1.28839200	3.07161500
H	2.91329500	-3.15480000	2.43873400
O	4.65678700	-1.72776500	1.05299700
H	5.41510100	-1.13022700	0.99107300

72-s

B3LYP SCF energy in DMF: -1960.429588 a.u.

M06 SCF energy in DMF: -1959.694682 a.u.

M06 Free energy in DMF: -1959.17721 a.u.

C	2.59063100	-0.00716500	-0.85278600
C	1.35168500	1.90833800	-0.51458100
C	2.50238900	2.69550900	-0.44004600
C	3.74661000	2.08128200	-0.55776100
C	3.78928400	0.70603700	-0.77165900
H	2.59195200	-1.07679800	-1.03449100
H	2.42221200	3.76464500	-0.28798000
H	4.65859100	2.66356500	-0.48972300
C	0.00655300	2.51517000	-0.40870900
N	-1.08816000	1.87614700	-0.21990100
C	-1.43316800	4.23342300	-0.37615600
C	-2.18396800	2.87867200	-0.27249400
H	-1.72859800	4.83300100	-1.23829100
H	-2.74261400	2.69009700	-1.19858400
O	-0.03583400	3.85502900	-0.55450000
H	-1.49248200	4.84372600	0.52775100
N	1.39489900	0.57283700	-0.71515900
C	-3.20307000	2.78123000	0.89794000
C	-3.95231600	1.44077200	0.80491700
H	-3.27750100	0.59114500	0.93172000
H	-4.71687700	1.38172100	1.58795800
H	-4.45746600	1.33645500	-0.16301900
C	-4.22243300	3.92727900	0.73858600
H	-4.99357700	3.85651500	1.51354100
H	-3.75652600	4.91418000	0.83278400
H	-4.72368200	3.88096600	-0.23546900
C	-2.50619600	2.88596200	2.26580600
H	-1.96596800	3.83169100	2.38514400
H	-3.24857200	2.83178600	3.06976700
H	-1.79233300	2.06901400	2.41529900
C	5.09036000	-0.04232300	-0.85471200
F	6.12945400	0.77145600	-1.12429200
F	5.36977400	-0.67460100	0.31227900
F	5.05796300	-0.99513300	-1.81230400
Pd	-0.45931900	-0.76150900	-0.16402300

C	0.79454700	-1.46602300	2.37672700	H	2.52928300	4.55098100	1.10529000
C	2.19831300	-1.46067200	2.23227300	H	1.47967200	4.75514300	2.50651600
C	0.25285400	-0.72969300	3.45132000	H	1.81183000	3.13281800	1.89578100
C	3.01476200	-0.72736000	3.09193100	C	3.82452300	-3.55851900	0.32638200
H	2.66148700	-2.01701000	1.42468300	F	5.15045000	-3.66023000	0.54203100
C	1.07091900	0.00065900	4.31430400	F	3.19332300	-4.06152300	1.40861500
H	-0.81655500	-0.74161000	3.63352200	F	3.52543500	-4.36682600	-0.71524000
C	2.45654300	0.01263700	4.13788000	Pd	-0.38587300	0.16168700	0.08615000
H	4.09019200	-0.73086200	2.93649300	C	-2.44851800	0.76028500	-0.05784200
H	0.62102000	0.55126300	5.13615600	C	-2.59180400	-0.47983500	0.61107400
H	3.09233100	0.58012000	4.81148700	H	-2.47643500	1.65150300	0.56699700
C	-1.45233900	-2.01177300	1.35027800	H	-0.96315200	-1.21302000	0.45369900
C	-0.07021000	-2.26744100	1.44482100	C	-2.86055200	0.98955800	-1.49260800
H	-1.84996800	-1.20168600	1.95912300	H	-2.72311900	0.07935400	-2.08972300
C	0.51032800	-3.59429500	0.99128800	H	-3.93376500	1.23790600	-1.50985900
C	-2.50793600	-3.03432400	0.99558900	O	-2.10583500	2.07619800	-2.02842500
H	-2.23145100	-3.62717300	0.12021300	H	-2.47969100	2.28118700	-2.89738900
H	1.47024300	-3.47875700	0.48114200	C	-3.24287500	-1.67636700	-0.04828700
H	0.68670900	-4.23800500	1.86416100	C	-2.67323700	-2.95902400	-0.02286200
C	-3.87870000	-2.41759800	0.74456000	C	-4.53009500	-1.52887100	-0.59193400
H	-3.81621800	-1.68732700	-0.07426400	C	-3.35404400	-4.05589200	-0.55087500
H	-0.16228300	-4.12570100	0.31819400	H	-1.68427000	-3.10159700	0.40543100
H	-4.58351100	-3.20540600	0.43707400	C	-5.21469300	-2.62835200	-1.11568800
C	-2.59959600	-0.78175100	-3.22953400	H	-5.00874400	-0.55498700	-0.59383400
C	-1.22800200	-0.65110300	-2.84519500	C	-4.62770700	-3.89408600	-1.10239800
C	-0.48577600	-1.70852800	-2.18471500	H	-2.88766100	-5.03674800	-0.53067900
C	-1.13628000	-2.98417900	-2.20451000	H	-6.20814000	-2.49038300	-1.53294300
C	-2.44187400	-3.12345500	-2.61456300	H	-5.15713200	-4.74802300	-1.51513800
C	-3.19117600	-2.01028100	-3.09677200	C	-2.68561600	-0.47254900	2.14195800
H	-3.12048700	0.07389900	-3.64479000	H	-2.04642700	0.32455200	2.53327900
H	0.59953000	-1.68889500	-2.25119300	H	-2.30103000	-1.42167000	2.52923900
H	-0.56777600	-3.85000200	-1.88446700	C	-4.12427500	-0.26259500	2.63914000
H	-2.90901400	-4.10330200	-2.59572400	H	-4.79249700	-1.06418700	2.31096100
H	-4.22467100	-2.14443600	-3.39820700	H	-4.13398600	-0.24637900	3.73392000
N	-0.58879700	0.47667200	-3.17950100	H	-4.53270600	0.69009600	2.28492800
N	-0.05438700	1.42788500	-3.47442900				
H	-2.60628400	-3.74452200	1.83195800				
O	-4.32258600	-1.78866400	1.94921600				
H	-5.06983800	-1.21812400	1.72297100				

TS43-s

B3LYP SCF energy in DMF: -1619.939047 a.u.

M06 SCF energy in DMF: -1619.345122 a.u.

M06 Free energy in DMF: -1618.907884 a.u.

C	2.08045600	-1.75981800	0.27260500
C	2.52687400	0.38826500	-0.47405000
C	3.86012100	0.08617700	-0.72206200
C	4.31189100	-1.20501500	-0.45097700
C	3.40953300	-2.13561300	0.05515800
H	1.35224700	-2.45971000	0.66305000
H	4.52792500	0.84297200	-1.11536200
H	5.34715400	-1.47313900	-0.62910000
C	1.94705900	1.72236000	-0.69543700
N	0.72987700	2.00467200	-0.38265200
C	1.79181700	3.80833600	-1.46053400
C	0.53588700	3.45918800	-0.62436800
H	1.59061400	3.83797700	-2.53445400
H	-0.37421800	3.58014100	-1.21440100
O	2.70596300	2.67960200	-1.22723500
H	2.31368000	4.71460000	-1.15905400
N	1.64798900	-0.52202800	0.01347600
C	0.38050300	4.28409800	0.69458600
C	-0.85104100	3.79428500	1.47659000
H	-0.73423100	2.75842000	1.80881800
H	-0.99810900	4.41604700	2.36678300
H	-1.76086400	3.86166700	0.87007000
C	0.15270900	5.75742700	0.30088100
H	-0.00687900	6.36397200	1.19889300
H	1.00781000	6.18479400	-0.23350700
H	-0.73218900	5.86473400	-0.33729000
C	1.62578700	4.16917500	1.59272100

TS44-s

B3LYP SCF energy in DMF: -1619.934584 a.u.

M06 SCF energy in DMF: -1619.339568 a.u.

M06 Free energy in DMF: -1618.900974 a.u.

C	2.23422700	-1.54486400	0.26739000
C	2.46725500	0.68393300	-0.32730300
C	3.85023300	0.57796500	-0.40061800
C	4.44083100	-0.65340600	-0.11693400
C	3.62062000	-1.72329300	0.22529700
H	1.56616000	-2.35926200	0.51870200
H	4.45066500	1.43893500	-0.66825600
H	5.51749500	-0.77044500	-0.16127700
C	1.74516900	1.94467100	-0.56005200
N	0.48690900	2.08135800	-0.31096900
C	1.39268800	4.00718300	-1.31384400
C	0.16944800	3.52515800	-0.50355900
H	1.21866600	3.99293200	-2.39304900
H	-0.74524400	3.60953700	-1.09454500
O	2.42009700	2.99312800	-1.03093100
H	1.79702200	4.97301700	-1.01719600
N	1.66914300	-0.36394900	-0.00293000
C	-0.04739500	4.28632000	0.84694500
C	-1.17188700	3.61470200	1.65224600
H	-0.88500100	2.61122800	1.98174000
H	-1.39424500	4.20588900	2.54780400
H	-2.08935400	3.53515200	1.06181400
C	-0.47732700	5.72626400	0.50116300
H	-0.64858700	6.29711900	1.42019600
H	0.28374400	6.26008000	-0.07812900
H	-1.40849800	5.73558100	-0.07718700
C	1.23149300	4.31737400	1.70508300
H	2.05690400	4.84358000	1.21464600
H	1.02884700	4.84189800	2.64503600
H	1.57142200	3.30870200	1.96510900
C	4.18252200	-3.09366200	0.50415400

F	5.51582500	-3.06273600	0.68750600
F	3.62883400	-3.64068000	1.60771400
F	3.93408200	-3.94080300	-0.51983500
Pd	-0.41186100	0.01652300	-0.23074100
C	-2.48943500	-0.92806400	-0.98659400
C	-3.18220400	-1.88982600	-0.05890700
C	-2.86487900	-1.98210900	1.30674000
C	-4.24105300	-2.67376000	-0.55084200
C	-3.58069700	-2.82745900	2.15466300
H	-2.03838800	-1.39516100	1.69802700
C	-4.95937600	-3.51608700	0.30018300
H	-4.52345700	-2.61922200	-1.59680600
C	-4.63218200	-3.59911300	1.65453700
H	-3.31123500	-2.88574000	3.20544800
H	-5.77563900	-4.10944600	-0.10200200
H	-5.18741300	-4.26111700	2.31277100
C	-2.50986000	0.44771300	-0.70785800
C	-3.32574200	1.08879000	0.39963500
H	-4.15680200	0.42770600	0.68176600
H	-2.72888800	1.26543300	1.30255000
H	-0.70304800	-1.47586000	-0.22925500
O	-3.82094500	2.32203000	-0.12821000
H	-4.32872400	2.75034800	0.57655300
H	-2.33708000	1.11417600	-1.55349000
C	-2.23184200	-1.37922900	-2.42173000
H	-3.21961200	-1.46840600	-2.89560200
H	-1.71760300	-0.57109000	-2.95018600
C	-1.47247400	-2.69448700	-2.60669700
H	-1.96465600	-3.52643500	-2.09403500
H	-1.41563300	-2.94576800	-3.67074500
H	-0.44927700	-2.61688200	-2.22292600

TS45-s

B3LYP SCF energy in DMF: -1659.23932 a.u.

