

Supporting Information

Mechanism of Pd-Catalyzed Acylation/Alkenylation of Aryl Iodide: A DFT Study

Yujie Liang, Yuan-Ye Jiang, Yuxia Liu and Siwei Bi*

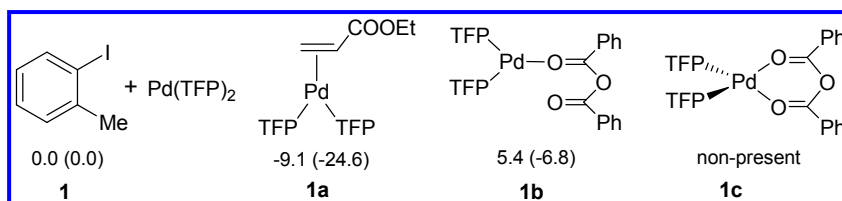
School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165,
People's Republic of China

Table of Contents

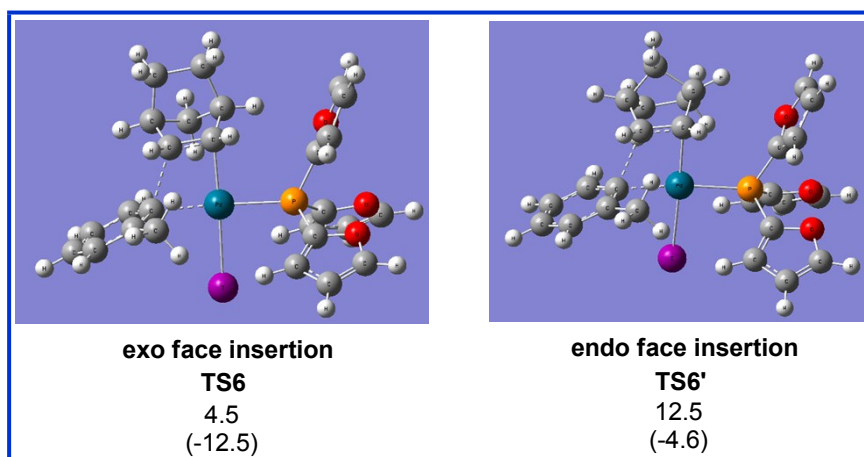
Complete Reference for Ref (14).....	S3
The transition states of migratory insertion of norbornene on 5	S4
Calculated relative solution-phase Gibbs free energies and enthalpies in parenthesis by B3LYP and M06 methods (kcal mol ⁻¹).....	S5
Relative stability of possible resting states of catalyst precursors.....	S6
C-I oxidative addition step with the Pd(0) complex bearing one TFP ligand.....	S7
C-O oxidative addition of the substrate benzoic anhydride.....	S8
The <i>cis</i> → <i>trans</i> isomerization of 4	S9
Dissociated of TFP and CsICsHCO ₃ for activating the C-O bond of benzoic anhydride.....	S10
Ethyl acrylate insertion into the Pd-C(sp ²) and Pd-C(sp ³) bonds of intermediate 10	S11
The transition states of competitive base-assisted deprotonation and β-H elimination on 21	S12
Ethyl acrylate insertion into the Pd-C bond of intermediate 4	S13
Cartesian coordinates, solution-phase energies for all of calculated structures	S14

Complete Reference for Ref (14):

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.



Scheme S1 Relative stability of possible resting states of catalyst precursors. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.



Scheme S2 The transition states of migratory insertion of norbornene from exo and endo face.

The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

Table S1. Calculated relative solution-phase Gibbs free energies and enthalpies in parenthesis by B3LYP and M06 methods (kcal mol⁻¹).

	B3LYP $\Delta G(\Delta H)$	M06 $\Delta G(\Delta H)$
TS6	4.5 (-12.5)	0.5 (-14.1)
TS6a	6.2 (-10.0)	4.6 (-11.6)
TS9	-0.5 (-30.4)	-3.1 (-33.0)
TS9b	0.7 (-20.1)	-0.6 (-19.8)
10	-35.0 (-63.4)	-36.3 (-66.1)
TS12	-9.9 (-39.9)	-11.2 (-40.1)
TS19	-19.9 (-49.6)	-27.4 (-57.4)
TS19a	-11.1(-40.3)	-16.3 (-45.9)
TS22	-29.3 (-55.8)	-27.7 (-55.2)
TS22a	-23.1 (-50.3)	-28.4 (-57.5)

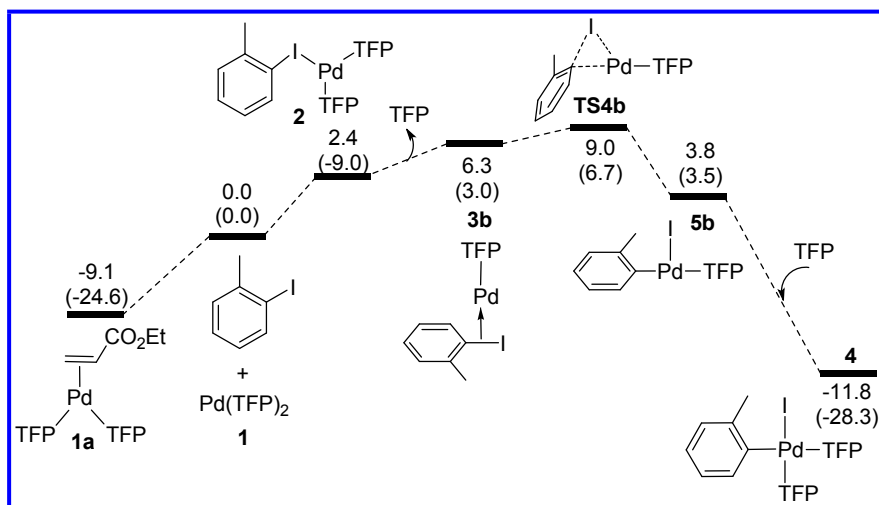


Fig. S1 Gibbs free energy profile calculated for the C-I oxidative addition step with the Pd(0) complex bearing one TFP ligand. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

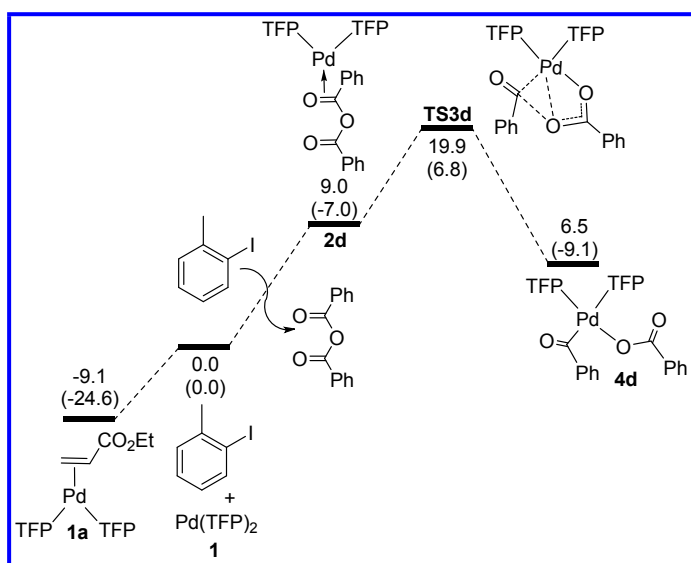


Fig. S2 Gibbs free energy profile calculated for the C-O oxidative addition of the substrate benzoic anhydride, for the purpose of comparing with the C-I oxidative addition. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

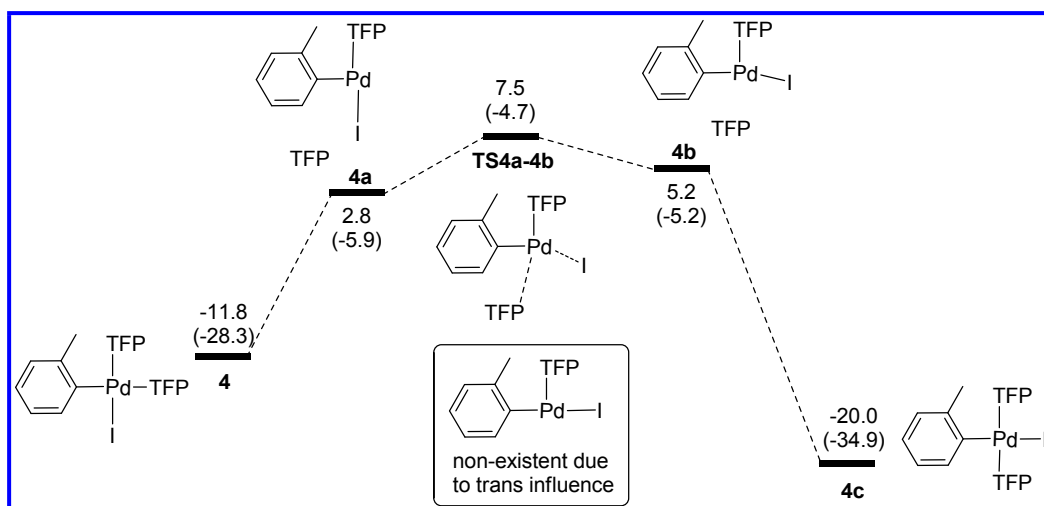


Fig. S3 Gibbs free energy profile calculated for the *cis*→*trans* isomerization of **4**. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

From **4**, the relative energy of the *cis*→*trans* transition state **TS4a-4b** is $\Delta G = 7.5$ and $\Delta H = -4.7$ kcal mol⁻¹, appreciably higher than the norbornene insertion transition state **TS6** in Fig. 1 ($\Delta G = 4.5$ and $\Delta H = -12.5$ kcal mol⁻¹). Thus, the path through the *cis*→*trans* isomerization can be excluded.

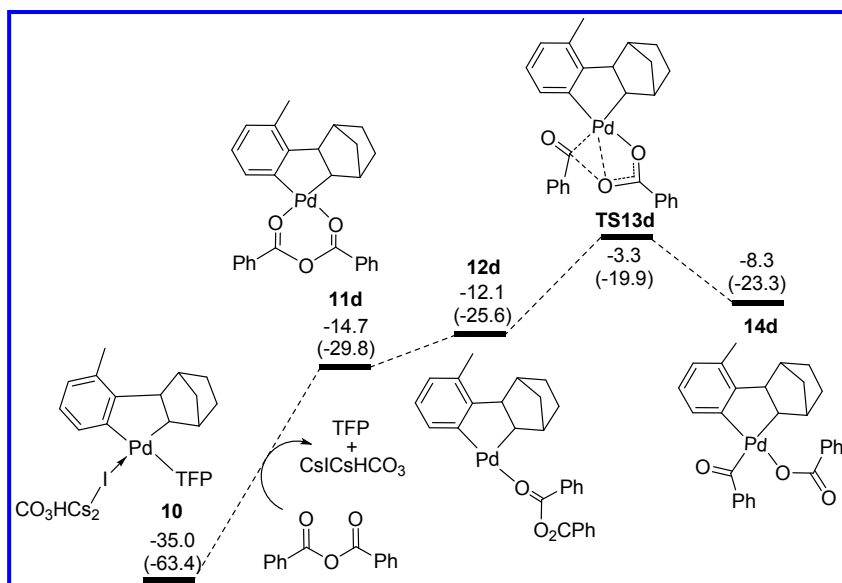


Fig. S4 The energy profiles is dissociated of TFP and CsICsHCO₃ for activating the C-O bond of benzoic anhydride. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

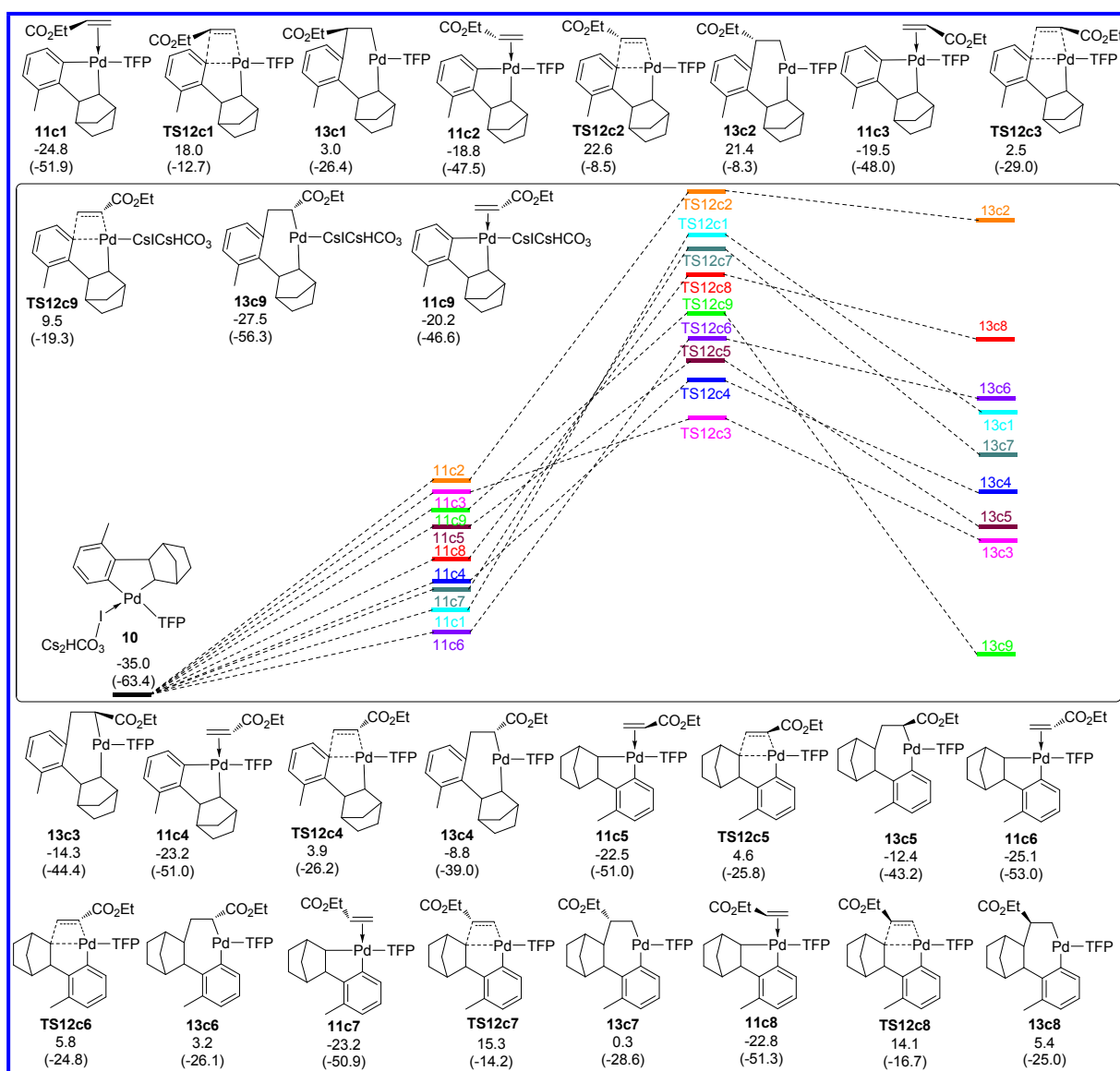


Fig. S5 Gibbs free energy profiles calculated for ethyl acrylate insertion into the Pd-C(sp²) and Pd-C(sp³) bonds of intermediate **10**. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

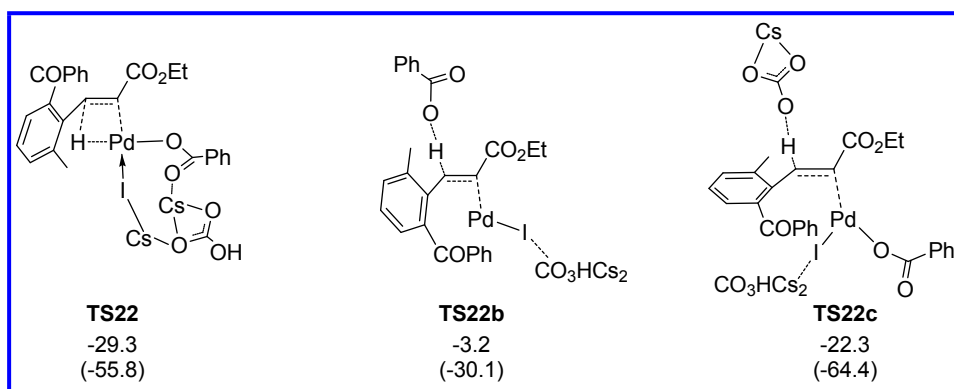


Fig. S6 The transition states of competitive base-assisted deprotonation and β -H elimination on **21**. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

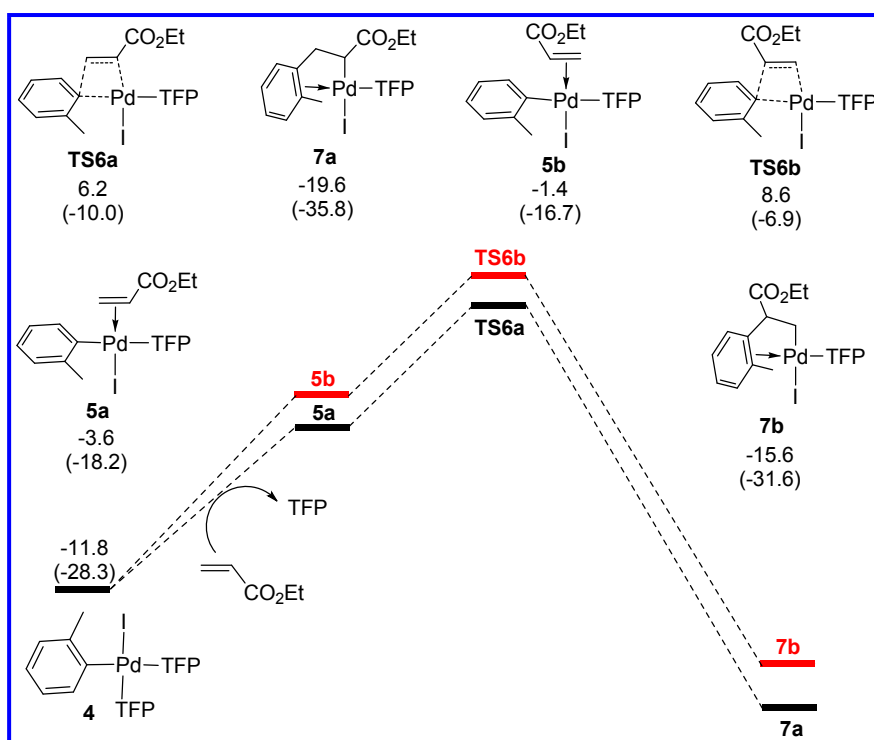


Fig. S7 Gibbs free energy profiles calculated for ethyl acrylate insertion into the Pd-C bond of intermediate 4. The free energies and the enthalpies in parentheses are given in kcal mol⁻¹.

Cartesian coordinates, SCF energies, enthalpies and free energies in solution for all of calculated structures

1a

M06/BSII SCF energy in solution: -2532.348618 a.u.

Solution-phase enthalpy: -2531.813051 a.u.

Solution-phase Gibbs energy: -2531.936468 a.u.

P	-2.09203900	-0.26692800	-0.08986100
C	-3.38774800	-0.35877600	-1.38634300
C	-4.67438300	-0.83171200	-1.41818800
O	-3.04118100	0.08687400	-2.64195700
C	-5.14718600	-0.66242900	-2.75626900
H	-5.20740200	-1.25697400	-0.58034400
C	-4.11530400	-0.10255700	-3.44964900
H	-6.12018400	-0.92515500	-3.14774700
H	-3.98817300	0.20642000	-4.47638000
C	-2.32696000	-1.87772700	0.74598000
C	-1.46894600	-2.92449400	0.94810600
O	-3.55410100	-2.18186000	1.29915300
C	-2.19971500	-3.92945000	1.65734200
H	-0.43861800	-2.96843800	0.62931900
C	-3.45119500	-3.42450600	1.84127900
H	-1.83650100	-4.89236700	1.98811700
H	-4.34236600	-3.80024400	2.32207700
C	-2.91132800	0.85609500	1.10973400
C	-4.03853300	1.63078700	1.09504900
O	-2.22068100	1.07479700	2.27801500
C	-4.04930500	2.36346400	2.32676700
H	-4.77397500	1.66793200	0.30499300
C	-2.92994500	1.98559700	3.00205400
H	-4.79441800	3.07266900	2.65966600
H	-2.50989500	2.24901900	3.96094900
Pd	-0.00606600	0.67367000	-0.73932700
P	1.86282200	-0.71375700	-0.14228400
C	1.75696200	-2.35449200	-0.94641300
C	0.99578100	-2.75540500	-2.01421600
O	2.54150300	-3.40430900	-0.52946700
C	1.33026100	-4.12172000	-2.27253000
H	0.28185400	-2.13951900	-2.54334300
C	2.26772600	-4.45737400	-1.34119300
H	0.92481400	-4.76391300	-3.04187600
H	2.81113700	-5.36580500	-1.12688000

C	3.58547600	-0.23288400	-0.50815500
C	4.11514500	0.95667300	-0.93555300
O	4.59488500	-1.15791600	-0.34950500
C	5.52770100	0.75567900	-1.04398900
H	3.57463500	1.87296100	-1.13455600
C	5.75577700	-0.53758000	-0.67987200
H	6.26727700	1.48088000	-1.35379600
H	6.64586100	-1.14547800	-0.60917800
C	1.92889300	-1.11187800	1.63894500
C	1.09020200	-0.72567100	2.65263800
O	2.94715400	-1.87867600	2.15611600
C	1.61626300	-1.28710800	3.85826200
H	0.20316600	-0.11734600	2.54295200
C	2.73789000	-1.97108000	3.49358800
H	1.21422600	-1.19197900	4.85731300
H	3.46770900	-2.54880800	4.04149000
C	-0.85037300	2.45563400	-1.66631100
C	0.54106800	2.61315000	-1.72145000
C	1.30577400	3.46863000	-0.79418800
O	2.47878900	3.77643200	-0.95560000
O	0.57321500	3.90541400	0.26409200
C	1.25400200	4.75024200	1.21384200
H	0.71170700	4.59800300	2.15090200
H	2.28233700	4.39852800	1.32873200
C	1.22070100	6.21111600	0.78555900
H	1.67660800	6.83966800	1.55993600
H	1.78061400	6.34919000	-0.14357800
H	0.18993900	6.54817400	0.63151000
H	-1.38976800	2.13312900	-2.55182100
H	1.08840000	2.37859900	-2.62953600
H	-1.43055300	2.99492000	-0.92342500

1b

M06/BSII SCF energy in solution: -2951.554635 a.u.

Solution-phase enthalpy: -2950.931575 a.u.

Solution-phase Gibbs energy: -2951.076743 a.u.

P	-0.35761700	2.27571600	0.37655300
C	-1.36558000	2.02021000	1.88725300
C	-1.76691100	2.81656000	2.92780300
O	-1.80374000	0.73574700	2.10468100
C	-2.49393700	1.97866500	3.83228300
H	-1.56509900	3.87271400	3.02893400
C	-2.48410000	0.73292800	3.28029900

H	-2.95529000	2.26695700	4.76679800	C	-1.95877700	-3.57857200	3.55809800
H	-2.88197900	-0.22350300	3.58369600	C	-2.43483400	-3.07537100	2.34831400
C	0.48250600	3.84551500	0.79105300	C	-1.53913200	-2.80773800	1.30138900
C	1.81820400	4.13364000	0.87386300	C	-0.16780500	-3.04662400	1.47715800
O	-0.24606300	4.98445400	1.06231500	C	0.30356500	-3.54010100	2.69138800
C	1.92464900	5.51847100	1.21840900	C	-0.59078400	-3.80846300	3.73135000
H	2.61932500	3.42840800	0.70338700	H	-2.65379700	-3.79222100	4.36561600
C	0.64632200	5.97892700	1.31770000	H	-3.49441000	-2.89235800	2.20853900
H	2.82952300	6.09151100	1.36571300	H	0.51363400	-2.83090400	0.66163400
H	0.21821300	6.94455400	1.54339000	H	1.36834400	-3.70617900	2.82628100
C	-1.64689500	2.81998100	-0.80519400	H	-0.22262200	-4.19617700	4.67764000
C	-2.86696500	3.42813600	-0.67767400	C	-1.98266100	-2.27124800	-0.00909300
O	-1.39253200	2.58049400	-2.13266600	O	-1.28303500	-2.10652100	-0.97576700
C	-3.39392000	3.57178500	-1.99850900	O	-3.35555900	-2.02869700	-0.03250700
H	-3.32851300	3.73053600	0.25128400	C	-3.87934800	-1.03780800	-0.86001700
C	-2.45722800	3.03900900	-2.83519600	O	-3.24819100	-0.07627900	-1.21287600
H	-4.33954600	4.01135900	-2.28527100	C	-5.30749000	-1.29193800	-1.18401200
H	-2.39946800	2.91363700	-3.90599800	C	-5.96643400	-2.47825100	-0.83111300
Pd	1.13047900	0.60880700	-0.21792000	C	-5.99766000	-0.28968500	-1.88284600
P	3.04775400	-0.63270700	-0.59013000	C	-7.30522600	-2.65777100	-1.17642600
C	4.40405100	0.32980300	-1.34414400	H	-5.42866200	-3.25283300	-0.29610100
C	4.38950600	1.60091300	-1.85625000	C	-7.33509500	-0.47296100	-2.22265600
O	5.66352200	-0.20381800	-1.48336000	H	-5.46638200	0.61927700	-2.14621600
C	5.70922700	1.86648100	-2.33946300	C	-7.99017900	-1.65695200	-1.86997200
H	3.52942300	2.25532800	-1.88137900	H	-7.81393400	-3.57872500	-0.90557300
C	6.43299200	0.73959800	-2.08427500	H	-7.86847400	0.30435500	-2.76263700
H	6.06798200	2.77127800	-2.81014900	H	-9.03399000	-1.79972800	-2.13685600
H	7.46215700	0.46158600	-2.25778600				
C	3.80903900	-1.30814200	0.92906400				
C	3.42620100	-1.15258500	2.23616200				
O	4.92263300	-2.11322300	0.87391700				
C	4.35413200	-1.89837600	3.03040700				
H	2.57972500	-0.57132900	2.57403700				
C	5.23326000	-2.45632300	2.14963700				
H	4.36685500	-2.00005300	4.10680600				
H	6.09735500	-3.09408400	2.26480300				
C	2.92940200	-2.09790700	-1.67232200				
C	1.81995000	-2.67857000	-2.23081200				
O	4.05352600	-2.80026200	-2.04333300				
C	2.28438700	-3.80199500	-2.98566500				
H	0.79906400	-2.34644700	-2.10126400				
C	3.63913300	-3.82191400	-2.83561400				
H	1.68848400	-4.49499700	-3.56323800				
H	4.42011500	-4.46532300	-3.21362500				

Pd-2TFP

M06/BSII SCF energy in solution: -2186.640689 a.u.

Solution-phase enthalpy: -2186.240392 a.u.

Solution-phase Gibbs energy: -2186.347288 a.u.

P	-2.35650700	0.02138000	-0.02044000
C	-3.12242900	1.68302800	-0.00437500
C	-4.34458700	2.18795800	-0.36958500
O	-2.34652000	2.69984600	0.49825300
C	-4.31943800	3.58692600	-0.07672100
H	-5.15790600	1.62259100	-0.80140300
C	-3.08606800	3.83625900	0.44840000
H	-5.10981200	4.30686700	-0.23786200
H	-2.59969500	4.72756400	0.81522200
C	-3.25476900	-0.69978700	-1.45676600
C	-3.67221500	-0.20868900	-2.66559900
O	-3.43079300	-2.05884700	-1.42947000

C	-4.14431000	-1.33062700	-3.42136700	Pd	0.19308300	-0.14432000	0.03766000
H	-3.64127600	0.82448100	-2.97961000	C	-3.63124300	-1.81186100	-0.13574200
C	-3.97358100	-2.42163800	-2.62541000	C	-3.93081900	-0.56170300	-0.67648100
H	-4.55690900	-1.31922400	-4.42070600	C	-4.63178700	-2.69174600	0.31019000
H	-4.18287500	-3.47396100	-2.74278800	C	-5.26340100	-0.15920800	-0.78129600
C	-3.20933000	-0.77790000	1.39455600	H	-3.13397300	0.09360300	-1.01316200
C	-4.36065200	-0.52232100	2.09193900	C	-5.96048800	-2.25496000	0.18899400
O	-2.57919800	-1.86906300	1.94117300	C	-6.28070400	-1.00835500	-0.34736600
C	-4.44800600	-1.51211800	3.11960600	H	-5.49638200	0.81638900	-1.19921400
H	-5.05481000	0.28202500	1.89577600	H	-6.75569900	-2.91503700	0.52805300
C	-3.34467800	-2.30034500	2.97576000	H	-7.32109400	-0.70383900	-0.42390000
H	-5.22401900	-1.61890200	3.86492500	I	-1.56367800	-2.35715900	-0.00658500
H	-2.97315900	-3.16527300	3.50443300	C	-4.33438500	-4.04902000	0.89954800
Pd	-0.06051000	-0.07913700	-0.02620400	H	-3.70109200	-3.96975000	1.79127400
P	2.26295700	-0.03091500	-0.02661700	H	-5.26012200	-4.55850600	1.18435900
C	3.05841800	-0.96671400	1.32181300	H	-3.80091000	-4.68985000	0.18703600
C	2.48036100	-1.70930900	2.31795000	P	2.37248500	-0.93572200	-0.00700300
O	4.42602400	-1.00523900	1.45686100	C	3.16202200	-0.98916200	-1.66308400
C	3.54722600	-2.23498100	3.11178700	C	4.02711000	-1.85492200	-2.28015200
H	1.41766100	-1.85289400	2.45509500	O	2.80195100	-0.00086400	-2.54691600
C	4.69747800	-1.77484700	2.54215500	C	4.21546400	-1.36994200	-3.61328800
H	3.46853200	-2.86738100	3.98509900	H	4.46856600	-2.73361800	-1.83202500
H	5.74426500	-1.89867400	2.77727000	C	3.45168700	-0.24549800	-3.71383500
C	3.06907700	-0.68113600	-1.52802800	H	4.83144900	-1.80322200	-4.38922100
C	2.50126400	-1.21144500	-2.65701600	H	3.26535500	0.46099900	-4.50876800
O	4.43801400	-0.69601900	-1.65472300	C	3.65192800	0.00128400	0.91951900
C	3.57578600	-1.57205600	-3.52869800	C	4.95016400	0.35464800	0.65983200
H	1.44032900	-1.32578700	-2.83016700	O	3.26780200	0.53607000	2.12391600
C	4.72031300	-1.23642100	-2.86779900	C	5.39089500	1.14695200	1.76784500
H	3.50544200	-2.01949700	-4.51034500	H	5.51546300	0.08213400	-0.21991200
H	5.76940700	-1.31378300	-3.11232400	C	4.32989200	1.21955500	2.62150300
C	2.96009400	1.64569800	0.14454000	H	6.36407200	1.59736800	1.90827800
C	2.30820300	2.84267100	0.28710900	H	4.17334600	1.69444600	3.57839200
O	4.31798700	1.86021300	0.15013900	C	2.78077400	-2.63320300	0.57375100
C	3.31699900	3.85147000	0.38513300	C	3.83515800	-3.19939600	1.24076600
H	1.23490100	2.96918900	0.31789800	O	1.81073900	-3.58836600	0.37122000
C	4.50965200	3.19648200	0.29573400	C	3.50230700	-4.57535800	1.45366300
H	3.17432700	4.91638200	0.50533300	H	4.73730600	-2.68788200	1.54460300
H	5.53936500	3.52154700	0.31680800	C	2.26837000	-4.75221200	0.90388000
				H	4.09944900	-5.32630100	1.95245300
				H	1.60566000	-5.59982700	0.81426100
				P	-0.50779900	2.07041500	0.09279700
				C	0.73905700	3.32682500	0.58428600
				C	0.68268900	4.50997900	1.27458400

2

M06/BSII SCF energy in solution: -2468.862408 a.u.