M06 SCF energy in DMF: -1658.628484 a.u.

M06 Free energy in DMF: -1658.163962 a.u.

C	-2.56654200	0.53468300	0.10423100
C	-0.84712000	1.98677400	0.62118800
C	-1.72182200	2.93538400	1.13981800
C	-3.08848700	2.65660400	1.12195500
C	-3.51346900	1.44202200	0.59307800
H	-2.86462300	-0.42417800	-0.30387400
H	-1.34533300	3.86649700	1.54558900
H	-3.80114900	3.37233400	1.51579000
C	0.60720300	2.19563500	0.54947500
N	1.41819700	1.31944900	0.05944500
C	2.56814000	3.19613800	0.88837300
C	2.76023900	1.96381900	-0.02566700
H	2.93393100	3.02957800	1.90488100
H	3.50321400	1.28576200	0.39862900
O	1.11032600	3.35336300	0.97482200
H	2.97181100	4.12952400	0.50096000
N	-1.26117400	0.80232000	0.11450200
C	3.19358900	2.30087500	-1.49102400
C	3.29296000	1.01080900	-2.32297300
H	2.32499900	0.50927800	-2.41357700
H	3.64210400	1.24717100	-3.33426100
H	4.00727000	0.30625200	-1.88263400
C	4.59423800	2.94421500	-1.42688000
H	4.95954100	3.14238200	-2.44015600
H	4.59485200	3.89776400	-0.88860200
H	5.31428900	2.27891400	-0.93628400
C	2.20598600	3.26582800	-2.17209200
H	2.11906800	4.21968300	-1.64066900
H	2.54989600	3.49171800	-3.18724600
H	1.20527400	2.82812000	-2.25750100
C	-4.97478100	1.09022500	0.50026300
F	-5.72904400	1.84735500	1.32072100
F	-5.44589500	1.26627300	-0.75493300
F	-5.19257300	-0.20398800	0.82211700
Pd	0.45812100	-0.59633300	-0.29301000

C	-0.73446200	-2.27231300	-0.67960500
C	-1.25784500	-2.89480900	0.47081800
C	-1.51943100	-2.22339000	-1.84511900
C	-2.55355700	-3.41481300	0.46509300
H	-0.65013800	-2.97985400	1.36760900
C	-2.81334700	-2.75414600	-1.84803100
H	-1.12701200	-1.77136000	-2.75111000
C	-3.33374900	-3.34811100	-0.69461600
H	-2.94961900	-3.88280800	1.36242900
H	-3.41067200	-2.70538200	-2.75461300
H	-4.33675100	-3.76501600	-0.70134700
C	2.08872000	-1.90342100	-0.31713400
C	1.22753200	-2.78663000	-1.04873900
H	2.83084900	-1.36929900	-0.91131000
C	0.99248100	-3.71998400	-0.54498400
C	1.38389800	-2.92008900	-2.54402900
C	2.54615500	-2.32761900	1.06853100
H	1.71136700	-2.79905400	1.60352400
H	3.29994400	-3.11680200	0.93162300
H	0.55899800	-3.47149600	-2.99933700
H	1.48423200	-1.95209600	-3.04146900
C	3.16415400	-1.22914300	1.94010800
H	2.41521700	-0.46228100	2.17082300
H	3.97668600	-0.73180400	1.39475800
C	3.72320400	-1.76163900	3.25359300
H	2.92682300	-2.27191300	3.81899400
H	2.30486200	-3.48909400	-2.72724600
O	4.79606900	-2.65888700	2.96238400
H	5.07867200	-3.05706900	3.79742300
H	4.07418500	-0.92043900	3.87155200

TS46-s

B3LYP SCF energy in DMF: -1659.235777 a.u.

M06 SCF energy in DMF: -1658.623605 a.u.

M06 Free energy in DMF: -1658.157055 a.u.

C	-2.53449100	0.57119600	-0.63087700
C	-1.02110100	1.79270100	0.61775200
C	-1.99845200	2.69079600	1.03011700
C	-3.30455600	2.50975100	0.57534500
C	-3.56940300	1.44306800	-0.27679500
H	-2.71957200	-0.27910800	-1.27612100
H	-1.74196800	3.51848200	1.68013400
H	-4.09120800	3.19304000	0.87376600
C	0.40136300	1.95151700	0.95916100
N	1.33458200	1.29524400	0.35935100
C	2.18590100	2.63329100	2.09819200
C	2.62719600	1.86525600	0.83263500
H	2.30290900	2.04493500	3.01228700
H	3.30137900	1.04481100	1.09043400
O	0.74332400	2.83520300	1.89907000
H	2.63664800	3.61479700	2.23167500
N	-1.28787000	0.73186400	-0.18352900
C	3.32623600	2.75466300	-0.25089600
C	3.57848900	1.93271000	-1.52619700
H	2.64285800	1.59227300	-1.98042000
H	4.10506000	2.54632000	-2.26583700
H	4.19676300	1.05469100	-1.31911600
C	4.68530300	3.20577700	0.32119200
H	5.22172700	3.80877700	-0.41941700
H	4.57556400	3.81753200	1.22300000
H	5.31596800	2.34525400	0.57245700
C	2.48030600	3.98996500	-0.61447800
H	2.31191600	4.65248700	0.24062400
H	2.99893100	4.57745900	-1.37980800
H	1.50581500	3.70795000	-1.02845300
C	-4.95492200	1.16641100	-0.79810200
F	-4.94787500	0.95915000	-2.13322200
F	-5.47826100	0.05300100	-0.23395000
F	-5.80167200	2.18164200	-0.54575700
Pd	0.40224800	-0.62614900	-0.41197700
C	2.10143100	-1.85269900	-0.41675500

C	2.36557000	-2.38263500	0.86328100
C	3.17834900	-1.55756700	-1.26721400
C	3.68093300	-2.56304500	1.29500300
H	1.54666700	-2.66230500	1.51949500
C	4.49319700	-1.75955700	-0.83715300
H	2.99759300	-1.16898300	-2.26385500
C	4.74804800	-2.25727900	0.44346300
H	3.87123800	-2.96028300	2.28852200
H	5.31774600	-1.52726900	-1.50574500
H	5.77096000	-2.41774600	0.77211700
C	-0.65236300	-2.36314900	-0.90756200
C	0.59635700	-2.84695600	-1.42015400
H	-1.34645200	-1.97987700	-1.66086400
H	0.98056500	-3.74079000	-0.93670000
C	0.87812900	-2.78464700	-2.90112600
H	1.91999800	-3.01020400	-3.13585900
H	0.25808500	-3.55220600	-3.38295800
H	0.61317300	-1.81723900	-3.33551900
C	-1.28959000	-3.11228600	0.25240800
H	-1.70520000	-4.04429800	-0.16474700
H	-0.51171100	-3.42132300	0.95759100
C	-2.40632600	-2.38858800	1.01242100
H	-3.22181300	-2.11834100	0.33011500
H	-2.02460500	-1.45502100	1.44228000
C	-2.99351300	-3.23038400	2.13809500
H	-3.37481200	-4.18267200	1.73586300
O	-1.97504000	-3.46206500	3.11305800
H	-2.34532100	-4.04764200	3.78816300
H	-3.84781900	-2.69948100	2.58591100

TS47-s

B3LYP SCF energy in DMF: -1659.238402 a.u.

M06 SCF energy in DMF: -1658.625544 a.u.

M06 Free energy in DMF: -1658.162133 a.u.

C	-2.53917700	-0.34927000	-0.21240400
C	-1.85237700	1.82499600	0.15914800
C	-3.15664100	2.30655800	0.12997800
C	-4.19322400	1.39985600	-0.09176100
C	-3.87757300	0.05594900	-0.26689100
H	-2.25916800	-1.38908100	-0.33523800
H	-3.35769000	3.36068900	0.27809900
H	-5.22278000	1.73811900	-0.12082800
C	-0.68144500	2.69388300	0.35842000
N	0.52913200	2.24716800	0.33739300
C	0.46292200	4.53298700	0.87699200
C	1.43650500	3.42563100	0.41031600
H	0.48862400	4.69144700	1.95822300
H	2.19699700	3.23558000	1.17201700
O	-0.86747900	3.99859900	0.55212900
H	0.56273400	5.48647100	0.36244800
N	-1.54736900	0.51655800	-0.00605500
C	2.16574000	3.72903300	-0.94099000
C	3.03611200	2.52964500	-1.35545700
H	2.43516500	1.63356800	-1.53652700
H	3.57598000	2.76387000	-2.27975000
H	3.78258700	2.29721100	-0.58787600
C	3.09148600	4.94039100	-0.70887900
H	3.66530700	5.15038800	-1.61783800
H	2.53806100	5.85059800	-0.45506400
H	3.80524300	4.74348100	0.09952700
C	1.16729000	4.04151600	-2.07135400
H	0.54325900	4.91369300	-1.85013200
H	1.71177100	4.26175400	-2.99579600
H	0.50735100	3.19130200	-2.27674400
C	-4.94312600	-0.97010000	-0.55011300
F	-6.15921500	-0.55635600	-0.14339200
F	-5.03278300	-1.23760500	-1.87278500
F	-4.68067300	-2.14191400	0.06896400
Pd	0.61312800	0.08730000	0.43644600
C	0.40047100	-1.98948900	0.48484000
C	-0.21911600	-2.51806200	1.63355000

C	0.15420100	-2.59065200	-0.76111700
C	-1.10367500	-3.59320700	1.52826400
H	-0.00661200	-2.09199200	2.61054800
C	-0.73323900	-3.66802200	-0.86209000
H	0.65129700	-2.22362700	-1.65468200
C	-1.36369000	-4.17004100	0.28020600
H	-1.58214700	-3.98650400	2.42130300
H	-0.92223100	-4.11903000	-1.83263400
H	-2.04395200	-5.01319100	0.20085800
C	2.55057500	-0.14879100	1.14751600
C	2.42917100	-1.54625500	0.86948300
H	3.16136200	0.41384000	0.44192000
H	2.34068400	-2.18398000	1.74532000
C	3.20464000	-2.15831500	-0.28554300
C	2.62762100	0.33390200	2.58277100
H	1.95915600	-0.23155600	3.24003700
H	3.65194000	0.20430500	2.96090400
H	2.83571900	-1.78314000	-1.24630500
H	4.22970900	-1.77901900	-0.19113000
C	3.27068700	-3.68991800	-0.28738700
H	3.64222000	-4.03873300	0.68512200
C	2.27588100	-4.12494100	-0.42726100
H	4.17996300	-4.23540300	-1.38098600
H	3.81243100	-3.90988400	-2.36752900
H	2.38234500	1.39681200	2.66904500
O	5.50889600	-3.76451700	-1.15151000
H	6.05355000	-4.05523000	-1.89620600
H	4.14704900	-5.33580300	-1.36878700

73-s

B3LYP SCF energy in DMF: -1117.085647 a.u.

M06 SCF energy in DMF: -1116.732077 a.u.

M06 Free energy in DMF: -1116.503583 a.u.