Solution-phase enthalpy: -2468.333902 a.u.

Solution-phase Gibbs energy: -2468.46462 a.u.

O	2.04547700	3.05260800	0.26282800	C	2.08375300	1.08788000	-2.28870100
C	2.02590900	4.99193400	1.37840200	C	3.26843900	1.55054800	-2.80019900
H	-0.21283800	4.97183500	1.66496600	O	1.66129000	0.00882000	-3.02468200
C	2.80467200	4.06850700	0.74583000	C	3.58827200	0.71624100	-3.91715800
H	2.36328300	5.89813500	1.86256300	H	3.84205800	2.38205200	-2.41578200
H	3.86588200	3.98023100	0.56957400	C	2.57873600	-0.19604400	-4.00371400
C	-1.05776300	2.79574100	-1.50321200	H	4.45460600	0.78316900	-4.56065600
C	-0.82286800	3.97901100	-2.15123700	H	2.37541200	-1.02233700	-4.66824400
O	-1.83390800	1.98831300	-2.30233100	C	0.05432200	2.91959100	-1.54440700
C	-1.49421900	3.90046100	-3.41376500	C	0.22309800	3.81452400	-2.56846400
H	-0.23683200	4.80251100	-1.76917300	O	-1.17812100	3.11619800	-0.97042800
C	-2.09038500	2.67613900	-3.44727700	C	-0.96612100	4.60764500	-2.62483300
H	-1.52355200	4.65306500	-4.18966800	H	1.09297500	3.88815300	-3.20587400
H	-2.69924700	2.16131500	-4.17529500	C	-1.77633500	4.13773000	-1.63332400
C	-1.90562100	2.60719700	1.15911700	H	-1.18840800	5.41244700	-3.31205800
C	-2.91846100	3.52112800	1.02617400	H	-2.76374700	4.40435500	-1.28785300
O	-2.05466000	1.93601900	2.34846800	C	2.28789300	2.54340000	0.08520800
C	-3.73022600	3.41224100	2.19981600	C	2.45962900	3.88466800	0.30994800
H	-3.06193900	4.18684300	0.18692500	O	3.22325300	1.83907000	0.80317100
C	-3.15637600	2.43931600	2.96262300	C	3.56677900	4.01274900	1.20925900
H	-4.62078200	3.97734200	2.43816200	H	1.86928800	4.68064400	-0.11984500
H	-3.39786700	2.00290500	3.92017800	C	3.98955000	2.74409800	1.46864400

TS3

M06/BSII SCF energy in solution: -2468.853806 a.u.

Solution-phase enthalpy: -2468.326912 a.u.

Solution-phase Gibbs energy: -2468.452618 a.u.

Pd	-0.15746300	-0.24778300	0.27274700	H	4.78162300	2.32907900	2.07357800
C	-0.41432800	-1.05696800	2.32398900	P	-2.18698900	-0.90279300	-0.88915000
C	-1.42502900	-2.03091300	2.42819500	C	-2.68201500	0.00115500	-2.40763600
C	-0.34518400	0.02724800	3.22642500	C	-3.88313400	0.28050100	-3.00609400
C	-2.43662500	-1.88765500	3.37072100	O	-1.67029700	0.58692500	-3.12880400
H	-1.41750200	-2.87899800	1.75382100	C	-3.59473900	1.07531800	-4.16025200
C	-1.39100600	0.13437400	4.16420200	H	-4.85323900	-0.04232300	-2.65592600
C	-2.42349600	-0.79379500	4.24303600	C	-2.23994200	1.22616900	-4.18203300
H	-3.23148200	-2.62707000	3.42087000	H	-4.30069100	1.48215300	-4.87117000
H	-1.36621400	0.96987200	4.86129800	H	-1.55636200	1.74284100	-4.83813200
H	-3.20095800	-0.67967100	4.99385300	C	-2.18864000	-2.61730600	-1.54765800
I	1.65132800	-1.95586500	1.51212000	C	-2.57065800	-3.18438700	-2.73495600
C	0.76126500	1.05923600	3.26745500	O	-1.62393900	-3.58227000	-0.74669800
H	0.50621900	1.95296400	2.68611900	C	-2.22913600	-4.57252300	-2.65926900
H	0.93513300	1.38052700	4.30120800	H	-3.03654500	-2.66712600	-3.56120600
H	1.69777300	0.66651700	2.86652100	C	-1.66279100	-4.75423100	-1.43360200
P	1.05449000	1.54976400	-0.84505300	H	-2.38206200	-5.32838700	-3.41715100
				H	-1.25096300	-5.60993200	-0.92001800
				C	-3.79526400	-0.91399800	-0.00829400
				C	-4.84528800	-1.79250100	0.05790800
				O	-4.02697600	0.13679600	0.84442400

C	-5.77729400	-1.24915600	0.99834000
H	-4.93633300	-2.71420300	-0.49894900
C	-5.22783600	-0.08197300	1.43891300
H	-6.72352400	-1.67314900	1.30515300
H	-5.54591500	0.67350100	2.14141900

4

M06/BSII SCF energy in solution: -2468.893558 a.u.

Solution-phase enthalpy: -2468.364603 a.u.

Solution-phase Gibbs energy: -2468.487173 a.u.

Pd	0.19937600	-0.70629900	-0.00728400
C	1.94404000	-1.79396800	-0.11704700
C	2.65932600	-2.13119800	1.03510400
C	2.40336300	-2.21626500	-1.37941900
C	3.85168500	-2.85916600	0.94997100
H	2.28431200	-1.83865400	2.00948900
C	3.59909200	-2.94758900	-1.44370600
C	4.32633400	-3.26580400	-0.29604900
H	4.39493000	-3.11279900	1.85749100
H	3.95931600	-3.27646900	-2.41705100
H	5.24888800	-3.83562300	-0.37656600
I	-0.96319300	-3.12341000	0.39517200
C	1.63334200	-1.93472900	-2.64915600
H	1.36395700	-0.87526700	-2.73792600
H	2.21461000	-2.21243600	-3.53556000
H	0.69789400	-2.50821200	-2.66422100
P	-2.10966800	0.28015400	-0.10193800
C	-3.08962100	-0.04122100	1.40269500
C	-4.39327600	-0.38094700	1.64642500
O	-2.40008700	0.01974600	2.58783900
C	-4.51390000	-0.54128100	3.06241400
H	-5.16378400	-0.50842900	0.90053600
C	-3.27736500	-0.28712400	3.57671500
H	-5.39892800	-0.81916600	3.61757000
H	-2.87174500	-0.28544600	4.57704700
C	-2.52792700	2.04611600	-0.38110500
C	-3.45885300	2.89320700	0.15616000
O	-1.86639600	2.67922900	-1.40411900
C	-3.36890700	4.11810700	-0.57864200
H	-4.13611100	2.66006600	0.96465000
C	-2.39138500	3.92929100	-1.50886700
H	-3.95549800	5.01483000	-0.43318300
H	-1.96050200	4.55308200	-2.27695100
C	-3.11021400	-0.46034500	-1.43609200

C	-2.80149600	-1.35242100	-2.42616700
O	-4.40845500	-0.02388800	-1.60176800
C	-3.96838500	-1.48455700	-3.24173900
H	-1.86172700	-1.87217400	-2.53398100
C	-4.90619300	-0.66258000	-2.69344400
H	-4.08983500	-2.11262400	-4.11309400
H	-5.92899300	-0.42566400	-2.94656100
P	1.66715100	1.14900300	0.06793200
C	1.11023800	2.89548000	0.04754400
C	1.53686200	4.03884700	-0.57411000
O	0.12678300	3.20346700	0.95278300
C	0.77282800	5.11229900	-0.01784900
H	2.30024100	4.10522000	-1.33404400
C	-0.06198500	4.54810400	0.89938400
H	0.83665000	6.16115800	-0.27241000
H	-0.82423900	4.93726800	1.55612000
C	2.62597600	1.14011900	1.62695100
C	3.82396100	1.68013300	2.01485600
O	2.00864000	0.57086000	2.71061600
C	3.95931300	1.41262700	3.41212400
H	4.51966700	2.20649000	1.37761300
C	2.82980600	0.74214000	3.77799100
H	4.78606300	1.68280300	4.05416300
H	2.47195200	0.33436900	4.71116500
C	3.00724000	1.22237000	-1.16868500
C	4.26410500	0.68531400	-1.21446800
O	2.69747500	1.78193800	-2.38627900
C	4.76968100	0.94560700	-2.52793800
H	4.75271800	0.14103000	-0.41999300
C	3.78282300	1.60760000	-3.19167800
H	5.73766600	0.66777000	-2.92058700
H	3.69143500	2.01220900	-4.18829100

5

M06/BSII SCF energy in solution: -1712.126715 a.u.

Solution-phase enthalpy: -1711.635409 a.u.

Solution-phase Gibbs energy: -1711.737204 a.u.

Pd	0.83330800	0.01881100	-0.08317700
P	-1.70497700	-0.05014000	-0.10123900
C	-2.35082300	-1.30814000	-1.24944800
C	-1.71476400	-2.18191600	-2.09074800
O	-3.71388100	-1.47239000	-1.36243600
C	-2.73567600	-2.92560400	-2.75918700
H	-0.64569800	-2.29773800	-2.18756900

C	-3.92019900	-2.45526400	-2.27467800
H	-2.60184700	-3.70951000	-3.49122800
H	-4.95359800	-2.70384000	-2.46640700
C	-2.48285100	-0.37905300	1.50930900
C	-1.93825100	-0.65483600	2.73540200
O	-3.85446000	-0.34399900	1.61059500
C	-3.03153700	-0.80057000	3.64399500
H	-0.88520500	-0.76859200	2.94699500
C	-4.16132000	-0.60287600	2.90652100
H	-2.98003200	-1.02742300	4.69957800
H	-5.21488100	-0.61058300	3.14378100
C	-2.71245700	1.37713300	-0.67792400
C	-3.25468300	1.70171100	-1.89249300
O	-2.93281300	2.40135100	0.20880600
C	-3.85226400	2.99514300	-1.74358400
H	-3.25053800	1.08365200	-2.77865800
C	-3.63039000	3.36740100	-0.45348300
H	-4.38496400	3.56023200	-2.49570400
H	-3.89329000	4.23611900	0.13085500
I	0.83849800	-2.54788100	0.72185700
C	3.62794400	-0.08592900	1.04606000
C	5.01560700	-0.26469400	1.04246600
C	5.66171400	-0.63875600	-0.13475700
C	4.91097300	-0.84324100	-1.29251200
C	3.51690000	-0.67679700	-1.30771200
C	2.88148900	-0.27424000	-0.11930300
H	3.13240900	0.18813400	1.97289200
H	5.58081300	-0.11756500	1.95992000
H	6.73936900	-0.77941300	-0.15243700
H	5.41067600	-1.14752900	-2.21063000
C	2.74489500	-0.97666000	-2.57286500
H	2.02123900	-0.18813200	-2.81608500
H	3.41670700	-1.09565100	-3.43017600
H	2.17259200	-1.90629400	-2.45996400
C	1.83179300	2.15016800	-0.77419800
C	2.50237600	2.95314700	0.32682900
C	0.26793000	3.24945300	0.55927700
C	0.47492500	2.32735800	-0.63729100
H	2.33914900	1.85403200	-1.68406200
H	-0.25021600	2.22048200	-1.43726300
C	1.45733800	2.85263100	1.45895300
H	1.63538300	3.56806000	2.26962700
H	1.36474500	1.84424200	1.87382100
C	2.29523900	4.44585300	-0.11122600

H	2.85996300	5.10821300	0.55365300
H	2.64533500	4.63045800	-1.13173100
C	0.75521600	4.65114400	0.05178300
H	0.53156700	5.41756200	0.80212200
H	0.26224600	4.94914100	-0.87901100
H	3.53080400	2.67795900	0.55917200
H	-0.72617600	3.24336900	1.00396300

TS6

M06/BSII SCF energy in solution: -1712.120143 a.u.

Solution-phase enthalpy: -1711.629832 a.u.

Solution-phase Gibbs energy: -1711.728383 a.u.