C	2.26622800	-0.55970700	0.01878200
C	0.56150200	1.01887900	-0.17453700
C	1.46027100	2.07145800	-0.08285200
C	2.81855800	1.78785700	0.06154600
C	3.22033500	0.45753500	0.11055200
H	2.54228600	-1.60431400	0.06058500
H	1.10295900	3.09338800	-0.12508900
C	3.54114000	2.59244500	0.13634800
H	-0.88832900	1.20451600	-0.33913400
N	-1.68284200	1.09833100	-0.42742100
C	-2.85896300	2.24466100	-0.53883100
C	-3.06105800	0.70323600	-0.60240900
H	-3.16675000	2.75781500	-1.44983700
H	-3.39443200	0.41041300	-1.60448300
O	-1.40191500	2.42873700	-0.40656300
H	-3.31730700	2.72260300	0.32773300
N	0.96403200	-0.28329500	-0.11999900
C	-4.06711500	0.09667100	0.41717900
C	-4.15386800	-1.42362100	0.18139400
H	-3.20440000	-1.92705900	0.40543900
H	-4.91629800	-1.86505600	0.83245600
H	-4.42423900	-1.65263800	-0.85584300
C	-5.44903700	0.72279000	0.14669800
H	-6.19856400	0.28333300	0.81342200
H	-5.45024800	1.80481800	0.31965400
H	-5.77188200	0.54370300	-0.88534600
C	-3.63906200	0.36713300	1.86992100
H	-3.59322300	1.43771900	2.09756900
H	-4.36174800	-0.08054000	2.56058300
H	-2.65748800	-0.06871500	2.08667000
C	4.67759500	0.08251300	0.21680800
F	5.40778300	1.07684500	0.75590800
F	4.85158800	-1.01745700	0.97845400
F	5.20326500	-0.18932800	-0.99753700
Pd	-0.55210100	-1.65093200	-0.25798500
H	0.42775100	-2.81426100	-0.11021100

74-s

B3LYP SCF energy in DMF: -1116.610925 a.u.

M06 SCF energy in DMF: -1116.280699 a.u.

M06 Free energy in DMF: -1116.065146 a.u.

C	-2.30774200	0.45189600	0.00464600
C	-0.41547100	-0.85431600	-0.27779200
C	-1.18289300	-2.02247500	-0.22669200
C	-2.55856300	-1.94085600	-0.05203000
C	-3.12627900	-0.67326800	0.06693600
H	-2.72870800	1.44551900	0.08321000
H	-0.69447400	-2.98351400	-0.32265200
H	-3.16800600	-2.83670800	-0.01452600
C	1.05007100	-0.96571000	-0.45680700
N	1.91886500	-0.04938000	-0.26151300
C	2.93500900	-2.12039100	-0.86790700
C	3.24234100	-0.62609100	-0.58441400
H	3.28030700	-2.45949900	-1.84591500
H	3.59591800	-0.13849100	-1.50265900
O	1.47957700	-2.18970500	-0.85931600
H	3.30241200	-2.80499400	-0.09894100
N	-0.97091500	0.38344000	-0.16983300
C	4.31111200	-0.34641200	0.51054300
C	4.53519100	1.17424800	0.60579800
H	3.62288600	1.69371500	0.91563500
H	5.31699800	1.40072600	1.33965400
H	4.85126200	1.59075200	-0.35814900
C	5.62842900	-1.02273900	0.08382100
H	6.42334300	-0.79722300	0.80339500
H	5.53398000	-2.11347300	0.03316100
H	5.95883800	-0.66761900	-0.89968500
C	3.86828900	-0.88069100	1.88388800
H	3.70776400	-1.96451200	1.87660700
H	4.63770800	-0.67109300	2.63521800
H	2.93938000	-0.40423400	2.21489200
C	-4.60174900	-0.49911200	0.29910900
F	-5.31269500	-1.53410100	-0.19574600
F	-4.89480100	-0.41598900	1.61852800
F	-5.07196500	0.62930200	-0.27658800
Pd	0.09123500	2.18983600	-0.24381800

75-s

B3LYP SCF energy in DMF: -1619.959628 a.u.

M06 SCF energy in DMF: -1619.35898 a.u.

M06 Free energy in DMF: -1618.916278 a.u.

C	3.18599500	-0.78967600	0.40356300
C	2.03581600	0.49820300	-1.13407400
C	3.02303400	0.34188700	-2.10082200
C	4.14406300	-0.42225300	-1.77845500
C	4.22579200	-0.99204400	-0.50972100
H	3.21867900	-1.21978400	1.39840300
H	2.91977200	0.80328400	-3.07565200
H	4.93780000	-0.56530000	-2.50365800
C	0.82067400	1.30113600	-1.33573900
N	-0.08824900	1.42365900	-0.42163900
C	-0.70961800	2.53084300	-2.38746300
C	-1.04744300	2.46926400	-0.88111900
H	-1.36006700	1.89461300	-2.99291300
H	-2.06446100	2.10406600	-0.73182800
O	0.64598700	1.96138000	-2.47385700
H	-0.66677400	3.53116900	-2.81301100
N	2.11429800	-0.05849000	0.09606400
C	-0.89352800	3.82945700	-0.12123200
C	-1.13206900	3.62918900	1.38579300
H	-0.38929000	2.95898200	1.82906200
H	-1.06369800	4.59392800	1.90068700
H	-2.12822400	3.21822800	1.58207500
C	-1.97686900	4.78528900	-0.66237400
H	-1.93716400	5.73604700	-0.12034100
H	-1.84549900	5.01020900	-1.72594400
H	-2.98032400	4.36525100	-0.52826100
C	0.50075400	4.44930400	-0.33051500

H	0.70814900	4.66963600	-1.38296200
H	0.56702200	5.39565100	0.21679400
H	1.29658100	3.79903500	0.04939500
C	5.39969600	-1.85895500	-0.13605500
F	6.55331800	-1.36993200	-0.63563200
F	5.54409100	-1.96306700	1.20102600
F	5.25791200	-3.11275300	-0.62116400
Pd	0.16717000	0.14255500	1.18776300
C	-3.93449100	-1.75311500	-0.56868800
C	-3.48041800	-2.17957500	-1.82534800
C	-4.99617100	-2.45681900	0.02429800
C	-4.06397600	-3.27245100	-2.47296600
H	-2.66232500	-1.64580500	-2.30453700
C	-5.58141500	-3.54964300	-0.61804100
H	-5.37127100	-2.14886500	0.99691500
C	-5.11786400	-3.96238400	-1.87071500
H	-3.69537400	-3.58196500	-3.44753000
H	-6.40186200	-4.07901100	-0.14038800
H	-5.57471100	-4.81179900	-2.37114300
C	-2.59212900	-0.99939400	1.43783400
C	-3.28485500	-0.56186600	0.12548000
H	-3.37231800	-1.26385700	2.17198200
H	-2.50846500	-0.18457900	-0.55055400
C	-4.30174300	0.56974800	0.36438500
H	-3.82918000	1.44399100	0.82352900
H	-4.75714000	0.89360400	-0.57764600
H	-5.10795300	0.24274400	1.03072400
C	-1.66989400	0.02420800	2.10120900
C	-1.05689900	-0.47848500	3.39706300
H	-0.83369500	0.32019200	4.10512500
H	-2.12396900	1.00900100	2.21268300
H	-2.03587200	-1.92826500	1.25361700
O	0.28244700	-1.00461600	2.98810100
H	0.19178700	-1.95068900	2.78014900
H	-1.60631300	-1.27697200	3.90734800

76-s

B3LYP SCF energy in DMF: -1619.952414 a.u.

M06 SCF energy in DMF: -1619.351742 a.u.

M06 Free energy in DMF: -1618.909501 a.u.

C	2.65007700	-0.67921300	0.07324200
C	1.97870700	1.50442700	-0.28609600
C	3.28464700	1.97998900	-0.25679600
C	4.31323200	1.06328600	-0.03719600
C	3.98996000	-0.28001400	0.13562100
H	2.36289600	-1.71820900	0.19486400
H	3.49373900	3.03405000	-0.39437600
H	5.34436000	1.39578500	0.00249200
C	0.80120400	2.36948700	-0.45578200
N	-0.41450800	1.94590700	-0.29563100
C	-0.36674300	4.15736200	-1.07444200
C	-1.29604000	3.15468300	-0.36343900
H	-0.47947600	4.14583700	-2.16181200
H	-2.16810100	2.92313800	-0.97839000
O	0.98082500	3.64593900	-0.77750100
H	-0.41429500	5.17968600	-0.70604000
N	1.66837400	0.19831700	-0.13109400
C	-1.78641300	3.64231100	1.04153900
C	-2.60642300	2.53938100	1.72510000
H	-2.01470200	1.63267800	1.88314800
H	-2.95849900	2.88445300	2.70354500
H	-3.48595800	2.28175400	1.12875000
C	-2.70475700	4.86106000	0.81626900
H	-3.12660400	5.18834600	1.77254600
H	-2.17143600	5.71544900	0.38712900
H	-3.53931600	4.61338300	0.15023700
C	-0.61456000	4.04154000	1.95795200
H	-0.01277600	4.85418800	1.53896000
H	-1.00537200	4.39098500	2.91951300
H	0.04804900	3.19453100	2.16749500
C	5.06115100	-1.31935400	0.33879200

F	6.17922300	-0.78744600	0.87063300
F	4.64505100	-2.30693900	1.15960800
F	5.41253300	-1.90064100	-0.83053800
Pd	-0.46872400	-0.16604000	-0.61147000
C	-2.74131400	-2.30242200	0.58371900
C	-2.99297500	-3.68152800	0.52338400
C	-1.94855500	-1.82385000	1.64375800
C	-2.45579700	-4.55915300	1.47200500
H	-3.62431500	-4.07379200	-0.26988600
C	-1.41149500	-2.69598000	2.59278900
H	-1.76007400	-0.75706900	1.73424900
C	-1.65916100	-4.06986400	2.50769000
H	-2.66759200	-5.62262000	1.40115900
H	-0.80483400	-2.30130000	3.40375200
H	-1.24219600	-4.74832300	3.24672000
C	-2.32805700	-0.65179800	-1.38194300
C	-3.34846000	-1.34766000	-0.44808100
H	-2.77472800	0.22250600	-1.86393700
H	-3.96735600	-1.96804600	-1.11192600
C	-4.31331600	-0.35955100	0.22686400
H	-4.75421000	0.31987800	-0.51113100
H	-5.12985700	-0.90318700	0.71426800
H	-3.81303600	0.23860200	0.98894400
C	-1.64838200	-1.56662900	-2.40500600
H	-1.19624200	-0.95557100	-3.18948400
C	-2.39278700	-2.71979400	-3.05250800
H	-2.75730100	-3.45208700	-2.32780100
H	-3.25369700	-2.32926500	-3.60582900
H	-1.73660100	-3.22942500	-3.76549100
O	-0.45052600	-2.06436900	-1.64227000
H	-0.76231600	-2.76567000	-1.04073900

TS2 (M06)

M06/BS1 SCF energy in gas phase: -1618.899218 a.u.

M06/BS2 SCF energy in DMF: -1619.34322 a.u.

M06/BS2 Free energy in DMF: -1618.901635 a.u.