Pd	-0.96141700	0.28214500	-1.21083300
P	-2.14792300	-1.39538000	-2.52815400
C	-1.85164800	-1.18040700	-4.31107400
C	-0.96918000	-0.37039900	-4.97554400
O	-2.54381800	-1.94895800	-5.22085900
C	-1.12536100	-0.64836000	-6.36871100
H	-0.26976200	0.30998200	-4.51218200
C	-2.08814700	-1.60985100	-6.45359500
H	-0.58739100	-0.19801900	-7.19100100
H	-2.54458000	-2.13500000	-7.27966300
C	-1.74679900	-3.13356100	-2.15823900
C	-0.87784100	-3.70666600	-1.26887500
O	-2.43620800	-4.11823800	-2.82923800
C	-1.03512100	-5.12153500	-1.39825100
H	-0.19049100	-3.17579300	-0.62717400
C	-1.98754900	-5.30796200	-2.35575600
H	-0.50456600	-5.89130300	-0.85559900
H	-2.43788700	-6.18509500	-2.79648800
C	-3.97749900	-1.48778500	-2.50486400
C	-4.96310500	-1.08796000	-3.36460900
O	-4.54212900	-2.07189400	-1.39766300
C	-6.20723900	-1.45185500	-2.75793500
H	-4.81910600	-0.61313000	-4.32357000
C	-5.89092700	-2.04344100	-1.57334000
H	-7.19982900	-1.29872000	-3.15818600
H	-6.47437500	-2.48229100	-0.77816800
I	1.48301100	-0.73867600	-1.90032500
C	-3.39905200	2.10276100	-1.57169400
C	-4.77715300	2.32221900	-1.57887900
C	-5.57423700	1.72620200	-0.60212800
C	-4.98693900	0.89467200	0.35251100
C	-3.60966300	0.63924600	0.35887000

C	-2.79784600	1.26845400	-0.61486700	C	3.31455200	-0.88669900	-3.41085000
H	-2.78491900	2.59949400	-2.31616800	H	1.12874200	-1.10086900	-2.87680600
H	-5.21890000	2.96621700	-2.33516200	C	4.33676500	-0.44845600	-2.62154200
H	-6.64596200	1.90464400	-0.58156700	H	3.38874800	-1.22687000	-4.43411900
H	-5.61041000	0.42340000	1.10964600	H	5.39789100	-0.32426700	-2.77954800
C	-3.04269700	-0.33174200	1.36778200	C	2.38076400	1.54170400	0.72703200
H	-2.04451700	-0.04097100	1.71419300	C	2.69723500	1.99533400	1.97993000
H	-3.69633700	-0.42615700	2.24188500	O	2.65055200	2.51932600	-0.19626300
H	-2.94214400	-1.32867800	0.92052700	C	3.20080600	3.32480600	1.81815100
C	-1.17941600	2.23803900	0.29704200	H	2.60254700	1.44102400	2.90247700
C	-1.13377800	3.65742300	-0.25785800	C	3.15011400	3.58766100	0.48245900
C	0.90843000	2.76883800	-0.68968700	H	3.56050500	3.98715000	2.59309600
C	0.10808400	1.67559600	0.01458200	H	3.42693100	4.43713800	-0.12329200
H	-1.65527800	2.06327000	1.25521500	I	-0.83526700	-2.74605800	-0.85268200
H	0.60429800	1.02438500	0.73117600	C	-3.68434200	0.08703800	-0.63912800
C	-0.19894100	3.49928600	-1.47785100	C	-4.36900900	-1.12331300	-0.54101300
H	0.12741400	4.46239200	-1.88565700	C	-4.42199800	-1.78605300	0.68075600
H	-0.61870900	2.88986300	-2.28382300	C	-3.78970400	-1.23401600	1.79551200
C	-0.18954700	4.42057000	0.73000900	C	-3.09857800	-0.02147100	1.72266600
H	-0.23145800	5.49408200	0.51599200	C	-3.04196100	0.66694100	0.47415700
H	-0.48872400	4.28717600	1.77523900	H	-3.66908300	0.60345400	-1.59188500
C	1.21930300	3.82570900	0.41516700	H	-4.84446500	-1.54714100	-1.42010000
H	1.89767000	4.59267800	0.02417600	H	-4.94532600	-2.73364900	0.76907100
H	1.69959200	3.38039500	1.29240600	H	-3.83616900	-1.75381300	2.74929100
H	-2.10278100	4.13357100	-0.41300000	C	-2.50937500	0.56952500	2.98570000
H	1.77454000	2.41826300	-1.25028300	H	-3.06444300	1.46322300	3.30387600

7

M06/BSII SCF energy in solution: -1712.162992 a.u.

Solution-phase enthalpy: -1711.669768 a.u.

Solution-phase Gibbs energy: -1711.768498 a.u.

Pd	-0.67990800	-0.07888800	-0.10105300	C	-0.86648900	1.96284700	0.24987900
P	1.59578300	0.00012800	0.13298900	H	-2.67086000	2.58604900	1.34343900
C	2.20285500	-1.16137500	1.39312500	H	-0.29400300	2.22458700	1.14310700
C	1.58692500	-2.17206000	2.08259300	C	-1.77263400	2.58052300	-1.88081000
O	3.53554700	-1.10858600	1.74116400	H	-1.80903100	3.24601200	-2.75163600
C	2.58961400	-2.77450300	2.90327900	H	-1.83408300	1.54572700	-2.23112900
H	0.55272900	-2.46583100	1.97764700	C	-2.35312900	4.40575200	-0.46387500
C	3.74333000	-2.09259600	2.65211200	H	-2.75170100	5.10940000	-1.20325400
H	2.46563300	-3.60781200	3.58043800	H	-2.70585600	4.73479400	0.52007700
H	4.75397500	-2.17737100	3.02348700	C	-0.79495600	4.31748500	-0.55396300
C	2.52651800	-0.32808600	-1.38874800	H	-0.40022200	4.99974000	-1.31643600
C	2.13427600	-0.80981000	-2.60914000	H	-0.29836800	4.56323400	0.39103600
O	3.88426300	-0.10389700	-1.38958400	H	-3.86407000	2.88814800	-1.07475600

H	0.42912900	2.66830700	-1.42005000
---	------------	------------	-------------

8

M06/BSII SCF energy in solution: -2016.383976 a.u.

Solution-phase enthalpy: -2015.864521 a.u.

Solution-phase Gibbs energy: -2015.986237 a.u.

Pd	0.20618500	0.05957200	0.54317700
P	1.90592900	1.20741800	-0.53624900
C	2.10393500	-2.72205100	0.12184100
C	3.22117500	-3.20773700	-0.60352900
C	0.81847800	-2.94436300	-0.40006800
C	3.01508200	-3.86730100	-1.82371700
C	0.63708500	-3.61693200	-1.61172500
H	-0.07222400	-2.61578800	0.13418500
C	1.73540400	-4.07790900	-2.33546700
H	3.88012800	-4.23189100	-2.37443800
H	-0.37365400	-3.78458900	-1.97885900
H	1.60360900	-4.60185100	-3.27975900
C	-2.37997900	-1.25616100	1.26867600
O	-3.58486100	-0.84206400	1.42063200
O	-1.41101800	-0.44476000	1.73520400
O	-2.06899600	-2.34371600	0.69204800
Cs	-4.05819400	-1.92630900	-1.38618100
C	2.31301400	-2.07832800	1.48960800
C	1.98409500	-3.07577800	2.65818600
C	0.86153700	-1.21276600	3.26848000
C	1.51689900	-0.79139300	1.93733300
C	0.53626100	-2.69889800	3.03498300
H	0.20020700	-3.21084200	3.94685900
H	-0.20746200	-2.85096500	2.25074900
C	2.75864900	-2.61386200	3.91514700
H	2.69607400	-3.37283600	4.70452800
H	3.82303400	-2.44405500	3.71255800
C	2.00058600	-1.31012200	4.32602100
H	1.57523700	-1.40098100	5.33391300
H	2.64961800	-0.42582700	4.32739900
H	2.16285900	-4.12066800	2.38575500
H	0.02418500	-0.58618300	3.57231600
H	2.21124700	0.03249700	2.10784000
H	3.37347200	-1.81715400	1.55211100
Cs	-2.93043200	2.04469600	1.93190900
I	-1.70034800	1.20942700	-1.63800400
C	1.54627700	3.00674400	-0.64450700
C	1.87665100	3.99478900	-1.53169600

O	0.83348200	3.54904500	0.39901300
C	1.33141700	5.21166800	-1.01615000
H	2.44185300	3.86166400	-2.44136000
C	0.71594600	4.88164800	0.15294600
H	1.39088300	6.19633000	-1.45906700
H	0.18399100	5.45174100	0.90023200
C	3.60358100	1.26746700	0.17495600
C	4.83333900	0.85584300	-0.26281700
O	3.72730800	1.82650500	1.42397100
C	5.76807800	1.17823600	0.77437800
H	5.04812700	0.39467200	-1.21537000
C	5.04391800	1.76382700	1.76710300
H	6.83433900	0.99921400	0.77354400
H	5.29420800	2.17322000	2.73404500
C	2.30977100	0.75185800	-2.24688800
C	1.91645700	-0.33091000	-2.98246200
O	3.17776300	1.52706600	-2.99197700
C	2.56685700	-0.22243800	-4.25143800
H	1.24976400	-1.11255900	-2.64873000
C	3.30927000	0.91835500	-4.20117000
H	2.48871600	-0.90535100	-5.08564300
H	3.95848800	1.41722800	-4.90557600
C	4.64349100	-3.06717500	-0.09827400
H	5.34797600	-3.51013100	-0.81047300
H	4.93246900	-2.01906700	0.04567400
H	4.78917700	-3.57284800	0.86463900

TS9

M06/BSII SCF energy in solution: -2016.342019 a.u.

Solution-phase enthalpy: -2015.829025 a.u.

Solution-phase Gibbs energy: -2015.950897 a.u.

Pd	-1.37667500	-1.65786400	0.50684500
P	0.36855800	-1.49331300	-1.03833600
C	-4.19411700	-0.71498100	0.01013900
C	-5.08960700	0.33606000	-0.29593600
C	-3.33906400	-0.64142700	1.14207500
C	-5.09427700	1.48253800	0.50636900
C	-3.35492000	0.55820800	1.88612000
H	-3.13298000	-1.64447000	2.00430100
C	-4.21421900	1.61018900	1.58244100
H	-5.78329900	2.29167000	0.26985100
H	-2.66066700	0.66424300	2.71557200
H	-4.20483600	2.52504200	2.17272400
C	-2.11248000	-3.15582000	3.19021300

O	-1.61159300	-3.46750300	4.32395100
O	-1.62231400	-3.56886300	2.07469700
O	-3.14737600	-2.31935500	3.15222900
Cs	-2.22063900	-0.79590200	5.49937200
C	-4.05495900	-1.88773400	-0.93277600
C	-5.00736400	-3.10273800	-0.68816000
C	-2.94281300	-4.03459600	-0.59637700
C	-2.64234700	-2.55262300	-0.88869100
C	-4.19538100	-3.96166100	0.30116600
H	-4.64989900	-4.94749700	0.46828300
H	-4.00846800	-3.49053700	1.26511800
C	-4.97789500	-3.98617700	-1.95888100
H	-5.75756300	-4.75591200	-1.91168600
H	-5.14870700	-3.40761900	-2.87512300
C	-3.55065400	-4.62622700	-1.90475400
H	-3.61163900	-5.71936400	-1.82716800
H	-2.94792900	-4.39756300	-2.79153600
H	-6.01275300	-2.81058500	-0.36766900
H	-2.10027700	-4.60032100	-0.19989500
H	-2.12487300	-2.42370500	-1.84091200
H	-4.22266600	-1.51293900	-1.95169100
Cs	1.09781000	-4.00561700	2.97342400
I	0.41887200	-0.20663700	2.54633900
C	2.13553900	-1.77100700	-0.58659000
C	3.28072200	-1.03363500	-0.70048100
O	2.43537400	-2.99728500	-0.03108800
C	4.34828800	-1.84091200	-0.19349600
H	3.35467400	-0.03674000	-1.10670200
C	3.78455000	-3.01806700	0.18926900
H	5.39533500	-1.57759800	-0.13213400
H	4.18329900	-3.94092200	0.58521800
C	0.28253800	-2.50903200	-2.57074300
C	0.18541400	-2.23941300	-3.90940000
O	0.23922900	-3.86855100	-2.37409000
C	0.08052300	-3.50251900	-4.57603000
H	0.19971100	-1.25973400	-4.36293600
C	0.12154400	-4.45021500	-3.59883700
H	-0.01268800	-3.67598200	-5.63914800
H	0.07972100	-5.52889500	-3.60169100
C	0.44652500	0.18307900	-1.74039300
C	-0.32280600	1.27720100	-1.45066700
O	1.36761500	0.51397900	-2.71683600
C	0.14012000	2.34031700	-2.28772800
H	-1.11579200	1.30631200	-0.71684900

C	1.15966500	1.82210100	-3.02803600
H	-0.23626900	3.35284100	-2.32764800
H	1.81078900	2.22945600	-3.78763500
C	-6.02279900	0.26954400	-1.48721700
H	-6.71285700	1.12032400	-1.48783700
H	-5.47479800	0.29173800	-2.43935800
H	-6.62399300	-0.64706900	-1.49147500

10

M06/BSII SCF energy in solution: -2016.400056 a.u.

Solution-phase enthalpy: -2015.881605 a.u.

Solution-phase Gibbs energy: -2016.007614 a.u.

Pd	-0.15588000	0.90436300	-0.51613700
P	-2.56308900	0.50559400	-0.17093800
C	2.06995600	2.83761600	-0.06240700
C	3.19396800	3.63804900	-0.37609700
C	1.56039400	1.90079200	-0.99502100
C	3.80098000	3.48989000	-1.62979300
C	2.17549200	1.81019900	-2.25809200
H	3.89364800	-1.47069800	3.12719500
C	3.29199700	2.59217000	-2.57080100
H	4.66022000	4.10987900	-1.88018400
H	1.76929400	1.13358200	-3.00515200
H	3.74870600	2.52269900	-3.55726300
C	2.72856100	-2.55818500	2.08569900
O	2.58277600	-3.07238000	0.94977700
O	1.96550800	-2.55531700	3.07364700
O	3.92757100	-1.81664800	2.21993200
Cs	3.71637400	-1.02636300	-0.92279100
C	1.29654800	2.98022400	1.21954200
C	1.99771400	2.44468200	2.51322400
C	0.06284900	1.27840800	2.45817600
C	-0.02463900	2.12872400	1.17018600
C	1.57020400	0.96503000	2.53869300
H	1.85957600	0.43685400	3.45426500
H	1.93030700	0.39580200	1.67739200
C	1.23150100	3.00294500	3.73439900
H	1.77682200	2.79506800	4.66281400
H	1.09306800	4.08873000	3.67351000
C	-0.11801100	2.21585300	3.68690500
H	-0.26625100	1.62782800	4.60127400
H	-0.98973400	2.87033800	3.57632600
H	3.07468200	2.63312400	2.54492300
H	-0.60910100	0.41845900	2.48641200

H	-0.91421600	2.76980900	1.16761100	C	2.72417900	3.50659800	-1.21756600
H	1.06020700	4.04492700	1.37398000	H	4.35166200	4.49153700	-0.20133000
Cs	-0.45244900	-2.86779800	1.13546400	H	1.01889800	2.41241500	-1.95801000
I	0.02474400	-1.25658600	-2.48627000	H	2.91123400	4.01214800	-2.16410200
C	-3.54237900	-0.80993100	-1.00416200	C	3.16619600	-3.26895400	0.01938400
C	-4.45001500	-0.81764900	-2.02466700	O	2.69583100	-3.15441600	-1.13919400
O	-3.29992100	-2.10326500	-0.59472900	O	2.70786900	-3.86031100	1.01864200
C	-4.79146800	-2.18784800	-2.26353200	O	4.36870600	-2.54878500	0.21459600
H	-4.83213200	0.04856300	-2.54357900	Cs	3.32436400	-0.32783300	-1.90614700
C	-4.07139100	-2.91954200	-1.37314200	C	1.75429900	1.67348500	2.55259800
H	-5.48004700	-2.57034200	-3.00396200	C	2.66729600	0.57281200	3.19267900
H	-3.99367500	-3.97645500	-1.16685700	C	0.66717500	-0.46292100	2.99553900
C	-3.29958000	0.44035700	1.51836300	C	0.39722900	0.91247200	2.35336500
C	-4.13403100	1.23926300	2.24819800	C	2.12712000	-0.73276000	2.57363200
O	-2.89000900	-0.62336900	2.29955700	H	2.55935000	-1.63688400	3.01804000
C	-4.25204300	0.64334800	3.54634400	H	2.25485200	-0.78356700	1.48848000
H	-4.61966500	2.13714000	1.89661100	C	2.22604200	0.40425500	4.66540000
C	-3.48492600	-0.47835400	3.52181000	H	2.92552800	-0.24389800	5.20681900
H	-4.83349100	1.00698800	4.38215200	H	2.18767000	1.36151500	5.19808600
H	-3.25883300	-1.24489900	4.24777000	C	0.82285000	-0.27262500	4.53278200
C	-3.35525700	1.99528000	-0.84581300	H	0.79977000	-1.24086300	5.04891800
C	-2.79140500	3.06755600	-1.48469800	H	0.01523700	0.33906200	4.94982700
O	-4.72394200	2.16524100	-0.78413100	H	3.73967100	0.75205600	3.07155500
C	-3.86187300	3.94775800	-1.83641400	H	-0.07278900	-1.23001800	2.74220200
H	-1.73457300	3.19448700	-1.67464700	H	-0.45447500	1.42979800	2.80893000
C	-5.00215900	3.35170000	-1.38759200	H	1.63736100	2.48479000	3.28879400
H	-3.78836200	4.89394000	-2.35373400	Cs	-0.14235400	-3.32126100	-0.07694100
H	-6.04635700	3.62646700	-1.41546800	I	-0.70994300	-0.18864200	-2.41118500
C	3.72935000	4.67951400	0.58408200	C	4.11965600	3.57670600	2.32831100
H	4.50267400	5.28953500	0.10498300	H	4.80610900	4.39159600	2.07432700
H	2.93719200	5.35631100	0.92890500	H	3.50030800	3.91191700	3.16995000
H	4.17161400	4.23399900	1.48361000	H	4.72368100	2.73978000	2.69987300

11

M06/BSII SCF energy in solution: -1751.950214 a.u.

Solution-phase enthalpy: -1751.408592 a.u.

Solution-phase Gibbs energy: -1751.536144 a.u.

Pd	-0.12218100	0.70137000	0.37486700	C	-5.50482500	-1.04017700	-0.05896700
C	2.19894300	2.27904800	1.24799300	C	-4.29085500	-1.31898100	0.58667300
C	3.27281600	3.19120100	1.13395300	C	-4.10932500	-2.55732500	1.22376500
C	1.39751300	1.96326400	0.12204100	C	-5.12705000	-3.50681000	1.21070100
C	3.53094400	3.78202000	-0.11067000	C	-6.32848300	-3.23176100	0.54921400
C	1.65911300	2.60729600	-1.10109800	C	-6.51461700	-2.00053800	-0.08372400
H	4.59624500	-2.71112100	1.14520400	H	-5.64481900	-0.08063500	-0.54325900
				H	-3.18230800	-2.74377100	1.75688400
				H	-4.99099800	-4.45620000	1.72114400
				H	-7.12159600	-3.97422500	0.53552300
				H	-7.44948500	-1.78584500	-0.59300400
				C	-3.18570200	-0.33287600	0.61637900

O	-2.04069800	-0.61065400	0.94224900	H	-0.44616600	3.23439500	-5.79736300
O	-3.55162800	0.90472400	0.18985300	H	0.61070300	4.30300800	-4.86847700
C	-3.13637100	2.06090300	0.89679000	C	1.27043400	2.17391700	-4.90307000
O	-2.98909500	2.02724400	2.09030400	H	1.23498000	1.58428000	-5.82694900
C	-3.05845600	3.24125500	0.01703000	H	2.28773300	2.56792300	-4.80590200
C	-3.07379200	3.13526300	-1.38175900	H	-1.61668000	3.45909000	-3.60036900
C	-2.95028100	4.49971500	0.63090000	H	1.29528100	0.28108200	-3.73641100
C	-2.98725000	4.28942100	-2.15807300	H	2.30452100	2.30697500	-2.33298500
H	-3.11825100	2.15838300	-1.84978500	H	0.82897200	4.19481800	-2.59009800
C	-2.86895000	5.64671500	-0.15164700	Cs	-0.44226600	-2.67078400	-2.84470100
H	-2.93067600	4.55590600	1.71428400	I	-0.50919500	-1.35682300	0.82585200
C	-2.88861700	5.54172900	-1.54655000	C	-1.44396700	5.65427100	-1.65051400
H	-2.98683500	4.20884300	-3.24111600	H	-1.99457900	6.46111300	-1.15559400
H	-2.78634600	6.62099200	0.32141300	H	-0.49281400	6.07074700	-2.00602300
H	-2.82089300	6.43839400	-2.15702800	H	-2.01076000	5.36582000	-2.54387100

TS12

M06/BSII SCF energy in solution: -1751.930961 a.u.

Solution-phase enthalpy: -1751.391281 a.u.

Solution-phase Gibbs energy: -1751.514391 a.u.

Pd	0.92098800	0.78736900	-0.77274300	C	4.75948800	-2.94042400	-0.37657200
C	-0.41563600	3.38545900	-1.06039000	C	3.89053500	-2.37223800	-1.31727900
C	-1.21962100	4.49470600	-0.70324700	C	3.79175000	-2.94053800	-2.59530200
C	-0.17096900	2.34982400	-0.13004400	C	4.54583200	-4.06569800	-2.92671500
C	-1.77824300	4.53471300	0.58068000	C	5.39685400	-4.63920700	-1.97776700
C	-0.71981400	2.43398000	1.15942300	C	5.50215200	-4.07429900	-0.70423200
H	-3.94555100	0.50104600	-4.73380400	H	4.84002400	-2.48460900	0.60420100
C	-1.52862500	3.51857300	1.50849600	H	3.14563500	-2.47042400	-3.33030700
H	-2.38777600	5.38997300	0.86683300	H	4.47737900	-4.49111200	-3.92481200
H	-0.51281100	1.65664000	1.88858700	H	5.98232700	-5.51844300	-2.23351500
H	-1.94474100	3.58670900	2.51208000	H	6.16814000	-4.51488400	0.03267100
C	-3.19505600	-0.89819300	-3.68190200	C	3.07197900	-1.16484900	-0.96142600
O	-3.17054100	-1.37742100	-2.52214300	O	2.08688900	-0.86561700	-1.69951100
O	-2.57224500	-1.24236000	-4.70750500	O	3.41439200	-0.51595400	0.07711200
O	-4.02233800	0.24318800	-3.80024100	C	2.92342600	1.37239700	0.11213700
Cs	-3.54196000	0.79153400	-0.52909500	O	3.66557500	1.94339300	-0.62368500
C	0.27309100	3.26493700	-2.39429300	C	2.71812100	1.60126400	1.56755800
C	-0.64064900	2.96669100	-3.63491900	C	2.32842900	0.60979300	2.47394700
C	0.87455100	1.28731000	-3.68308200	C	2.95332800	2.91358000	2.01249300
C	1.24943700	2.04498100	-2.40538000	C	2.17677100	0.93420800	3.82197000
C	-0.66228500	1.42529900	-3.69034300	H	2.14820600	-0.39760600	2.12391100
H	-1.14381500	1.02131200	-4.58613800	C	2.79275900	3.22782300	3.35908400
H	-1.13152000	0.96074400	-2.81552300	H	3.26430300	3.67019000	1.29987800
C	0.18282300	3.29471300	-4.90168300	C	2.40262800	2.23876800	4.26666900

M06/BSII SCF energy in solution: -1751.941825 a.u.

Solution-phase enthalpy: -1751.400855 a.u.

Solution-phase Gibbs energy: -1751.527096 a.u.

Pd	-0.08136300	0.99586500	0.52523900
C	2.65664600	1.02083400	1.58955600
C	4.05827900	1.22478400	1.61375000
C	1.90008700	1.41372300	0.46457400
C	4.67188400	1.80273200	0.49548500
C	2.53799000	2.01659300	-0.62953300
H	2.42479600	-4.80056800	0.98264300
C	3.92296800	2.19788200	-0.61727100
H	5.74628300	1.97592400	0.51209300
H	1.95777100	2.34162400	-1.48701200
H	4.41682000	2.67295100	-1.46278900
C	1.06714800	-4.20556000	-0.21720100
O	0.88498600	-3.59716700	-1.29857700
O	0.24261600	-4.67815200	0.59153800
O	2.43374000	-4.30545000	0.14678800
Cs	3.05184800	-1.58031700	-1.62346600
C	1.89720100	0.43275600	2.75195800
C	2.12960500	-1.09649300	3.02137700
C	-0.11237900	-0.94549900	2.75755000
C	0.35662300	0.48740400	2.51223600
C	1.04576000	-1.76753700	2.15487100
H	0.95255200	-2.84575300	2.31298000
H	1.17289300	-1.59610000	1.07923700
C	1.60535500	-1.40120800	4.44310900
H	1.86311700	-2.42475400	4.73792000
H	2.02918100	-0.72657900	5.19531700
C	0.06169400	-1.23598800	4.28065300
H	-0.46979900	-2.15715600	4.54650400
H	-0.34977800	-0.43187800	4.89988700
H	3.15661500	-1.42777800	2.84699900
H	-1.12244200	-1.14147800	2.39708700
H	-0.17646100	1.24726100	3.08027300
H	2.15174800	0.99404100	3.66368200
Cs	-1.98061800	-2.74717700	-0.64252500
I	-0.29189100	0.28639800	-2.41771400
C	4.89632900	0.88460700	2.82801800
H	5.91154200	1.28066600	2.72171900
H	4.46830100	1.30927100	3.74439300
H	4.98068900	-0.19630200	2.99422400
C	-5.47114100	1.28124000	-0.04735700
C	-4.44825100	0.56695300	0.58956900

C	-4.76539100	-0.61512300	1.27422900
C	-6.08104800	-1.08043700	1.31373900
C	-7.09151500	-0.37348500	0.65598700
C	-6.78311800	0.80863000	-0.02275200
H	-5.21550000	2.20538300	-0.55500100
H	-3.97795100	-1.14387500	1.80370000
H	-6.32080300	-1.98690400	1.86480800
H	-8.11584100	-0.73637800	0.68227700
H	-7.56817200	1.36580300	-0.52746100
C	-3.02980700	1.08674600	0.52367800
O	-2.10477600	0.21402100	0.74937900
O	-2.83271800	2.28179600	0.24988600
C	-0.49321300	2.96525000	1.15268200
O	-0.73438700	3.20638400	2.29221900
C	-0.24931800	3.97078800	0.07811900
C	-0.74441500	3.86304700	-1.22553500
C	0.52784400	5.08089600	0.45328900
C	-0.45307700	4.86414100	-2.15206100
H	-1.36957300	3.02222000	-1.49215000
C	0.82114500	6.06814500	-0.48382400
H	0.89351600	5.15952900	1.47206200
C	0.33293600	5.95981000	-1.78919400
H	-0.84463300	4.78213000	-3.16196700
H	1.42414500	6.92403200	-0.19304300
H	0.55959000	6.73268100	-2.51906900

TS14

M06/BSII SCF energy in solution: -1751.931191 a.u.

Solution-phase enthalpy: -1751.391571 a.u.

Solution-phase Gibbs energy: -1751.515671 a.u.

Pd	0.10604900	1.13507400	0.59739300
C	2.68592800	1.12289600	1.98746400
C	4.09103700	1.03639800	2.08450500
C	2.10443100	1.73836900	0.84223300
C	4.87082800	1.47169200	0.99940600
C	2.91586400	2.15545600	-0.22984200
H	1.92673400	-4.16236200	0.83873600
C	4.29897500	2.00113000	-0.15929500
H	5.95492100	1.42164900	1.08473500
H	2.45644200	2.61725000	-1.09618500
H	4.93192700	2.34296600	-0.97527100
C	0.80747100	-3.75524100	-0.65233800
O	0.82892800	-3.33585100	-1.83395200
O	-0.14957600	-4.05788500	0.08632100

O	2.09942900	-3.83015300	-0.05764500
Cs	3.06405600	-1.35774500	-1.78804600
C	1.74027600	0.63461900	3.06615600
C	1.93598500	-0.86809200	3.48843100
C	-0.22875000	-0.80647100	2.84492300
C	0.24283800	0.62695800	2.60018400
C	1.02852700	-1.62634400	2.50310700
H	0.92618500	-2.69162900	2.73762700
H	1.33613700	-1.53256100	1.45678600
C	1.18107300	-1.07478700	4.82233700
H	1.42325500	-2.05568600	5.24717700
H	1.44570900	-0.32036300	5.57172700
C	-0.31607300	-1.00303200	4.38821500
H	-0.84396300	-1.93613900	4.61778700
H	-0.86313800	-0.18934800	4.87582800
H	2.97586800	-1.19293000	3.52250100
H	-1.14771500	-1.06217500	2.32053700
H	-0.37569700	1.38716800	3.07835200
H	1.86694900	1.27710200	3.94855000
Cs	-2.00956200	-2.13088100	-1.51623500
I	0.09862100	1.06197900	-2.42555100
C	4.81240200	0.55552800	3.32870100
H	5.77441900	1.07054400	3.42499700
H	4.23790700	0.75195100	4.23799400
H	5.02610700	-0.52032100	3.30239200
C	-5.29147000	1.20959900	0.16565900
C	-4.19864800	0.45791200	0.61780400
C	-4.41448200	-0.84935600	1.07823100
C	-5.69916500	-1.39792100	1.07808400
C	-6.77896900	-0.64900500	0.60224700
C	-6.57155700	0.65639600	0.14730000
H	-5.11337800	2.22879000	-0.16153300
H	-3.57617900	-1.41958500	1.46880500
H	-5.85933200	-2.40416000	1.45834800
H	-7.77857400	-1.07615200	0.59833800
H	-7.41070000	1.24588800	-0.21321100
C	-2.82112700	1.09057400	0.60573600
O	-1.83733800	0.24153000	0.55082400
O	-2.71845000	2.31993000	0.63250000
C	0.91462600	3.13345800	1.30228300
O	0.89201500	3.38685500	2.47727400
C	0.74077100	4.19797000	0.25029000
C	-0.43332600	4.30589700	-0.50097900
C	1.74452100	5.17276600	0.14211600

C	-0.58634500	5.38620300	-1.37374000
H	-1.22557800	3.57464200	-0.37822100
C	1.58728500	6.23622400	-0.74399600
H	2.64292100	5.09177000	0.74761100
C	0.41970400	6.34307000	-1.50543300
H	-1.50047600	5.47185000	-1.95430200
H	2.37065700	6.98436100	-0.83269500
H	0.29474300	7.17482300	-2.19389700

15

M06/BSII SCF energy in solution: -1751.961664 a.u.

Solution-phase enthalpy: -1751.41917 a.u.

Solution-phase Gibbs energy: -1751.543405 a.u.