C	-2.34471800	-0.66949900	0.06463800
C	-0.60209400	-2.06502900	-0.48835000
C	-1.45417900	-3.11484900	-0.78849800
C	-2.82562100	-2.91215500	-0.64538000
C	-3.27188900	-1.67510800	-0.21231400
H	-2.66740700	0.31344700	0.40654900
H	-1.05002200	-4.06355200	-1.12823100
H	-3.53381200	-3.70432000	-0.87027600
C	0.85740200	-2.17000800	-0.58048000
N	1.64861500	-1.19038400	-0.31248200
C	2.81720100	-3.08899400	-1.01770300
C	3.02028200	-1.74729500	-0.29716800
H	3.06733800	-3.05038700	-2.08336800
H	3.68070400	-1.08799100	-0.87730100
O	1.38907700	-3.33395600	-0.91889700
H	3.32759800	-3.93703200	-0.55645600
N	-1.03867600	-0.86018900	-0.06600700
C	3.59742700	-1.86518900	1.13489500
C	3.70088200	-0.47804800	1.76476800
H	2.71385400	-0.01291000	1.88781100
H	4.16186600	-0.55112900	2.75687300
H	4.33276100	0.18758300	1.15934300
C	5.00787200	-2.44867900	1.02842200
H	5.46982500	-2.48813300	2.02152800
H	5.01865100	-3.47113400	0.63269500
H	5.65092700	-1.82922700	0.38959200
C	2.72688200	-2.75415600	2.02107500
H	2.64576000	-3.78164500	1.64500900
H	3.16513400	-2.81797600	3.02377600
H	1.71430100	-2.34457500	2.13555700
C	-4.72932700	-1.34740400	-0.03239500
F	-5.50699000	-2.37676800	-0.34816300
F	-4.97363700	-1.00299300	1.23244500
F	-5.06323100	-0.30971100	-0.80155200
Pd	0.57950400	0.67295600	0.00885100

C	-0.77631300	2.20512300	0.32986800
C	-1.44242700	2.64619600	-0.81908000
C	-1.42985100	2.21670000	1.56471400
C	-2.77271400	3.04785000	-0.73724200
H	-0.92575400	2.67266600	-1.77854100
C	-2.75902300	2.63323900	1.64031900
H	-0.91127500	1.89060000	2.46561200
C	-3.43191200	3.04188000	0.49125000
H	-3.29233600	3.37736500	-1.63369700
H	-3.26686600	2.63727400	2.60190700
H	-4.46665400	3.36785400	0.55415400
C	2.09180000	2.07916200	-0.23755900
C	1.21829500	2.95077000	0.46070500
H	2.94122900	1.67950500	0.32637400
H	0.81066300	3.77107800	-0.12970200
C	1.44762500	3.24932500	1.90771400
C	2.37336900	2.38117300	-1.69274100
H	1.40429800	2.53238800	-2.21123500
H	0.58974400	3.73068100	2.38257600
H	1.72011600	2.35287900	2.47662300
C	3.14843200	1.28232500	-2.39003500
H	2.57341400	0.34874900	-2.41926900
H	4.09841900	1.10672700	-1.86769900
H	2.29315300	3.94704200	1.96425500
H	3.38137800	1.56247600	-3.42378300
O	3.10357300	3.59137200	-1.65806600
H	3.37534900	3.82169100	-2.55379000

TS4 (M06)

M06/BS1 SCF energy in gas phase: -1618.897463 a.u.

M06/BS2 SCF energy in DMF: -1619.338854 a.u.

M06/BS2 Free energy in DMF: -1618.898153 a.u.

C	-2.65266600	-0.34479400	0.33999900
C	-1.10284300	-1.78186300	-0.56658700
C	-2.07812000	-2.67295000	-0.98032000
C	-3.40983500	-2.36794800	-0.70735400
C	-3.69414600	-1.19387300	-0.03263200
H	-2.86409000	0.59822500	0.83445500
H	-1.79383800	-3.58094500	-1.50312100
H	-4.21266700	-3.03205300	-1.01475900
C	0.32960700	-2.03255400	-0.74818300
N	1.22730000	-1.27393500	-0.22927100
C	2.16568000	-2.95947200	-1.54001400
C	2.52006500	-1.96139600	-0.42906000
H	2.38312100	-2.58221500	-2.54516400
H	3.26769200	-1.22879800	-0.76485100
O	0.71953500	-3.09521700	-1.43798800
H	2.60033500	-3.95411800	-1.42360400
N	-1.38326000	-0.62447800	0.07484700
C	3.03280100	-2.62113000	0.87802700
C	3.19196300	-1.56110400	1.96374700
H	2.23665300	-1.07183600	2.19492200
H	3.56697900	-2.02356900	2.88453300
H	3.91163400	-0.79256000	1.65763600
C	4.40552300	-3.22928200	0.58765500
H	4.82334100	-3.66410500	1.50310500
H	4.36580700	-4.03213100	-0.15880000
H	5.11041900	-2.46720000	0.22958800
C	2.07961800	-3.70356600	1.38413500
H	1.96032700	-4.53671400	0.68117300
H	2.47344300	-4.12823700	2.31483900
H	1.08607000	-3.29594900	1.61306200
C	-5.09323800	-0.76986900	0.31540600
F	-5.25378100	-0.73176400	1.63827400
F	-5.32808100	0.45943900	-0.15144800
F	-5.99829100	-1.59578400	-0.19722000
Pd	0.34503600	0.70915300	0.18489300
C	2.10977200	1.74736400	-0.14796300
C	2.30082100	2.01239000	-1.51003200
C	3.20991100	1.57385300	0.68908300
C	3.59001300	2.05652200	-2.03214900

H	1.44649100	2.18390300	-2.16495000
C	4.49837600	1.62795200	0.15964900
H	3.07171000	1.38378800	1.75171200
C	4.69031300	1.86690800	-1.19771600
H	3.73511100	2.25681500	-3.09110700
H	5.35358100	1.48726000	0.81749200
H	5.69666700	1.92078800	-1.60470600
C	-0.64843700	2.51654400	0.50163300
C	0.66069400	3.00584300	0.74812800
H	-1.26472200	2.30144900	1.38589900
H	1.03565600	3.72561200	0.01858100
C	1.12243600	3.23693400	2.15477900
H	2.19306400	3.44350900	2.21646000
H	0.59256500	4.11818600	2.53981900
H	0.88180100	2.39311400	2.81125500
C	-1.42149400	3.05813000	-0.67463200
H	-0.72954000	3.15941700	-1.53341100
C	-1.98951400	4.42865700	-0.33109800
H	-2.56241400	4.83369100	-1.17414400
H	-2.65790700	4.35508000	0.53491900
H	-1.19571800	5.14784400	-0.10023300
O	-2.45605900	2.14564900	-0.97644400
H	-3.08170900	2.57133100	-1.57271300

TS12 (M06)

M06/BS1 SCF energy in gas phase: -1618.896525 a.u.

M06/BS2 SCF energy in DMF: -1619.339198 a.u.

M06/BS2 Free energy in DMF: -1618.898568 a.u.

C	-2.25975100	-0.80190500	0.12329100
C	-0.54694000	-2.26684400	-0.33239600
C	-1.41207400	-3.34400400	-0.43841000
C	-2.77462300	-3.11566200	-0.25519800
C	-3.19904300	-1.82849700	0.02962300
H	-2.56874300	0.21740100	0.35075300
H	-1.02432500	-4.33262100	-0.66422800
H	-3.49394800	-3.92537300	-0.33919400
C	0.90562800	-2.38714500	-0.49340600
N	1.70343500	-1.38113400	-0.40865000
C	2.83923400	-3.35453000	-0.94208200
C	3.07798100	-1.92736400	-0.42307300
H	3.01024700	-3.45705400	-2.01891100
H	3.68663100	-1.34987200	-1.13385500
O	1.42487000	-3.58589500	-0.70769200
H	3.39216700	-4.13391100	-0.41394900
N	-0.96361900	-1.01404900	-0.05757900
C	3.76314100	-1.84808900	0.96357400
C	3.88504800	-0.38913600	1.39713300
H	2.90164400	0.07807900	1.53967700
H	4.42433700	-0.32668900	2.34956000
H	4.45194000	0.19856300	0.66157300
C	5.17221500	-2.42762100	0.82542000
H	5.71018400	-2.32502800	1.77479000
H	5.17268000	-3.49478000	0.57301600
H	5.75086000	-1.89617800	0.05859500
C	2.97906000	-2.62121200	2.02199400
H	2.88065400	-3.68740400	1.78279900
H	3.49749100	-2.55659900	2.98558300
H	1.97384300	-2.20351800	2.16653100
C	-4.64151100	-1.47112600	0.26199000
F	-5.45405400	-2.46747000	-0.07136300
F	-4.84339400	-1.17187900	1.54535900
F	-4.96752800	-0.39389300	-0.45627500
Pd	0.64742800	0.51720400	-0.30672700
C	-0.70365700	2.06156100	-0.10364100
C	-1.55233500	2.36446200	-1.17265800
C	-1.14922500	2.23006400	1.21080400
C	-2.85019900	2.80475100	-0.92674000
H	-1.20046300	2.25653800	-2.19891000
C	-2.45144200	2.66993900	1.44874800
H	-0.49165700	2.01138800	2.05144000
C	-3.30126300	2.95875600	0.38317300

H	-3.50676800	3.03675100	-1.76172700
H	-2.79807600	2.79192600	2.47227400
H	-4.31114600	3.31227400	0.57303400
C	2.20640500	1.78097200	-0.88345200
C	1.24253800	2.77831200	-0.59780600
H	2.98878300	1.64165300	-0.13403100
H	0.78922600	3.24779300	-1.47379100
C	1.49383500	3.72517800	0.56936200
C	2.57989800	1.46577900	-2.30226100
H	1.72570800	1.57605800	-2.98176900
H	3.36238900	2.16073000	-2.63645300
H	2.97768800	0.45109100	-2.41368900
H	1.36648000	3.17588900	1.52041700
C	0.59673200	4.94764400	0.53343100
H	0.76716400	5.49509200	-0.40135400
H	-0.46532400	4.69623900	0.60672600
H	0.83483800	5.61869500	1.36669400
O	2.84983900	4.09891300	0.40819000
H	3.02428300	4.86709800	0.96342100

TS16 (M06)

M06/BS1 SCF energy in gas phase: -1618.895649 a.u.

M06/BS2 SCF energy in DMF: -1619.337068 a.u.

M06/BS2 Free energy in DMF: -1618.89538 a.u.