Pd	1.01411500	-0.12499400	0.20958700
C	2.88090300	-1.52419700	0.78735400
C	2.68079600	-2.88063900	0.37033200
C	3.44952500	-0.60878000	-0.17674400
C	3.02588900	-3.26180400	-0.92784200
C	3.77641900	-1.05627500	-1.47675800
H	-4.29512900	-1.46066200	2.43586000
C	3.56675500	-2.36866900	-1.85127100
H	2.87581100	-4.29805500	-1.22187400
H	4.22071700	-0.35860000	-2.17677200
H	3.81944000	-2.70172000	-2.85315000
C	-4.32368700	-1.03241000	0.57719300
O	-4.05702500	-1.48939000	-0.56046300
O	-4.72857600	0.09493200	0.92074600
O	-4.05487300	-1.94833900	1.63048300
Cs	-1.78042200	-3.32030500	-0.13337200
C	2.71295900	-0.96536500	2.22978900
C	2.10305300	-1.78878100	3.39894900
C	0.65912500	-0.04918300	3.20090900
C	1.69389400	0.19680400	2.10595500
C	0.57972300	-1.58951900	3.23457400
H	0.00074600	-1.97934100	4.08077300
H	0.17296700	-2.00050800	2.30337800
C	2.36064900	-0.95822200	4.68709300
H	2.12953200	-1.56111400	5.57271500
H	3.40667500	-0.64527800	4.76920300
C	1.37467200	0.24468800	4.55067700
H	0.64790600	0.26354900	5.37163700
H	1.88337900	1.21379100	4.54180100
H	2.46486400	-2.81128500	3.49589600
H	-0.27969900	0.48694200	3.06053700

H	2.09775500	1.20888400	2.07449300	C	3.32713700	-3.93220800	0.36443800
H	3.70081400	-0.60482400	2.52234000	C	4.51473400	-2.04212400	-0.51456200
Cs	-3.11440200	1.26207200	-1.53950600	H	-3.79070800	4.43407700	-0.51750900
I	0.04596900	-0.87365400	-2.50674500	C	4.35472200	-3.42066100	-0.42268100
C	2.18959500	-3.99756100	1.27343500	H	3.15724000	-5.00614800	0.38648600
H	1.99045500	-4.89349300	0.67509700	H	5.28274600	-1.62602800	-1.16021900
H	2.94477800	-4.27709700	2.01704800	H	5.00361100	-4.08832000	-0.98244000
H	1.28093300	-3.74855000	1.82568300	C	-2.50987500	3.58596900	-1.64881000
C	-1.34487800	4.61904000	1.27193300	O	-2.25744800	2.50616000	-2.23757100
C	-1.51439600	3.22634600	1.28165900	O	-1.82153900	4.61981300	-1.52859000
C	-2.73250500	2.68792200	1.72312300	O	-3.75563200	3.57723800	-0.97376500
C	-3.76678900	3.53163800	2.13646100	Cs	-3.36714100	0.42644100	-0.39069700
C	-3.59334500	4.91766900	2.11510200	C	2.72984900	-0.77572200	2.87134800
C	-2.37844500	5.45965100	1.68259500	C	2.41619100	-1.64303900	4.08748700
H	-0.38992400	5.01590300	0.94306600	C	0.96685100	0.09642900	4.20592800
H	-2.88494400	1.61371500	1.73678700	C	1.77481800	0.31050500	2.93069800
H	-4.70511700	3.09746400	2.47130700	C	0.89627600	-1.44334000	4.28003100
H	-4.39851000	5.57349600	2.43743200	H	0.54366200	-1.81091700	5.25079300
H	-2.23706700	6.53763600	1.67024700	H	0.28637300	-1.87860600	3.48584800
C	-0.36362900	2.35516500	0.81424800	C	2.96436700	-0.79089700	5.28366200
O	-0.67656900	1.10351200	0.60584600	H	2.95247500	-1.39788300	6.19551400
O	0.75088400	2.85769200	0.65169100	H	3.99743600	-0.46673600	5.12126100
C	4.08909900	0.72609300	0.19655900	C	1.95684500	0.39861300	5.37373000
O	4.73505900	0.82048500	1.23422200	H	1.42503100	0.39847700	6.33225400
C	4.05496200	1.87386900	-0.76590600	H	2.44022000	1.37444700	5.26441300
C	3.08800700	2.01897400	-1.77291600	H	2.80857400	-2.66071600	4.06638300
C	5.03763200	2.86694800	-0.61007200	H	0.02244600	0.63971300	4.25452600
C	3.11484500	3.13189800	-2.61319500	H	2.07381000	1.31665700	2.64192000
H	2.30081100	1.28160800	-1.89087300	H	3.76595000	-0.52393700	2.68798000
C	5.06639500	3.97099900	-1.45550800	Cs	0.74872200	2.81462600	-1.86383200
H	5.76952100	2.75079500	0.18232300	I	-0.03378900	-1.36918900	-1.32375900
C	4.10385700	4.10485400	-2.46160000	C	1.31160800	-3.77440400	1.81142600
H	2.35609700	3.23760200	-3.38365200	H	0.37922800	-3.23535500	1.62310300
H	5.83536900	4.72889400	-1.33181600	H	1.18553700	-4.79329100	1.43201100
H	4.12385000	4.96845200	-3.12166700	H	1.45158800	-3.84491900	2.89451500
				C	-2.01026700	4.15667600	1.92542500
				C	-1.83040300	2.79825500	2.22117500
				C	-2.72030200	2.16460800	3.10141500
				C	-3.76770300	2.87978000	3.68617100
				C	-3.94246200	4.23316600	3.38451000
Pd	0.93460200	-0.44455200	1.18982700	C	-3.06449800	4.86723200	2.50033000
C	2.68499400	-1.69847900	1.09156400	H	-1.33760500	4.63194300	1.22023300
C	2.47306400	-3.10461700	1.10580900	H	-2.56936400	1.11419900	3.33308200
C	3.70681300	-1.18243200	0.24195000	H	-4.44122200	2.38520200	4.38215700

TS16

M06/BSII SCF energy in solution: -1751.941349 a.u.

Solution-phase enthalpy: -1751.401344 a.u.

Solution-phase Gibbs energy: -1751.524073 a.u.

H	-4.75733800	4.79156000	3.83840700	H	-1.38587700	4.97043400	-1.50341900
H	-3.19918400	5.91938100	2.26151200	H	-1.08398500	3.63730600	-0.34405800
C	-0.67874900	2.04121100	1.58968300	C	1.07835800	5.42601200	-2.26716200
O	-0.82148300	0.75619800	1.56810400	H	0.61087900	6.41294800	-2.35755500
O	0.28681000	2.67537000	1.13182400	H	2.15655600	5.55888700	-2.40268200
C	4.02264100	0.28458900	0.13192900	C	0.45731800	4.40457900	-3.27213000
O	4.23604800	0.98260600	1.11910100	H	-0.33077800	4.86884200	-3.87508300
C	4.14053700	0.89647800	-1.24023400	H	1.19527900	3.98359100	-3.96222200
C	3.59177500	0.30293100	-2.38918200	H	0.81832400	5.48455400	-0.02891900
C	4.78346500	2.14190000	-1.34983800	H	-0.88821500	2.65249000	-2.81084500
C	3.70001900	0.94147100	-3.62794900	H	1.55567500	1.78450400	-2.13391200
H	3.05487500	-0.63673200	-2.31048600	H	2.59393600	3.52925200	-0.44858300
C	4.89503700	2.77391900	-2.58644300	Cs	-0.08977900	-2.41085500	-1.61247100
H	5.18873300	2.59341800	-0.44999100	I	0.72597300	-0.54882600	2.22663700
C	4.35531500	2.17188200	-3.73076400	C	2.43279900	3.14484500	2.55119700
H	3.27168600	0.47488400	-4.51111500	H	1.74191600	2.53940700	3.14959500
H	5.40786700	3.72905400	-2.66395700	H	3.00989100	3.78050100	3.23224500
H	4.44912000	2.65990600	-4.69770200	H	1.81725400	3.79444500	1.91822100

17

M06/BSII SCF energy in solution: -1751.963009 a.u.

Solution-phase enthalpy: -1751.422174 a.u.

Solution-phase Gibbs energy: -1751.549345 a.u.

Pd	0.85392500	1.43348600	0.36082900	C	-4.20858000	0.38010800	-1.73791200
C	2.83655700	1.38273000	0.74257500	C	-3.42888700	1.17462900	-0.88508000
C	3.34444600	2.25706800	1.73207500	C	-4.05533700	2.14925600	-0.09334800
C	3.73351400	0.49794000	0.09815200	C	-5.43804100	2.33437100	-0.16049700
C	4.72284400	2.29341000	1.98053300	C	-6.20906100	1.53783600	-1.01283400
C	5.11459400	0.54512500	0.38794400	C	-5.59130900	0.55990700	-1.79759900
H	-5.11039500	-2.67009300	-0.93121300	H	-3.71860600	-0.38893800	-2.32649000
C	5.61373200	1.45857100	1.30421200	H	-3.44405900	2.76365200	0.56067800
H	5.10199800	2.98551900	2.72994300	H	-5.91298700	3.10401200	0.44352400
H	5.79038200	-0.13135700	-0.12719200	H	-7.28543800	1.68098000	-1.06639900
H	6.67967700	1.50958400	1.50785100	H	-6.18884900	-0.06288700	-2.45886400
C	-3.26472300	-3.03232600	-0.61521200	C	-1.92621900	0.95118500	-0.82427800
O	-2.39430200	-3.06669400	0.28828200	O	-1.33899100	1.45757800	0.20383400
O	-3.16416400	-3.20224000	-1.84611200	O	-1.38670600	0.29765000	-1.73474700
O	-4.55597700	-2.68791700	-0.13400500	C	3.27988900	-0.50959300	-0.90023500
Cs	-3.17978700	-0.83433000	2.10349900	O	2.39123700	-0.28420200	-1.72612300
C	1.57662200	3.53971900	-0.81816100	C	3.91702800	-1.87337700	-0.90603500
C	0.72517400	4.79646200	-0.87235600	C	4.32974100	-2.50876900	0.27568300
C	-0.16886600	3.31401400	-2.33072400	C	4.00496000	-2.56760000	-2.12505400
C	1.03977500	2.63646200	-1.70366400	C	4.81788200	-3.81624200	0.23553600
C	-0.66784300	4.21079300	-1.17260900	H	4.24154800	-1.98718400	1.22314100
				C	4.51402200	-3.86392300	-2.16562500
				H	3.68393500	-2.06794800	-3.03461700
				C	4.91706600	-4.49252100	-0.98212800
				H	5.12006500	-4.30637300	1.15689300
				H	4.59967600	-4.38466200	-3.11585800

H	5.30766100	-5.50627700	-1.01124400
---	------------	-------------	-------------

18

M06/BSII SCF energy in solution: -1825.053775 a.u.

Solution-phase enthalpy: -1824.539358 a.u.

Solution-phase Gibbs energy: -1824.669931 a.u.

Pd	-1.12367500	-1.78303000	0.20963100
C	-3.00388900	-1.50301100	-0.49919500
C	-4.07458700	-2.35958600	-0.15513900
C	-3.26053700	-0.40785900	-1.34964500
C	-5.32955900	-2.15768000	-0.74938400
C	-4.54123500	-0.20421100	-1.89724600
H	3.91902800	3.83116000	1.11443100
C	-5.56796900	-1.09954000	-1.62529700
H	-6.14152700	-2.83713000	-0.49805400
H	-4.71773300	0.65196300	-2.54398600
H	-6.54975500	-0.96347600	-2.07034900
C	2.84886000	3.44796300	-0.41012500
O	1.69744000	3.57229400	-0.88952600
O	3.86118300	2.87439400	-0.86840500
O	2.98794000	3.99534600	0.88993100
Cs	0.14013500	2.69562800	1.57180200
C	-1.13410300	-3.69401900	-1.04329700
C	-0.33362300	-2.80578300	-1.72323500
H	-0.74122600	-2.11956300	-2.45814800
H	-2.18156900	-3.79227100	-1.29697300
Cs	2.06337900	0.94956700	-2.49766600
I	-1.98227300	-0.53189500	2.46207800
C	-3.94543500	-3.44951800	0.88749500
H	-3.00449900	-4.00144500	0.81126400
H	-3.96192900	-3.00982100	1.89213300
H	-4.77285500	-4.16406600	0.81457200
C	3.96848400	-0.12164400	1.35733900
C	2.98950500	-1.10223200	1.58073400
C	3.29373900	-2.20359700	2.39364300
C	4.55487100	-2.32198500	2.97802400
C	5.52875500	-1.34614200	2.74706900
C	5.23347300	-0.24870300	1.93404000
H	3.74236400	0.73414400	0.72741400
H	2.52733800	-2.95297800	2.56109300
H	4.77906400	-3.17456900	3.61436200
H	6.51310900	-1.44079600	3.19897100
H	5.98828500	0.51083100	1.74624100
C	1.62429300	-0.96675600	0.94273100

O	0.88144900	-2.00890400	0.98945000
O	1.31222600	0.12221000	0.40309300
C	-2.21058000	0.60552900	-1.70471500
O	-1.17008800	0.29882400	-2.28728700
C	-2.46816500	2.04048700	-1.33987000
C	-3.41651400	2.39675800	-0.36516400
C	-1.68852200	3.04671000	-1.93452900
C	-3.57719700	3.73449800	0.00220100
H	-4.00618200	1.62521000	0.11699400
C	-1.85196200	4.38119500	-1.57212800
H	-0.95224100	2.76786600	-2.67946200
C	-2.79914900	4.72736000	-0.60141200
H	-4.31100700	4.00036300	0.75842600
H	-1.23403400	5.14541900	-2.03341700
H	-2.93014500	5.76869100	-0.31820900
H	-0.68968400	-4.46498600	-0.42212300
C	1.15346000	-2.91054100	-1.73444900
O	1.60545000	-3.99763500	-1.09993500
O	1.87198000	-2.11699300	-2.32614800
C	3.04114300	-4.15165200	-0.98260900
H	3.17153600	-4.73381700	-0.06823500
H	3.48985700	-3.16656400	-0.84268500
C	3.61992100	-4.86898100	-2.19299500
H	3.49172200	-4.26831900	-3.09809600
H	4.69200600	-5.04084100	-2.04196900
H	3.13484200	-5.83957900	-2.34125100

TS19

M06/BSII SCF energy in solution: -1825.030151 a.u.

Solution-phase enthalpy: -1824.516651 a.u.

Solution-phase Gibbs energy: -1824.646709 a.u.