C	2.67238800	-0.31062400	-0.38029400
C	1.18282500	-1.77367500	0.57952300
C	2.19282500	-2.61477600	1.01475300
C	3.51100100	-2.26688500	0.72862100
C	3.74801000	-1.10452600	0.01602100
H	2.84502700	0.61908800	-0.91363800
H	1.94531800	-3.51752800	1.56456300
H	4.33910000	-2.89024500	1.05370500
C	-0.23793200	-2.07481100	0.77674800
N	-1.17057300	-1.35713700	0.26090200
C	-2.02726800	-3.07557400	1.58785400
C	-2.43425100	-2.09126700	0.48155000
H	-2.25575800	-2.71131400	2.59528700
H	-3.20289900	-1.38899800	0.83431400
O	-0.57839800	-3.14760700	1.47721400
H	-2.41944800	-4.08787400	1.47101000
N	1.41596200	-0.62737400	-0.09817300
C	-2.94742800	-2.76704200	-0.81602800
C	-3.18755100	-1.70688300	-1.88627900
H	-2.25950900	-1.18681400	-2.15647100
H	-3.58756500	-2.17562100	-2.79333200
H	-3.91479300	-0.96026700	-1.54371300
C	-4.28122700	-3.44378500	-0.49686100
H	-4.69875800	-3.89216400	-1.40586300
H	-4.18535000	-4.24940700	0.24132200
H	-5.01400200	-2.71976700	-0.11723200
C	-1.95508900	-3.79774300	-1.35307900
H	-1.78030800	-4.62881800	-0.65902900
H	-2.34888500	-4.23473500	-2.27807900
H	-0.98788800	-3.34063400	-1.60063200
C	5.12976900	-0.62944600	-0.33605200
F	5.27993600	-0.56523500	-1.65912400
F	5.32643200	0.60017700	0.14865600
F	6.06602300	-1.43114300	0.15851400
Pd	-0.37559200	0.63176500	-0.25056800
C	-2.16375500	1.62235800	-0.02054100
C	-2.40828000	1.88920200	1.33175300
C	-3.22613600	1.51551000	-0.91795300
C	-3.71783600	2.00136000	1.78794700
H	-1.57816300	2.01503500	2.02797600
C	-4.53414500	1.64731300	-0.45607300
H	-3.03918700	1.33832300	-1.97655700
C	-4.78071000	1.88565600	0.89342700
H	-3.90867300	2.19680000	2.84060200
H	-5.36171600	1.56878800	-1.15781900
H	-5.80228000	1.99651000	1.24770500
C	0.55070800	2.48455100	-0.62660000

C	-0.75766100	2.92184300	-0.95613900
H	1.18009900	2.17247900	-1.47002200
C	1.31268400	3.08007100	0.53074200
H	0.60385400	3.29737000	1.35076100
C	2.01308700	4.36381800	0.10803400
H	2.57701700	4.79038800	0.94648400
H	2.71563200	4.15396500	-0.70691300
H	1.30631600	5.12807300	-0.23060900
O	2.26042500	2.11843100	0.95674100
H	2.86711400	2.54253200	1.57367300
C	-1.37739300	4.17231000	-0.39878600
H	-0.92153500	5.02423800	-0.92336600
H	-2.45547800	4.20446500	-0.57725300
H	-1.19917900	4.30285000	0.67200600
H	-1.06610600	2.70113300	-1.97966700

TS17 (M06)

M06/BS1 SCF energy in gas phase: -1618.897016 a.u.

M06/BS2 SCF energy in DMF: -1619.340461 a.u.

M06/BS2 Free energy in DMF: -1618.898558 a.u.

C	-2.32634500	-0.72150600	0.04946600
C	-0.57077700	-2.08828600	-0.53770000
C	-1.41423900	-3.13572700	-0.86883000
C	-2.78733200	-2.94718800	-0.72434700
C	-3.24469800	-1.72653200	-0.25700300
H	-2.65623800	0.24940000	0.41865800
H	-1.00186300	-4.07229400	-1.23146900
H	-3.48847400	-3.73846500	-0.97302600
C	0.89007900	-2.18458900	-0.61834700
N	1.67723200	-1.21582500	-0.30364400
C	2.85309200	-3.09000500	-1.06631200
C	3.04803700	-1.77714500	-0.29245100
H	3.11532900	-3.01010400	-2.12674700
H	3.71692900	-1.09748900	-0.83757600
O	1.42445000	-3.33658000	-0.99303800
H	3.35816600	-3.95626900	-0.63417700
N	-1.01855500	-0.89847000	-0.08658000
C	3.60860600	-1.94884500	1.14016300
C	3.71162200	-0.58427400	1.81763100
H	2.72370400	-0.12801900	1.96496500
H	4.17898700	-0.68870000	2.80381700
H	4.33688300	0.10368000	1.23027100
C	5.01814600	-2.53360800	1.02798000
H	5.46990300	-2.60923700	2.02366500
H	5.02999800	-3.54179300	0.59716400
H	5.66955400	-1.89471000	0.41733900
C	2.72564900	-2.86328600	1.98693900
H	2.65065500	-3.87943100	1.58029100
H	3.14918200	-2.95585800	2.99376300
H	1.71137900	-2.45688200	2.09807600
C	-4.70602200	-1.41877000	-0.07257700
F	-5.47119100	-2.45015800	-0.41208600
F	-4.95684100	-1.10476400	1.19866100
F	-5.05044600	-0.36902000	-0.82038000
Pd	0.57309200	0.63726900	0.06820800
C	-0.80513000	2.11798900	0.42512300
C	-1.47518500	2.55704300	-0.72171300
C	-1.44069000	2.16123600	1.66931500
C	-2.79139200	2.99920600	-0.62654500
H	-0.97391200	2.55005500	-1.68960300
C	-2.75452900	2.62035600	1.75801800
H	-0.91572300	1.83847600	2.56802600
C	-3.43063000	3.03397200	0.61228900
H	-3.31786200	3.32391000	-1.52086200
H	-3.24732600	2.65766100	2.72665000
H	-4.45365300	3.39328900	0.68540800
C	2.07836200	2.09716500	-0.01724500
C	1.17274200	2.91530200	0.70316300
H	2.85403800	1.60343100	0.57516500
C	2.50131500	2.48523700	-1.41536900
H	1.59533900	2.72679100	-2.00720900

C	3.26911400	1.38597500	-2.12203200
H	2.64694600	0.49359200	-2.26459500
H	4.15961000	1.11799500	-1.53772900
H	3.60524900	1.72007100	-3.11041900
O	3.29981300	3.63910100	-1.23992400
H	3.64183800	3.91783600	-2.09689400
H	1.18139500	2.76603000	1.78518000
C	0.80078000	4.30385700	0.28071200
H	-0.06277300	4.67900900	0.83616300
H	1.67345100	4.93411600	0.49636700
H	0.60507100	4.38946100	-0.79066200

TS21-s (M06)

M06/BS1 SCF energy in gas phase: -1618.896118 a.u.

M06/BS2 SCF energy in DMF: -1619.339002 a.u.

M06/BS2 Free energy in DMF: -1618.89593 a.u.

C	-2.09399600	-1.09787300	0.15689200
C	-0.22198000	-2.27747600	-0.47760700
C	-0.95686700	-3.42028500	-0.74993100
C	-2.33543500	-3.37889400	-0.55256100
C	-2.90583300	-2.20399500	-0.09107200
H	-2.51415800	-0.15977600	0.51934000
H	-0.45755500	-4.31435400	-1.11049800
H	-2.95817400	-4.24461800	-0.75966400
C	1.23436500	-2.20764100	-0.63439900
N	1.92092700	-1.15719500	-0.34904000
C	3.24978800	-2.85720100	-1.26233700
C	3.34487100	-1.53400500	-0.48416900
H	3.40958100	-2.73797200	-2.33918400
H	3.86142100	-0.76681800	-1.07989600
O	1.87438900	-3.28026400	-1.07588200
H	3.89511000	-3.65560800	-0.88980400
N	-0.78190600	-1.13310700	-0.03683500
C	4.06935700	-1.63715200	0.87970000
C	4.02956300	-0.28223200	1.58212000
H	3.00190900	0.01049400	1.83247700
H	4.59987700	-0.32577400	2.51738900
H	4.48381300	0.50147900	0.95865200
C	5.53067300	-1.99947900	0.60985000
H	6.09130800	-2.01450900	1.55141700
H	5.64694100	-2.99020600	0.15427100
H	6.01081700	-1.26408700	-0.04907000
C	3.42671900	-2.68508500	1.78600500
H	3.44993100	-3.69349700	1.35527800
H	3.97302800	-2.73412400	2.73519900
H	2.38605600	-2.43214300	2.02662500
C	-4.37896500	-2.07013900	0.18200000
F	-5.06407800	-3.08584000	-0.33351600
F	-4.60318500	-2.03378100	1.49522600
F	-4.84476800	-0.93293700	-0.33798000
Pd	0.62047000	0.58180000	-0.00405200
C	-0.93249800	1.89962700	0.18154200
C	-1.64346300	2.10245100	-1.00334300
C	-1.56087700	2.03171900	1.41907400
C	-3.00254500	2.39583500	-0.94499400
H	-1.14489900	2.02049900	-1.96994600
C	-2.92170500	2.33089600	1.46725400
H	-0.99719400	1.90718600	2.34273500
C	-3.64162800	2.50853600	0.28886800
H	-3.56379900	2.53800700	-1.86561900
H	-3.41525900	2.43452200	2.43067200
H	-4.70197800	2.74339800	0.33044600
C	2.02437500	2.13774500	-0.21202500
C	0.99259700	2.96307400	0.28453800
C	2.74830200	1.80114600	0.53415200
H	2.52448100	2.18648000	-1.62805200
H	1.72487600	2.39490900	-2.34826800
H	0.93728200	3.06489400	1.37094800
C	0.51174400	4.21052700	-0.42126800
H	0.25595700	3.97631400	-1.47072600
C	1.64840900	5.22983400	-0.38860400

H	2.53427000	4.89389900	-0.93586400
H	1.31501900	6.16747800	-0.84839400
H	1.93023900	5.44427000	0.64840000
O	-0.59767700	4.70053100	0.28356300
H	-0.85019400	5.55077700	-0.09042500
H	3.29520500	2.95976300	-1.75203900
H	2.98517600	1.23304700	-1.91101700

Pd₂dba₃

B3LYP SCF energy in DMF: -2450.37728 a.u.

M06 SCF energy in DMF: -2449.240202 a.u.

M06 Free energy in DMF: -2448.54958 a.u.