Pd	-0.30731400	-1.46973300	-0.01024000
C	-2.39800200	-1.79560800	0.33544100
C	-2.65144500	-2.78789100	1.31243500
C	-3.31139500	-0.70970500	0.20145900
C	-3.82269800	-2.71102200	2.07958900
C	-4.46705800	-0.66411500	0.99331400
H	3.28040100	3.87159100	-3.33569000
C	-4.73508900	-1.67332000	1.91582600
H	-4.01233300	-3.48180800	2.82326500
H	-5.16668100	0.15664100	0.87467000
H	-5.64429000	-1.64288800	2.50941400
C	2.25810600	2.50725800	-4.17429000
O	1.09607400	2.06834900	-4.33251100

O	3.35556300	2.06539800	-4.58657700
O	2.33220100	3.66038300	-3.35588400
Cs	0.08980400	2.39737600	-1.44481700
C	-1.90883500	-2.63306800	-1.39662300
C	-0.59965900	-2.36475200	-1.91413900
H	-0.50057900	-1.51571500	-2.58323400
H	-2.71412100	-2.10831000	-1.89352600
Cs	2.25769800	-0.77004200	-4.75548200
I	-0.13003600	0.21146400	2.16463000
C	-1.67204300	-3.90039400	1.60906100
H	-1.08807700	-4.19988500	0.73455000
H	-0.95215400	-3.56171200	2.36505800
H	-2.18674600	-4.78177300	2.00871200
C	4.69613100	-0.02726400	-1.74127500
C	3.92247900	-0.85023800	-0.90760200
C	4.56248000	-1.73258200	-0.02643600
C	5.95488400	-1.79997400	0.01427100
C	6.72164500	-0.98459000	-0.82299700
C	6.08974800	-0.09746200	-1.69835000
H	4.20494500	0.67370600	-2.41117600
H	3.95359300	-2.35111000	0.62388600
H	6.44341600	-2.48476500	0.70297100
H	7.80715300	-1.03554800	-0.78800100
H	6.68118900	0.54718100	-2.34384800
C	2.41378500	-0.77178800	-0.97176200
O	1.78757800	-1.52159800	-0.14151800
O	1.87919900	-0.01304400	-1.81052300
C	-3.09109500	0.38378300	-0.79135200
O	-2.51669400	0.18980300	-1.86635500
C	-3.56875400	1.77503300	-0.48230300
C	-3.52931100	2.30970200	0.81633500
C	-3.95384900	2.59749300	-1.55580000
C	-3.87742600	3.64491300	1.03259900
H	-3.18493100	1.69382100	1.64111200
C	-4.32093200	3.92244900	-1.33237200
H	-3.96428200	2.17967700	-2.55803100
C	-4.28081900	4.44893800	-0.03600600
H	-3.82901500	4.05612400	2.03705100
H	-4.63570000	4.54585100	-2.16488500
H	-4.56062700	5.48457400	0.13813600
H	-2.12235900	-3.65625300	-1.10825300
C	0.40654900	-3.41312600	-2.17113300
O	0.25573600	-4.51595500	-1.40630200
O	1.28528500	-3.30074200	-3.01782700

20

M06/BSII SCF energy in solution: -1825.058223 a.u.

Solution-phase enthalpy: -1824.541819 a.u.

Solution-phase Gibbs energy: -1824.671784 a.u.

Pd	-1.26869200	1.13400800	-0.33665100
C	-3.20441500	1.63822200	1.02788100
C	-3.93348200	2.44061000	0.10000600
C	-3.55246900	0.25286800	1.15907600
C	-5.00828100	1.88232900	-0.59635000
C	-4.65679600	-0.25467400	0.45214500
H	4.62910300	-3.27856600	-1.15179200
C	-5.38694500	0.55580000	-0.40593300
H	-5.56108900	2.50384500	-1.29527000
H	-4.95295700	-1.28730500	0.59361600
H	-6.23877500	0.14965800	-0.94314100
C	3.63461400	-2.86027900	0.41381400
O	2.54656200	-3.05711800	1.00073900
O	4.61062300	-2.14271900	0.73129900
O	3.74176600	-3.51880300	-0.83709700
Cs	0.70123500	-2.80483100	-1.43106100
C	-2.18083400	2.31055100	1.96076500
C	-0.79127500	1.83373600	1.55310200
H	-0.48426800	0.92690100	2.07636000
H	-2.40479000	2.04890800	2.99752800
Cs	2.83747200	-0.30797300	2.41253100
I	-2.09403900	-0.18301800	-2.68020700
C	-3.61730000	3.90636400	-0.11128200
H	-2.54636200	4.08572900	-0.23809300
H	-4.12942300	4.27577200	-1.00428200
H	-3.95534600	4.51410600	0.73904900
C	4.05935900	0.81523300	-1.44129900
C	2.85415000	1.51321700	-1.61485400
C	2.84464600	2.69773000	-2.36501000
C	4.02384600	3.17959700	-2.93254800
C	5.22354600	2.48551200	-2.75235500
C	5.23840900	1.30438800	-2.00592700

H	4.07192800	-0.10604400	-0.86506500	C	-3.70708000	-1.76424000	3.72721700
H	1.90579900	3.22367800	-2.49993000	H	-1.83406400	-2.48099000	4.49757800
H	4.00737500	4.09548800	-3.51785900	H	-5.44746700	-1.09614300	2.65787700
H	6.14252400	2.86240100	-3.19440400	H	-4.19349000	-1.74351500	4.69871400
H	6.16839000	0.75977500	-1.86367500	C	3.17263700	0.20030500	3.42985800
C	1.58897800	0.97866000	-0.98720600	O	2.21734000	-0.35657200	2.83379200
O	0.55752000	1.73607400	-1.11812200	O	3.22403200	1.30033900	4.01511400
O	1.60976800	-0.11866700	-0.39329200	O	4.38462600	-0.52735700	3.36001800
C	-2.88201100	-0.65750600	2.15938400	Cs	3.54094300	-1.53831900	0.40336700
O	-2.47526900	-0.23050600	3.23667600	C	-1.73698800	-1.91362600	-0.15918900
C	-2.73981200	-2.12635100	1.85963200	C	-0.76275800	-0.73087600	-0.32301100
C	-2.75593500	-2.66444800	0.56135300	H	-0.07093100	-0.64116700	0.51699000
C	-2.52941700	-2.98567300	2.95211300	H	-2.46011000	-1.91859600	-0.97126700
C	-2.58618600	-4.03848100	0.37147100	Cs	0.87275800	2.33491800	2.30790700
H	-2.88128200	-2.01629000	-0.30143400	I	1.05688200	-3.53347400	-2.11010500
C	-2.35985600	-4.35341000	2.75840500	C	-0.29269000	-2.69407500	2.35225700
H	-2.50507800	-2.55651600	3.94833300	H	0.40871600	-1.86829000	2.53155100
C	-2.39112600	-4.88541800	1.46529300	H	-0.12849100	-3.42175000	3.15483000
H	-2.62681100	-4.44862300	-0.63546000	H	-0.01543700	-3.17599700	1.41003900
H	-2.20598700	-5.00723400	3.61232000	C	2.98093200	3.85832800	-1.07770300
H	-2.26734400	-5.95446800	1.31308900	C	2.04103500	3.12512800	-1.81678000
H	-2.25161600	3.39125100	1.85155600	C	1.45439600	3.71018100	-2.94747400
C	0.33399100	2.79632700	1.54419400	C	1.79080800	5.01151300	-3.32149200
O	-0.01680800	4.03032100	1.12193000	C	2.71768400	5.74064600	-2.57207400
O	1.47968700	2.51175800	1.87992400	C	3.31547900	5.16022900	-1.44978900
C	1.04465100	5.00153600	0.97543800	H	3.45485300	3.38320800	-0.22410200
H	0.67488000	5.68941900	0.21112300	H	0.74328000	3.13146600	-3.52592700
H	1.93541100	4.49232100	0.60135000	H	1.33252200	5.45626700	-4.20091200
C	1.32390200	5.72617500	2.28449000	H	2.97959000	6.75387700	-2.86565900
H	1.70625800	5.02976600	3.03611200	H	4.04738800	5.71902700	-0.87190300
H	2.07549700	6.50821200	2.12425400	C	1.69205400	1.71842300	-1.38460500
H	0.41449600	6.19917800	2.67050500	O	0.80151200	1.13089200	-2.10917600

21

M06/BSII SCF energy in solution: -1825.057153 a.u.

Solution-phase enthalpy: -1824.540557 a.u.

Solution-phase Gibbs energy: -1824.67256 a.u.

Pd	0.53459400	-0.93344400	-1.90020200	C	-4.68126300	-1.18486700	0.13099700
C	-2.44377100	-1.86562000	1.19579700	O	-4.70212500	-1.94868000	-0.82604400
C	-1.73530200	-2.22859800	2.36681400	C	-5.59910000	0.00846000	0.14751500
C	-3.79381000	-1.44831100	1.32077200	C	-5.39588300	1.12263000	0.97715500
C	-2.38421600	-2.17766300	3.60956400	C	-6.67024700	0.02084300	-0.76144500
C	-4.40672100	-1.39583600	2.58288800	C	-6.25324600	2.22190900	0.90435700
H	5.01289600	0.01094700	3.86985300	H	-4.55855400	1.13521200	1.66716900
				C	-7.53096200	1.11299400	-0.82561300
				H	-6.80373800	-0.83985900	-1.40871300
				C	-7.32419000	2.21699100	0.00849700
				H	-6.08460200	3.08194300	1.54714100

H	-8.36246900	1.10771400	-1.52519900	C	4.72209000	3.14792100	-1.68775100
H	-7.99485600	3.07075600	-0.04248300	C	3.69318400	3.50143200	-0.80300500
H	-1.18050500	-2.84681000	-0.23545600	C	3.84095300	4.64858100	-0.01044300
C	-1.46358700	0.59752700	-0.48966700	C	5.00003300	5.42160400	-0.09499700
O	-2.35370600	0.58344300	-1.49147200	C	6.02423500	5.05763600	-0.97411100
O	-1.28096000	1.56549600	0.23874600	C	5.88227000	3.91885200	-1.77274500
C	-3.09141400	1.79879600	-1.77177400	H	4.59253300	2.26780900	-2.30982800
H	-4.04658600	1.44564700	-2.16483600	H	3.03812900	4.92570600	0.66373900
H	-3.26363200	2.32996500	-0.83382700	H	5.10352500	6.30999900	0.52254700
C	-2.35375000	2.66565400	-2.77928800	H	6.92606600	5.66068300	-1.04036900
H	-2.96612600	3.54119500	-3.02691700	H	6.67296400	3.63555500	-2.46294800
H	-1.39957600	3.00777900	-2.37185700	C	2.44403200	2.64466600	-0.72491600
H	-2.15715900	2.10788900	-3.70046300	O	1.56774500	3.03798100	0.12189900

TS22

M06/BSII SCF energy in solution: -1825.036748 a.u.

Solution-phase enthalpy: -1824.526526 a.u.

Solution-phase Gibbs energy: -1824.661762 a.u.

Pd	-0.34037200	2.15186700	0.46142900	C	-3.44408700	0.24160300	6.58633000
C	-2.14202900	-0.49257300	1.78994000	C	-2.59464000	-2.39036900	6.98570100
C	-2.31151500	-1.25850500	0.61129600	H	-2.26665600	-2.45473700	4.86084800
C	-3.00002400	-0.73812900	2.89887200	C	-3.44775800	-0.30133200	7.86739300
C	-3.31453300	-2.23842700	0.57542100	H	-3.76006400	1.26502300	6.41300700
C	-3.96937600	-1.74685300	2.83207500	C	-3.02158800	-1.61918300	8.06923500
H	2.42447000	-1.96112700	-5.27454800	H	-2.25384600	-3.40974800	7.14239100
C	-4.13440800	-2.49336700	1.66890900	H	-3.77883800	0.29892100	8.71003400
H	-3.44833800	-2.80815600	-0.34037500	H	-3.02031400	-2.04188600	9.07017500
H	-4.61501100	-1.92283700	3.68624900	H	-1.77460500	1.65542700	0.90338100
H	-4.90251400	-3.25903400	1.61344400	C	1.44310200	0.80562100	2.38609300
C	2.19137400	-1.93625400	-3.37910900	O	1.10765900	1.58463500	3.42821200
O	1.38674600	-1.62391900	-2.47169100	O	2.58537400	0.43634800	2.14522400
O	3.35219100	-2.39830000	-3.30930000	C	2.17969900	2.07366000	4.27598300
O	1.70497600	-1.68188200	-4.68374300	H	1.72111800	2.16684100	5.26263600
Cs	0.21881100	1.06717400	-3.63981500	H	2.96760300	1.31863700	4.31182200
C	-1.05986700	0.52464000	1.97697000	C	2.70250700	3.40922500	3.77203900
C	0.28860900	0.39174800	1.55060000	H	3.48829100	3.77262500	4.44433800
H	0.55519000	-0.38272700	0.84097400	H	3.12056800	3.30910600	2.76655000
H	-1.19027600	1.13503300	2.86106800	H	1.90092300	4.15416200	3.74243000
Cs	3.82645300	-0.99260100	-0.50362400				
I	-1.71751300	3.97886000	-1.02662700				
C	-1.49290700	-1.04972600	-0.63892500				
H	-0.53428600	-1.58118900	-0.62333600				
H	-2.04218600	-1.41722700	-1.51162200				
H	-1.26964800	0.01237400	-0.79300500				

23

M06/BSII SCF energy in solution: -1825.044162 a.u.

Solution-phase enthalpy: -1824.531672 a.u.

Solution-phase Gibbs energy: -1824.665694 a.u.

Pd	0.39477900	-0.05649700	1.21922200
----	------------	-------------	------------

C	3.02596700	-1.43008000	-0.31906500
C	2.50589500	-2.71035400	-0.65071100
C	4.42945900	-1.30273000	-0.10538100
C	3.38233200	-3.80036900	-0.73329500
C	5.27244900	-2.41374200	-0.22547300
H	-4.49156600	-4.10564300	-2.25090300
C	4.75108200	-3.66766200	-0.52597000
H	2.96832600	-4.77817800	-0.96617300
H	6.33808900	-2.29317100	-0.05727700
H	5.40443300	-4.53280300	-0.59482400
C	-3.13542300	-2.79197100	-2.48087300
O	-2.06700200	-2.35116600	-1.99311500
O	-3.79883100	-2.39905400	-3.46292700
O	-3.69799900	-3.86526500	-1.74391300
Cs	-2.77329100	-2.35920900	0.98292100
C	2.22479100	-0.18237900	-0.26056900
C	1.05659500	0.13593800	-0.94475400
H	0.50486700	-0.59354500	-1.52377100
H	2.76524100	0.66689800	0.13790900
Cs	-2.71501200	0.46364800	-3.07953400
I	-0.47194700	-0.58828400	3.69335300
C	1.04013200	-2.98045400	-0.88144200
H	0.68588900	-2.66195200	-1.86824400
H	0.83585600	-4.05321000	-0.80710200
H	0.41992100	-2.45969300	-0.14403500
C	-4.28685400	2.90808200	0.19177000
C	-2.95842000	2.86725900	0.63623100
C	-2.38760200	4.02579100	1.18032800
C	-3.12793700	5.20538300	1.26494200
C	-4.44822400	5.24054800	0.80793300
C	-5.02858400	4.08713100	0.27327700
H	-4.72918500	1.99593500	-0.19768600
H	-1.36667100	3.97738200	1.54346000
H	-2.67791100	6.09725500	1.69379300
H	-5.02495300	6.15951100	0.87632400
H	-6.05999400	4.10600300	-0.07086600
C	-2.15993300	1.58069500	0.52667800
O	-0.94540500	1.65870600	0.90583700
O	-2.73277000	0.56281200	0.06080100
C	5.08307700	-0.01508500	0.33974300
O	4.64268300	0.61733400	1.29215100
C	6.30644000	0.46986500	-0.38155400
C	6.64380100	0.05175900	-1.67862500
C	7.10210700	1.43727000	0.25553700

C	7.76068200	0.58631400	-2.32199800
H	6.02673100	-0.68090800	-2.18840500
C	8.22328700	1.95873600	-0.38213700
H	6.81810800	1.76381200	1.25062100
C	8.55455800	1.53415800	-1.67347700
H	8.00965000	0.26326700	-3.32908900
H	8.83916300	2.69830400	0.12222400
H	9.42799400	1.94462000	-2.17332700
H	1.24799500	-1.23975400	1.68324500
C	0.73771500	1.53567700	-1.33326100
O	1.48269900	2.45649200	-0.71430700
O	-0.09747200	1.80361300	-2.18822100
C	1.13797100	3.83997800	-0.95569300
H	1.29113500	4.05972800	-2.01775500
H	0.07734600	3.97098800	-0.72569300
C	2.02416900	4.68756400	-0.06297000
H	1.79311600	5.74816400	-0.21289900
H	1.85950000	4.44030100	0.99030200
H	3.08258200	4.52876400	-0.29360500

E-Pro

M06/BSII SCF energy in solution: -960.1273215 a.u.