C	-2.36545200	0.51582800	2.17742600
C	1.68532900	2.08160000	-0.95364700
C	2.35156700	-2.25816900	-0.54506900
C	-5.45227100	4.08293100	-0.23440000
C	-4.33146200	4.40750500	0.53344100
C	-5.34751200	3.09114100	-1.21610500
C	-2.99986700	2.74351300	-0.66045800
C	-4.13984300	2.42835200	-1.42811800
C	-3.12112300	3.74611100	0.32216900
C	1.01610500	-2.09075900	-0.82054200
C	-0.02731000	-2.52984000	0.15781600
C	-1.45494600	-2.31627400	-0.15588200
C	-1.96258900	-1.89377500	-1.38742200
C	-1.03073800	0.18356500	2.19265700
C	-5.92109300	-0.56224700	2.77355000
C	-5.76616300	-1.87980200	3.21202300
C	-4.80171500	0.19742300	2.43621000
C	-3.36279900	-1.67387600	2.97598600
C	-3.50436300	-0.34593400	2.52201700
C	-4.48248500	-2.42916800	3.31574800
C	0.01284400	1.25433000	2.16184000
C	6.03964800	-1.36512500	3.28512900
C	5.72494500	-0.06735800	2.86686300
C	5.02901700	-2.32671700	3.35893200
C	3.38565700	-0.69160000	2.59050100
C	3.71839800	-1.99293900	3.01536100
C	4.41698800	0.26757100	2.52209400
C	1.44784500	0.88665300	2.12091200
C	5.59024300	3.84361600	-0.53948600
C	4.49575700	4.33625500	0.17540300
C	5.41367200	2.75841300	-1.40516200
C	3.04765600	2.64840500	-0.83370000
C	4.16089800	2.16633100	-1.55256900
C	3.24022200	3.74659900	0.02795100
C	1.97546200	-0.39881800	2.25778000
C	5.70826700	-2.03566900	-3.20217600
C	4.42264800	-1.78727900	-3.69806600
C	5.87950900	-2.34893000	-1.85164700
C	3.47540500	-2.15264100	-1.48542000
C	4.77430900	-2.40959000	-1.00335600
C	3.31720300	-1.84407600	-2.85320600
C	-1.68262400	2.09104500	-0.83631400
C	-6.03063500	-2.22206500	-2.74009300
C	-5.72173400	-2.52580900	-1.40954300
C	-5.01231500	-1.81939200	-3.60801400
C	-3.37467800	-2.01129900	-1.80791100
C	-3.69998500	-1.71760500	-3.14727500
C	-4.41172600	-2.42282700	-0.94630400
C	-1.36371500	1.24287700	-1.89961900
C	-0.04397000	0.80718100	-2.44113200
C	1.30517700	1.13098700	-1.90514000
O	-0.30052600	2.45279000	2.19573000
O	-0.07397400	0.09482300	-3.46147300
O	0.28359100	-3.07637900	1.22672600
Pd	-1.64441200	-0.05526800	-0.09686000
Pd	1.62518900	0.05550200	0.04651600
H	-5.23823300	-1.58881000	-4.64542300
H	-7.05359800	-2.30413500	-3.09610400
H	-6.50581900	-2.84713600	-0.72948800

H	-4.19724100	-2.66678900	0.08920900
H	-2.90991600	-1.40924000	-3.82683400
H	-1.28071900	-1.71169200	-2.21289000
H	-2.11965200	-2.74804300	0.58630700
H	0.69340700	-1.83716500	-1.82329700
H	2.60440100	-2.64991300	0.43640100
H	2.32957300	-1.64697000	-3.25741700
H	4.28253600	-1.55236200	-4.74952000
H	6.56646800	-1.99139300	-3.86657100
H	6.87221000	-2.55106200	-1.45956100
H	4.90878000	-2.66051500	0.04546400
H	-6.39538900	4.59768700	-0.07451500
H	-6.21194100	2.83416600	-1.82248900
H	-4.08808500	1.66461300	-2.19789100
H	-2.25337900	3.99837300	0.92514500
H	-4.39646200	5.17899200	1.29600800
H	-0.90052700	2.53672500	-0.23499800
H	-2.14592000	1.00007400	-2.61390400
H	0.93254100	2.67442100	-0.44841800
H	2.06653900	0.74974500	-2.57991400
H	2.39117100	4.14115900	0.58008400
H	4.61691900	5.18377200	0.84436600
H	6.56881900	4.30202700	-0.42919900
H	6.25706100	2.37281600	-1.97146300
H	4.05170000	1.32612700	-2.23085600
H	-6.63602900	-2.47262200	3.48002300
H	-6.91248000	-0.12433600	2.69980000
H	-4.92315300	1.22445300	2.10222600
H	-4.35526200	-3.44857800	3.66925400
H	-2.37497100	-2.11292300	3.07303600
H	-2.60529000	1.56789100	2.04720500
H	-0.71721200	-0.82230700	2.44833500
H	2.09826800	1.75082400	2.22548700
H	1.30474200	-1.23951200	2.41156400
H	2.93556600	-2.74374800	3.08197500
H	5.25874200	-3.33650100	3.68780800
H	7.06073600	-1.62095100	3.55324800
H	6.50335400	0.68876300	2.81045100
H	4.19935200	1.28150900	2.20113700

PyrOx

B3LYP SCF energy in DMF: -988.7051501 a.u.

M06 SCF energy in DMF: -988.3809406 a.u.

M06 Free energy in DMF: -988.1614726 a.u.

C	2.18451300	-1.05400000	-0.31205300
C	0.37856900	0.35556400	-0.20290600
C	1.18246500	1.44370600	0.15387000
C	2.55510500	1.24780100	0.27400300
C	3.06840900	-0.02539100	0.03697800
H	2.55756100	-2.05817700	-0.49628900
H	0.74230400	2.41632400	0.33359300
H	3.20808100	2.06877500	0.54945000
C	-1.08906200	0.51757900	-0.34459900
N	-1.91761600	-0.40521100	-0.64782900
C	-3.00594300	1.68806200	-0.26479400
C	-3.26038600	0.21058800	-0.67323100
H	-3.31243800	2.40726100	-1.02698000
H	-3.62626300	0.16869400	-1.70751200
O	-1.55882900	1.77344400	-0.12318200
H	-3.44939600	1.97157900	0.69277100
N	0.87021100	-0.87569500	-0.43186400
C	-4.28886600	-0.57109900	0.19683000
C	-4.45408800	-1.98395600	-0.39244700
H	-3.50976600	-2.53608500	-0.37544200
H	-5.19243100	-2.55614400	0.18048500
H	-4.79987300	-1.94102900	-1.43225400
C	-5.64245200	0.16124800	0.13338800
H	-6.40400200	-0.39521800	0.69115600
H	-5.58792300	1.16571500	0.56790600
H	-5.99361600	0.26058200	-0.90056500
C	-3.81838400	-0.68059100	1.65755200

H	-3.69998400	0.30085700	2.13021100
H	-4.55075300	-1.23976600	2.25031900
H	-2.86047700	-1.20635400	1.72706400
C	4.54556400	-0.28861900	0.10172000
F	5.17049800	0.54334100	0.96373500
F	4.81677700	-1.55383000	0.49356600
F	5.14036700	-0.11990800	-1.10468800

PhN₂⁺

B3LYP SCF energy in DMF: -340.943213 a.u.

M06 SCF energy in DMF: -340.7597225 a.u.

M06 Free energy in DMF: -340.6907705 a.u.

C	0.09435000	-1.24527100	0.00001500
C	2.16538100	0.00001900	-0.00013000
C	1.47980800	1.22209600	-0.00007200
C	0.09432500	1.24525100	0.00003300
C	-0.56314100	-0.00000800	0.00003000
H	-0.47330600	-2.16806900	0.00002900
H	2.02827300	2.15716400	-0.00010400
H	-0.47332700	2.16805100	0.00010400
H	3.25060100	0.00000900	-0.00021500
C	1.47981700	-1.22208500	-0.00007800
H	2.02833100	-2.15712400	-0.00009800
N	-1.93389600	-0.00002400	0.00005400
N	-3.04664900	0.00001800	0.00016000

dba

B3LYP SCF energy in DMF: -731.4842219 a.u.

M06 SCF energy in DMF: -731.0825859 a.u.

M06 Free energy in DMF: -730.8709009 a.u.

C	-2.35142200	1.01794900	0.00003800
C	-1.04362700	0.68863200	0.00072200
C	-5.93273300	-0.12050300	-0.00070600
C	-5.80327300	-1.51072700	-0.00026500
C	-4.79489100	0.68464200	-0.00061200
C	-3.39191500	-1.28666400	0.00035900
C	-3.50515000	0.11886000	-0.00006900
C	-4.52850300	-2.08915100	0.00026300
C	-0.00726000	1.74930100	0.00081700
C	6.05806900	-1.03563600	-0.00042100
C	5.73156300	0.32543200	-0.00019300
C	5.04031000	-1.99134000	-0.00043100
C	3.36057200	-0.22261100	0.00002300
C	3.70594900	-1.58796000	-0.00021500
C	4.40045000	0.72973600	0.00002700
C	1.42459600	1.38586400	0.00067200
C	1.94016700	0.13787600	0.00026500
O	-0.31212800	2.94907600	-0.00010200
H	-6.68739300	-2.14167400	-0.00033900
H	-6.91818600	0.33614600	-0.00112100
H	-4.89601100	1.76671900	-0.00095200
H	-4.42350200	-3.17028200	0.00059400
H	-2.41090400	-1.75134600	0.00075600
H	-2.58551500	2.08154900	-0.00045500
H	-0.72895000	-0.34906900	0.00127800
H	2.07719700	2.25552300	0.00076900
H	1.26597000	-0.71526900	0.00008800
H	2.91567200	-2.33422200	-0.00022400
H	5.28473200	-3.04961100	-0.00060900
H	7.09896300	-1.34581700	-0.00059600
H	6.51992000	1.07273800	-0.00019900
H	4.16761000	1.79880900	0.00017700

N₂

B3LYP SCF energy in DMF: -109.5184114 a.u.

M06 SCF energy in DMF: -109.4845892 a.u.

M06 Free energy in DMF: -109.4974292 a.u.

N	0.00000000	0.00000000	0.55248900
N	0.00000000	0.00000000	-0.55248900

(E)-(S)-sub1

B3LYP SCF energy in DMF: -271.7743709 a.u.

M06 SCF energy in DMF: -271.6410306 a.u.

M06 Free energy in DMF: -271.5315136 a.u.

C	-0.36229000	-0.04457400	-0.29028700
C	-1.49487500	0.00112000	0.41611200
H	-0.40000500	-0.06218200	-1.38109000
H	-1.43084400	0.01291700	1.50579300
C	-2.87802400	0.04205100	-0.16240700
C	1.01722100	-0.05502200	0.30877500
H	0.92803700	-0.07413500	1.40656600
H	-3.41508700	0.94384900	0.15968300
H	-2.86231000	0.02754100	-1.25685500
C	1.82617300	1.17963500	-0.09818800
H	1.35027500	2.09713800	0.26334200
H	1.91473900	1.24060300	-1.18840300
H	-3.47520500	-0.81197400	0.18316400
H	2.83710500	1.13642400	0.32599700
O	1.66467100	-1.25541600	-0.15072800
H	2.58669900	-1.20611400	0.14359900

(E)-(R)-sub1

B3LYP SCF energy in DMF: -271.7743709 a.u.

M06 SCF energy in DMF: -271.6410306 a.u.

M06 Free energy in DMF: -271.5315136 a.u.

C	-0.36229000	-0.04457400	0.29028700
C	-1.49487500	0.00112000	-0.41611200
H	-0.40000500	-0.06218200	1.38109000
H	-1.43084400	0.01291700	-1.50579300
C	-2.87802400	0.04205100	0.16240700
C	1.01722100	-0.05502200	-0.30877500
C	0.92803700	-0.07413500	-1.40656600
H	-3.41508700	0.94384900	-0.15968300
H	-2.86231000	0.02754100	1.25685500
C	1.82617300	1.17963500	0.09818800
H	1.35027500	2.09713800	-0.26334200
H	1.91473900	1.24060300	1.18840300
H	-3.47520500	-0.81197400	-0.18316400
H	2.83710500	1.13642400	-0.32599700
O	1.66467100	-1.25541600	0.15072800
H	2.58669900	-1.20611400	-0.14359900

1a

B3LYP SCF energy in DMF: -502.8681659 a.u.

M06 SCF energy in DMF: -502.6002448 a.u.

M06 Free energy in DMF: -502.4175868 a.u.

C	1.00019700	-0.20755800	0.12547100
C	1.79212600	-1.13841500	-0.56158500
C	1.59497100	1.00107000	0.52319600
C	3.13512000	-0.87560300	-0.84458400
H	1.35076400	-2.08086500	-0.87731500
C	2.93572100	1.26874100	0.24177800
H	1.00583500	1.74097200	1.05878000
C	3.71249700	0.33041800	-0.44364800
H	3.72833400	-1.61410200	-1.37732900
H	3.37494500	2.21094700	0.55871800
H	4.75628600	0.53810200	-0.66196700
C	-1.40040300	0.46977800	-0.30517900
C	-0.46170500	-0.51021800	0.42497900
H	-1.36921900	1.46880500	0.14756400
H	-0.67967200	-1.50928100	0.03305900
C	-0.74370400	-0.52971300	1.93822000
H	-1.78673200	-0.79737900	2.13279700
H	-0.10734700	-1.26200700	2.44626300
H	-0.55610800	0.44978700	2.39218900
C	-2.84970000	0.01199800	-0.39533000
C	-3.86066300	1.07459300	-0.76569500
H	-4.81917300	0.61798000	-1.02059500

H	-4.00115600	1.74932100	0.08819000
H	-3.50166000	1.68761600	-1.59936800
O	-3.18134500	-1.14768200	-0.20017400
H	-1.07107800	0.61101000	-1.34532900

1b

B3LYP SCF energy in DMF: -502.8681659 a.u.

M06 SCF energy in DMF: -502.6002448 a.u.

M06 Free energy in DMF: -502.4175868 a.u.

C	1.00019700	-0.20755800	-0.12547100
C	1.79212600	-1.13841500	0.56158500
C	1.59497100	1.00107000	-0.52319600
C	3.13512000	-0.87560300	0.84458400
H	1.35076400	-2.08086500	0.87731500
C	2.93572100	1.26874100	-0.24177800
H	1.00583500	1.74097200	-1.05878000
C	3.71249700	0.33041800	0.44364800
H	3.72833400	-1.61410200	1.37732900
H	3.37494500	2.21094700	-0.55871800
H	4.75628600	0.53810200	0.66196700
C	-1.40040300	0.46977800	0.30517900
C	-0.46170500	-0.51021800	-0.42497900
H	-1.36921900	1.46880500	-0.14756400
H	-0.67967200	-1.50928100	-0.03305900
C	-0.74370400	-0.52971300	-1.93822000
H	-1.78673200	-0.79737900	-2.13279700
H	-0.10734700	-1.26200700	-2.44626300
H	-0.55610800	0.44978700	-2.39218900
C	-2.84970000	0.01199800	0.39533000
C	-3.86066300	1.07459300	0.76569500
H	-4.81917300	0.61798000	1.02059500
H	-4.00115600	1.74932100	-0.08819000
H	-3.50166000	1.68761600	1.59936800
O	-3.18134500	-1.14768200	0.20017400
H	-1.07107800	0.61101000	1.34532900

1c

B3LYP SCF energy in DMF: -502.8384586 a.u.

M06 SCF energy in DMF: -502.5708877 a.u.

M06 Free energy in DMF: -502.3864677 a.u.

C	-1.04902300	0.15548400	0.00436400
C	-2.05323600	1.05340500	-0.40411400
C	-1.45081800	-1.12489500	0.43223400
C	-3.39745900	0.67817100	-0.41233200
H	-1.78383800	2.05198400	-0.73287400
C	-2.79350700	-1.49941600	0.42581200
H	-0.70604200	-1.82588800	0.79622000
C	-3.77545500	-0.60071600	0.00030500
H	-4.15004200	1.38933800	-0.74190400
H	-3.07473900	-2.49211600	0.76670100
H	-4.82225000	-0.89077900	0.00047000
C	1.35588000	-0.35275400	-0.21670900
C	0.38585500	0.55923300	-0.00958200
H	1.07392200	-1.38914700	-0.39168500
C	0.69241100	2.02696800	0.19345700
C	2.84017300	-0.06607200	-0.24944400
H	3.02245800	0.82512200	-0.86951700
H	0.47925300	2.61233200	-0.71023200
H	0.07564700	2.44720500	0.99526900
C	3.62849700	-1.23285000	-0.84090500
H	3.31711600	-1.43262800	-1.87233300
H	3.47249400	-2.14217000	-0.25020900
H	1.73829000	2.18069200	0.46047500
H	4.70136800	-1.00944400	-0.85314400
O	3.26813500	0.20846000	1.10162500
H	4.21137900	0.42847600	1.05125500

1d

B3LYP SCF energy in DMF: -502.8444579 a.u.

M06 SCF energy in DMF: -502.5771751 a.u.

M06 Free energy in DMF: -502.3947861 a.u.

C	-0.89791700	0.26558100	-0.24228900
C	-1.50595200	-0.70805400	-1.04704100
C	-1.58177900	0.69493900	0.90695500
C	-2.75666200	-1.23869300	-0.71925800
H	-0.99320000	-1.05467200	-1.94126400
C	-2.83085500	0.16777600	1.23856100
H	-1.13418100	1.44757100	1.55071300
C	-3.42482100	-0.80244700	0.42602600
H	-3.20727700	-1.99205200	-1.36006300
H	-3.34172700	0.51497400	2.13280700
H	-4.39727400	-1.21240600	0.68403600
C	1.51940000	0.44743000	0.41769000
C	0.47541600	0.82878800	-0.61005100
H	1.43653600	0.89842200	1.40311900
H	0.76179800	0.37751200	-1.56500900
C	0.42757000	2.35828500	-0.80680600
H	1.40014800	2.73090300	-1.14623200
H	-0.32452700	2.63715600	-1.55332000
H	0.18140900	2.87561000	0.12701300
C	2.53572800	-0.40485400	0.21567800
C	3.56369000	-0.76293800	1.24872600
H	3.55515800	-1.84189000	1.45237500
H	4.57341900	-0.50711600	0.90059900
H	3.38269200	-0.23496500	2.18735500
O	2.68447600	-1.01937600	-1.00647900
H	3.48831500	-1.55891900	-0.98944500

(Z)-(S)-sub1

B3LYP SCF energy in DMF: -271.7717754 a.u.

M06 SCF energy in DMF: -271.6388996 a.u.

M06 Free energy in DMF: -271.5297446 a.u.

C	0.28522200	-0.34352700	0.73804600
C	1.61040900	-0.23327400	0.58611800
H	-0.10128400	-0.70463300	1.69174700
C	-0.78875900	-0.00183800	-0.25964000
H	-0.34444100	0.18755500	-1.24654300
C	-1.57985800	1.23941800	0.16630300
H	-0.93357100	2.12263500	0.20527700
H	-2.02672300	1.09219600	1.15560600
H	-2.38682500	1.44570100	-0.54781700
O	-1.65185500	-1.15142200	-0.33180700
H	-2.38755000	-0.91181700	-0.91514000
H	2.23394400	-0.51249900	1.43628900
C	2.37046300	0.23913600	-0.61968600
H	2.94991000	1.14126900	-0.38290500
H	3.09881900	-0.51858400	-0.93631100
H	1.72770700	0.47005200	-1.47259700

(Z)-(R)-sub1

B3LYP SCF energy in DMF: -271.7717754 a.u.

M06 SCF energy in DMF: -271.6388996 a.u.

M06 Free energy in DMF: -271.5297446 a.u.

C	0.28522200	-0.34352700	-0.73804600
C	1.61040900	-0.23327400	-0.58611800
H	-0.10128400	-0.70463300	-1.69174700
C	-0.78875900	-0.00183800	0.25964000
H	-0.34444100	0.18755500	1.24654300
C	-1.57985800	1.23941800	-0.16630300
H	-0.93357100	2.12263500	-0.20527700
H	-2.02672300	1.09219600	-1.15560600
H	-2.38682500	1.44570100	0.54781700
O	-1.65185500	-1.15142200	0.33180700
H	-2.38755000	-0.91181700	0.91514000
H	2.23394400	-0.51249900	-1.43628900
C	2.37046300	0.23913600	0.61968600
H	2.94991000	1.14126900	0.38290500
H	3.09881900	-0.51858400	0.93631100
H	1.72770700	0.47005200	1.47259700

DMF H⁺

B3LYP SCF energy in DMF: -248.9727722 a.u.

M06 SCF energy in DMF: -248.85724 a.u.

M06 Free energy in DMF: -248.769948 a.u.

N	-0.38140200	-0.02989600	0.00000000
C	-0.48550600	1.43591100	0.00000300
H	0.50369700	1.88737600	-0.00004800
H	-1.03652800	1.74142200	-0.89217900
H	-1.03644400	1.74142800	0.89223400
C	-1.64690000	-0.77665800	0.00001400
H	-1.44840500	-1.84792000	0.00004900
H	-2.21379300	-0.50151800	0.89210000
H	-2.21377300	-0.50157200	-0.89210200
C	0.74725000	-0.65774600	-0.00001700
H	0.75511800	-1.74476600	-0.00002200
O	1.87996700	0.00532100	-0.00000800
H	2.63114700	-0.61678400	0.00003700

(E)-sub2

B3LYP SCF energy in DMF: -271.7704678 a.u.

M06 SCF energy in DMF: -271.636863 a.u.

M06 Free energy in DMF: -271.527322 a.u.

C	-0.50412100	-0.00242000	0.32413900
C	-1.71344700	0.38006400	-0.09864000
H	-0.36576300	-1.02344500	0.68097300
C	0.71973200	0.87283000	0.34326600
H	0.48106000	1.86604300	-0.05545800
C	1.89252200	0.30121300	-0.45395400
H	1.58513400	0.13333600	-1.49741600
H	1.06338200	1.01607500	1.37825800
O	2.30612600	-0.92058500	0.16042200
H	2.98571600	-1.31255400	-0.40608200
H	2.71571600	1.03246500	-0.46569700
H	-1.84460300	1.40323700	-0.45706400
C	-2.93774500	-0.48782200	-0.12412900
H	-3.74116300	-0.06193700	0.49162000
H	-2.72692600	-1.49704100	0.24441300
H	-3.34320500	-0.57469200	-1.14101100

2a

B3LYP SCF energy in DMF: -502.8565174 a.u.

M06 SCF energy in DMF: -502.5897462 a.u.

M06 Free energy in DMF: -502.4058942 a.u.

C	-0.91564100	0.42713400	-0.16357800
C	-1.72515900	0.00354400	-1.22715200
C	-1.27978300	0.04163800	1.13754800
C	-2.86290500	-0.77710900	-1.00418500
H	-1.46160600	0.29072800	-2.24243700
C	-2.41426200	-0.73872400	1.36530900
H	-0.67160600	0.35498000	1.98216300
C	-3.21217800	-1.15134800	0.29433000
H	-3.47421700	-1.09184200	-1.84582400
H	-2.67645400	-1.02452000	2.38056200
H	-4.09592700	-1.75784000	0.47174600
C	1.62326400	0.62979600	0.05928500
C	0.31262100	1.29416100	-0.41695900
H	1.57736400	0.45504600	1.14079000
H	0.38998200	1.43437000	-1.50334600
C	0.15434600	2.68640200	0.22084600
H	1.00844200	3.32594600	-0.02895900
H	-0.75458600	3.18366200	-0.13382700
H	0.09564800	2.62067400	1.31304200
C	1.94893200	-0.68161700	-0.65278000
C	3.23035800	-1.33409100	-0.21435200
H	1.15430200	-1.43054200	-0.51776500
O	3.97642300	-0.90878100	0.64803200
H	3.47297800	-2.27908200	-0.74799800
H	2.01927500	-0.54523100	-1.74303300

H	2.44747300	1.33517800	-0.09924400
---	------------	------------	-------------

2b

B3LYP SCF energy in DMF: -502.8565174 a.u.

M06 SCF energy in DMF: -502.5897462 a.u.

M06 Free energy in DMF: -502.4058942 a.u.

C	-0.91564100	0.42713400	0.16357800
C	-1.72515900	0.00354400	1.22715200
C	-1.27978300	0.04163800	-1.13754800
C	-2.86290500	-0.77710900	1.00418500
H	-1.46160600	0.29072800	2.24243700
C	-2.41426200	-0.73872400	-1.36530900
H	-0.67160600	0.35498000	-1.98216300
C	-3.21217800	-1.15134800	-0.29433000
H	-3.47421700	-1.09184200	1.84582400
H	-2.67645400	-1.02452000	-2.38056200
H	-4.09592700	-1.75784000	-0.47174600
C	1.62326400	0.62979600	-0.05928500
C	0.31262100	1.29416100	0.41695900
H	1.57736400	0.45504600	-1.14079000
H	0.38998200	1.43437000	1.50334600
C	0.15434600	2.68640200	-0.22084600
H	1.00844200	3.32594600	0.02895900
H	-0.75458600	3.18366200	0.13382700
H	0.09564800	2.62067400	-1.31304200
C	1.94893200	-0.68161700	0.65278000
C	3.23035800	-1.33409100	0.21435200
H	1.15430200	-1.43054200	0.51776500
O	3.97642300	-0.90878100	-0.64803200
H	3.47297800	-2.27908200	0.74799800
H	2.01927500	-0.54523100	1.74303300
H	2.44747300	1.33517800	0.09924400

2c

B3LYP SCF energy in DMF: -502.8541351 a.u.

M06 SCF energy in DMF: -502.5885064 a.u.

M06 Free energy in DMF: -502.4055934 a.u.

C	-0.33365100	0.17648200	0.10559300
C	-1.13564600	-0.02008900	1.23845400
C	-0.91574000	-0.00905700	-1.15926200
C	-2.47788000	-0.39077800	1.11710600
H	-0.70291600	0.11779200	2.22638200
C	-2.25586800	-0.37715400	-1.28501100
H	-0.31695500	0.13539000	-2.05488700
C	-3.04320300	-0.57025600	-0.14614900
H	-3.07899500	-0.53890800	2.01016200
H	-2.68624000	-0.51436200	-2.27339600
H	-4.08609900	-0.85830900	-0.24418300
C	2.07116400	-0.51693300	-0.32163900
C	1.13151200	0.57364000	0.25156700
H	3.11052800	-0.17584800	-0.20294900
H	1.34182200	0.65319500	1.32656900
C	1.45136200	1.94544900	-0.38380500
H	2.52855700	2.12473800	-0.27570500
H	1.25450600	1.90119600	-1.46264200
C	1.96056600	-1.82318600	0.42018500
O	1.80564000	-2.91131700	-0.10012300
H	1.89157800	-0.69054200	-1.38700400
C	0.68064300	3.11380300	0.23447800
H	-0.40007200	3.01041900	0.09129800
H	0.98453600	4.06295400	-0.22026900
H	0.86820900	3.18761000	1.31231500
H	2.04686900	-1.73631700	1.52618800

2d

B3LYP SCF energy in DMF: -502.8541351 a.u.

M06 SCF energy in DMF: -502.5885064 a.u.

M06 Free energy in DMF: -502.4055934 a.u.

C	-0.33365100	0.17648200	-0.10559300
---	-------------	------------	-------------

C	-1.13564600	-0.02008900	-1.23845400
C	-0.91574000	-0.00905700	1.15926200
C	-2.47788000	-0.39077800	-1.11710600
H	-0.70291600	0.11779200	-2.22638200
C	-2.25586800	-0.37715400	1.28501100
H	-0.31695500	0.13539000	2.05488700
C	-3.04320300	-0.57025600	0.14614900
H	-3.07899500	-0.53890800	-2.01016200
H	-2.68624000	-0.51436200	2.27339600
H	-4.08609900	-0.85830900	0.24418300
C	2.07116400	-0.51693300	0.32163900
C	1.13151200	0.57364000	-0.25156700
H	3.11052800	-0.17584800	0.20294900
H	1.34182200	0.65319500	-1.32656900
C	1.45136200	1.94544900	0.38380500
H	2.52855700	2.12473800	0.27570500
H	1.25450600	1.90119600	1.46264200
C	1.96056600	-1.82318600	-0.42018500
O	1.80564000	-2.91131700	0.10012300
H	1.89157800	-0.69054200	1.38700400
C	0.68064300	3.11380300	-0.23447800
H	-0.40007200	3.01041900	-0.09129800
H	0.98453600	4.06295400	0.22026900
H	0.86820900	3.18761000	-1.31231500
H	2.04686900	-1.73631700	-1.52618800

2e

B3LYP SCF energy in DMF: -502.8364722 a.u.

M06 SCF energy in DMF: -502.5700182 a.u.

M06 Free energy in DMF: -502.3856912 a.u.

C	1.18774400	-0.20254700	0.18199000
C	2.09114100	-1.26009500	0.00374400
C	1.67072200	1.10899800	0.03895900
C	3.43293600	-1.02166900	-0.30545900
H	1.73846200	-2.28343200	0.10984800
C	3.00982200	1.35245300	-0.27076000
H	0.99483000	1.94956300	0.17238900
C	3.89798200	0.28723300	-0.44406400
H	4.11312400	-1.85900300	-0.43706600
H	3.36081600	2.37565400	-0.37610100
H	4.94050800	0.47684800	-0.68389100
C	-1.19808100	-0.02154400	-0.65859900
C	-0.27390700	-0.47731100	0.50752100
H	-1.15418300	1.07159500	-0.74580000
H	-0.38551800	-1.56549600	0.60175400
C	-0.69298500	0.15408500	1.84515300
H	-1.73082400	-0.09821500	2.08475900
H	-0.05978800	-0.20132400	2.66508500
H	-0.61721800	1.24705300	1.81261100
C	-2.62805900	-0.46394000	-0.51528100
C	-3.65550200	0.38355800	-0.40669000
H	-3.51193300	1.46359700	-0.41230900
H	-2.82946000	-1.53517700	-0.50364400
H	-0.78092500	-0.42461100	-1.59218300
O	-4.95009400	-0.04732000	-0.29048100
H	-5.52801800	0.72617900	-0.23069600

2f

B3LYP SCF energy in DMF: -502.8541438 a.u.

M06 SCF energy in DMF: -502.5869014 a.u.

M06 Free energy in DMF: -502.4034514 a.u.

C	-1.14715900	0.28677300	-0.12525700
C	-2.01110000	0.23130800	-1.22819700
C	-1.60655300	-0.22189700	1.10086900
C	-3.29346900	-0.31225200	-1.11554500
H	-1.67494400	0.62046100	-2.18643600
C	-2.88613000	-0.76734400	1.21780200
H	-0.96027300	-0.19189900	1.97406500
C	-3.73617600	-0.81432100	0.10940200
H	-3.94508700	-0.34140500	-1.98478300

H	-3.22071600	-1.15489100	2.17642200
H	-4.73283100	-1.23694400	0.20099000
C	1.32746400	-0.21346300	-0.05954300
C	0.25022100	0.87788300	-0.26652800
H	1.08832000	-1.06815700	-0.70474300
H	0.34626000	1.23505400	-1.30033400
C	0.45104200	2.08487900	0.66761000
H	1.41138100	2.57688500	0.48397000
H	-0.33674200	2.83012700	0.51522700
H	0.42756300	1.78317700	1.72088400
C	2.76122800	0.25685600	-0.37242800
C	3.73408300	-0.89157600	-0.34706300
H	2.78549300	0.67517200	-1.39028800
O	4.73522200	-0.94223400	0.34192000
H	3.47556500	-1.73555000	-1.02489100
H	3.10904700	1.02445700	0.32392200
H	1.28448200	-0.57967800	0.97389900

2g

B3LYP SCF energy in DMF: -502.8363013 a.u.

M06 SCF energy in DMF: -502.5685815 a.u.

M06 Free energy in DMF: -502.3843315 a.u.

C	1.10017100	0.23493200	-0.10614100
C	2.14651100	0.93727500	0.52200800
C	1.38718800	-1.05326700	-0.59980800
C	3.41158000	0.36749100	0.67628000
H	1.97075200	1.93578000	0.90888500
C	2.65014600	-1.62283600	-0.44664600
H	0.61838500	-1.60666500	-1.12995800
C	3.67103200	-0.91690200	0.19565100
H	4.19549900	0.93171200	1.17432800
H	2.84111700	-2.61664000	-0.84268700
H	4.65673000	-1.35872100	0.31040200
C	-1.35174000	0.06063000	-0.27751300
C	-0.25488200	0.84507600	-0.25206000
H	-1.21551900	-1.01311600	-0.16897700
C	-0.30849600	2.35456100	-0.34487400
C	-2.79075300	0.47437700	-0.42257000
H	-2.92419800	1.55314400	-0.30273200
H	-0.08398600	2.82686400	0.61996400
H	0.43220100	2.73102200	-1.05958300
C	-3.71157400	-0.23239700	0.57287700
H	-3.37957000	-0.02423100	1.60109700
H	-1.28881700	2.71387700	-0.66155200
H	-4.73244900	0.16630700	0.46880700
H	-3.14653800	0.22126700	-1.43311800
O	-3.68433800	-1.63453400	0.29977300
H	-4.16400100	-2.07796700	1.01370600

Allylic alcohol dissociated from 31

B3LYP SCF energy in DMF: -502.8290826 a.u.

M06 SCF energy in DMF: -502.5631196 a.u.

M06 Free energy in DMF: -502.3800036 a.u.

C	-1.13482000	0.30213700	-0.20793800
C	-1.83110000	-0.33072800	-1.24675500
C	-1.69922500	0.28445100	1.07773600
C	-3.05726400	-0.95925700	-1.01456800
H	-1.40871400	-0.32889600	-2.24874200
C	-2.92290800	-0.34426400	1.31411700
H	-1.18037300	0.76587100	1.90251300
C	-3.60797300	-0.96870000	0.26817100
H	-3.58002700	-1.44112600	-1.83645200
H	-3.34196600	-0.34656400	2.31680100
H	-4.56060800	-1.45754200	0.45212400
C	1.33099100	0.27190100	0.24413500
C	0.20709600	0.98081700	-0.48048100
H	1.27118900	0.27338900	1.33411100
H	0.39962200	0.90272500	-1.55680500
C	0.18044000	2.47844600	-0.10872200
H	1.12808500	2.95603200	-0.37891500

H	-0.62678700	2.99727600	-0.63677100
H	0.02719800	2.62241300	0.96605900
C	2.36077700	-0.33863800	-0.34819900
C	3.44653500	-1.06711500	0.38344000
H	3.39891300	-2.14015200	0.13477900
H	2.43849000	-0.34394500	-1.43629700
O	4.71383100	-0.52652100	-0.01269900
H	5.39389800	-1.12259700	0.33334000
H	3.29513400	-0.97902100	1.47023300