Solution-phase enthalpy: -959.7810795 a.u.

Solution-phase Gibbs energy: -959.8544585 a.u.

C	-0.53564400	1.92990700	0.14712100
C	-0.93539700	3.24655300	-0.19067900
C	-1.52688900	0.95738600	0.42192700
C	-2.29890100	3.55043800	-0.26548200
C	-2.88333700	1.29025500	0.32250800
C	-3.27130000	2.58460600	-0.01583500
H	-2.59863700	4.56117800	-0.53111300
H	-3.63439200	0.53699800	0.54302500
H	-4.32543800	2.84062600	-0.07600900
C	0.08457800	4.32000600	-0.49999900
H	0.74489500	4.02980100	-1.32544700
H	-0.41042300	5.25518800	-0.77783300
H	0.72851200	4.53114800	0.36333300
C	-1.18780300	-0.39661400	1.00531700
O	-0.54856100	-0.46836000	2.04471000
C	-1.69603200	-1.63312300	0.32702000
C	-1.60712400	-2.85084200	1.02240500
C	-2.21030700	-1.62467400	-0.97912800
C	-2.03842900	-4.03296700	0.42962100
H	-1.19423200	-2.84035000	2.02591800

C	-2.63441500	-2.81298200	-1.57553600
H	-2.27046500	-0.69152300	-1.53010200
C	-2.55341200	-4.01580600	-0.87151700
H	-1.97295700	-4.96992300	0.97601000
H	-3.02604100	-2.79943600	-2.58894400
H	-2.88763200	-4.93999900	-1.33564500
C	0.90356400	1.61968200	0.15975500
C	1.48696700	0.50428500	-0.30775200
C	2.95807300	0.35593200	-0.24800800
O	3.73770300	1.18953100	0.17651400
O	3.33446800	-0.84607000	-0.74879500
C	4.75104900	-1.13075600	-0.74303800
H	4.88402800	-1.85860500	-1.54770900
H	5.29631800	-0.21539500	-0.98703000
C	5.19892000	-1.69500000	0.59797500
H	4.61953000	-2.58702900	0.85797100
H	6.25833000	-1.97304100	0.54977300
H	5.07429400	-0.94966100	1.38835200
H	1.57315200	2.38935800	0.53860100
H	0.92731300	-0.31785300	-0.74265200

5a

M06/BSII SCF energy in solution: -1785.213234 a.u.

Solution-phase enthalpy: -1784.748698 a.u.

Solution-phase Gibbs energy: -1784.857725 a.u.

C	1.23927600	1.98763100	-0.26957000
C	1.08392100	1.50601600	-1.54639300
H	0.41681500	2.45222400	0.26404600
Pd	0.51524300	-0.24786700	-0.16480100
C	2.41692200	-0.97904300	-0.16197500
C	2.99731100	-1.55771500	-1.30285200
C	3.14165300	-0.85478500	1.02496500
C	4.34536800	-1.94584900	-1.22530300
C	4.47954200	-1.26121000	1.08186500
C	5.08578700	-1.80078200	-0.05193200
H	4.81208600	-2.38793700	-2.10371800
H	5.03367700	-1.16336700	2.01246000
H	6.12352000	-2.12328700	-0.02133100
P	-1.94282500	0.47555100	-0.07831700
C	-2.35754000	2.19717500	-0.57129100
C	-2.99134300	2.76642800	-1.64306500
O	-1.86252500	3.18787100	0.24497700
C	-2.89227600	4.18589300	-1.47277700
H	-3.48974100	2.23911800	-2.44304200

C	-2.20433600	4.38276200	-0.31531100
H	-3.29053600	4.95144400	-2.12396300
H	-1.89077500	5.25976200	0.23029100
C	-3.07281100	-0.44155000	-1.16236800
C	-2.85278900	-1.51143600	-1.98670100
O	-4.40579600	-0.08589300	-1.21680200
C	-4.11011000	-1.83665800	-2.58447800
H	-1.90952000	-2.02158200	-2.11581000
C	-5.00910000	-0.94575000	-2.08034400
H	-4.31377900	-2.63166200	-3.28777700
H	-6.06774800	-0.79146700	-2.22799200
C	-2.68716100	0.33847300	1.57960300
C	-3.96458800	0.20254700	2.05535900
O	-1.80512800	0.37085600	2.63032900
C	-3.86292800	0.14194300	3.47882500
H	-4.86098100	0.14865600	1.45487400
C	-2.53372600	0.25071600	3.76697900
H	-4.66929600	0.02726600	4.18962900
H	-1.96780400	0.25599300	4.68614700
H	2.67315400	-0.44020700	1.91300700
C	2.21691400	-1.82668200	-2.56982600
H	1.71677100	-0.92908600	-2.95279700
H	2.87038100	-2.20954600	-3.36114000
H	1.43380800	-2.57175600	-2.38330200
H	0.14428000	1.62494400	-2.07782200
H	1.95201900	1.21517100	-2.12624000
C	2.56086400	2.21835000	0.38977900
O	2.66123700	2.54714200	1.55579700
O	3.59227300	2.07454100	-0.46047700
C	4.92226400	2.24439900	0.08974000
H	5.55267000	1.61109200	-0.53752600
H	4.92856600	1.85807300	1.11042100
C	5.35157300	3.70306600	0.04044300
H	4.71530200	4.31502900	0.68639900
H	6.38632200	3.79651700	0.39026700
H	5.29889400	4.09270700	-0.98172800
I	-0.17761300	-2.71791100	0.58776300

TS6a

M06/BSII SCF energy in solution: -1785.199252 a.u.

Solution-phase enthalpy: -1784.735699 a.u.

Solution-phase Gibbs energy: -1784.842029 a.u.

C	0.92280200	1.02457000	-1.86454700
C	0.80115800	2.34750200	-1.37697900

H	1.30561000	0.24285900	-1.21497300
Pd	-1.21360200	1.02507300	-1.42144200
C	-1.17864500	3.16944000	-1.20433200
C	-1.37616800	3.77094600	0.05328700
C	-1.46170400	3.87193200	-2.38421300
C	-1.86758800	5.08490900	0.08051200
C	-1.97261300	5.16729400	-2.33090600
C	-2.16998700	5.77845900	-1.09063700
H	-2.02834400	5.56306900	1.04464000
H	-2.20375900	5.69845500	-3.25068000
H	-2.55285800	6.79406000	-1.03463400
P	-1.42457900	-1.36117100	-1.57021600
C	0.06242100	-2.38353600	-1.89723200
C	1.07839400	-2.82120600	-1.08887900
O	0.30460200	-2.76110000	-3.18867300
C	1.99961300	-3.51351400	-1.93633500
H	1.14984800	-2.68505700	-0.01850800
C	1.48130800	-3.43922400	-3.19384200
H	2.91977600	-4.00007500	-1.64455600
H	1.80793600	-3.79791400	-4.15775500
C	-1.98900400	-2.14204100	-0.02946300
C	-2.35729900	-1.62759200	1.18405700
O	-2.05167600	-3.51908400	0.01718000
C	-2.66767700	-2.74072000	2.02531200
H	-2.43012000	-0.57811900	1.42598300
C	-2.46915100	-3.85439900	1.26535400
H	-3.00001300	-2.71094600	3.05337700
H	-2.57167600	-4.91280800	1.45386600
C	-2.58477300	-1.93504100	-2.84867700
C	-3.40377700	-3.02479200	-2.96853100
O	-2.70941900	-1.13595900	-3.95535400
C	-4.07822000	-2.88673900	-4.22063200
H	-3.50941500	-3.82134600	-2.24689300
C	-3.61743900	-1.72757300	-4.77147300
H	-4.81179900	-3.55645600	-4.64714300
H	-3.82761300	-1.20454300	-5.69196400
H	-1.26994200	3.40336700	-3.34490200
C	-1.15805100	3.03578000	1.35352500
H	-0.28361500	2.37514100	1.32381500
H	-1.03058000	3.73305800	2.18856000
H	-2.02696900	2.40151900	1.56950700
H	1.06576900	2.54065800	-0.34389400
H	0.98087600	3.16234000	-2.06330200
C	1.17986800	0.76602700	-3.30628700

O	1.72903600	-0.23226000	-3.72980100
O	0.75033500	1.78118600	-4.09995100
C	0.97529200	1.62820400	-5.52125700
H	0.19140100	2.23192400	-5.98488000
H	0.83070700	0.57846700	-5.78683600
C	2.36219200	2.11282600	-5.91797300
H	3.13349500	1.48939900	-5.45690900
H	2.47921400	2.05596000	-7.00647500
H	2.51505800	3.15285000	-5.61058200
I	-3.89945100	1.15195200	-0.93014700

7a

M06/BSII SCF energy in solution: -1785.243399 a.u.

Solution-phase enthalpy: -1784.776774 a.u.

Solution-phase Gibbs energy: -1784.883137 a.u.

C	0.82550600	1.82538700	-1.14282600
C	2.27545900	1.77064300	-1.64248300
H	0.08091300	1.80335200	-1.93651300
Pd	0.74389900	-0.01779800	-0.11579700
C	3.00626900	0.57366300	-1.02054700
C	3.41365000	-0.55135100	-1.79236900
C	3.38501600	0.64271500	0.33955700
C	4.20800800	-1.52380800	-1.18426500
C	4.17900500	-0.34919500	0.92376900
C	4.59690500	-1.42841200	0.15653900
H	4.52983900	-2.38045400	-1.77143300
H	4.45363500	-0.27412200	1.97129700
H	5.21176400	-2.20892500	0.59514900
P	-1.54415500	-0.20532700	-0.19297700
C	-2.51831500	1.08478800	-1.04104600
C	-2.67751100	1.39544500	-2.36687100
O	-3.19699100	1.98547700	-0.27051700
C	-3.50384900	2.55953600	-2.41151000
H	-2.26638500	0.85182500	-3.20646200
C	-3.77938000	2.87320500	-1.11317600
H	-3.84526400	3.08825500	-3.29038200
H	-4.35318300	3.65624400	-0.64163200
C	-2.11579100	-1.68040700	-1.08639400
C	-1.46910300	-2.78062200	-1.58129800
O	-3.46417200	-1.77369400	-1.36322600
C	-2.46686300	-3.59900300	-2.19529900
H	-0.41398700	-2.98663700	-1.47957400
C	-3.64980000	-2.94251300	-2.02913100
H	-2.31954200	-4.54962200	-2.68818000

H	-4.66839400	-3.15818900	-2.31605600	C	-0.80157300	0.62383100	2.34693000
C	-2.32835700	-0.30027100	1.44225500	O	-1.87954100	0.80063300	2.94257300
C	-3.44797400	-0.93581700	1.90717200	O	-0.13285600	1.60466400	1.75465000
O	-1.71334400	0.37023000	2.46491600	O	-0.26664600	-0.57007700	2.14645000
C	-3.52503300	-0.64249700	3.30317100	Cs	-2.94441100	-1.94717900	1.77780400
H	-4.12750100	-1.53810800	1.32203800	C	2.33569000	2.87597200	0.13068200
C	-2.45048100	0.14976200	3.58181800	C	1.89547100	1.64989500	-0.68609300
H	-4.27475400	-0.98271900	4.00361300	H	2.72707800	1.18257200	-1.21296000
H	-2.08192500	0.61606800	4.48274300	H	2.54627000	3.70511000	-0.56132600
H	3.09753200	1.51914200	0.91143000	Cs	-2.54213200	2.90499500	0.40659200
C	3.04651400	-0.68989300	-3.25332000	I	-4.55912700	-0.05992200	-1.10918000
H	3.53172800	0.07761200	-3.87078000	C	0.69330200	-2.12379000	-1.78230400
H	3.35918000	-1.66560800	-3.63708000	C	0.81205900	-2.75392000	-2.99166100
H	1.96640100	-0.60023300	-3.41412500	O	-0.62735200	-1.80286900	-1.56285100
H	2.27957800	1.68179400	-2.73112600	C	-0.50451800	-2.81745100	-3.54963500
H	2.81699200	2.68901400	-1.39121800	H	1.72946700	-3.12077100	-3.42595800
C	0.46293300	2.90046800	-0.17900200	C	-1.33657900	-2.22589400	-2.64449300
O	-0.63501200	3.42231300	-0.09234300	H	-0.79010000	-3.24175500	-4.50230900
O	1.50519000	3.25938900	0.62913000	H	-2.39423000	-1.99877100	-2.61478500
C	1.23404400	4.27663800	1.61824900	C	3.46737400	-1.62407400	-1.18299500
H	1.95870700	4.08374700	2.41384600	C	4.56991200	-0.86357700	-0.89602200
H	0.22271100	4.13055000	2.00486700	O	3.80266600	-2.59443800	-2.09908900
C	1.40421200	5.67473800	1.04046400	C	5.64259500	-1.38621100	-1.68473300
H	0.66176400	5.85789900	0.25879900	H	4.61115400	-0.03480300	-0.20263100
H	1.26755900	6.42439200	1.82883400	C	5.11973100	-2.42605000	-2.39230600
H	2.40598500	5.80206300	0.61607200	H	6.66221200	-1.02934800	-1.71926200
I	0.95950700	-2.37674800	1.27552400	H	5.52719200	-3.11402500	-3.11798700

8a

M06/BSII SCF energy in solution: -2089.493346 a.u.

Solution-phase enthalpy: -2089.00008 a.u.

Solution-phase Gibbs energy: -2089.129612 a.u.

Pd	1.00639900	0.25842700	0.62448500	C	2.18914000	-5.12098500	1.26586200
P	1.80999900	-1.60084500	-0.43858100	H	1.65572100	-4.93246300	3.37903100
C	3.54796100	2.61105000	1.00352400	H	2.48132000	-6.13695400	1.04463900
C	4.86554400	2.74445400	0.51113400	C	5.14404600	3.20907300	-0.90316400
C	3.35577800	2.20780400	2.33299400	H	6.22074200	3.22874500	-1.10057600
C	5.93982900	2.45447400	1.36491300	H	4.68033400	2.55786000	-1.65395200
C	4.43526100	1.92373500	3.17076100	H	4.75859100	4.22130700	-1.08177100
H	2.33807100	2.11782700	2.70491800	H	1.50134900	3.20447300	0.75643900
C	5.73635500	2.04391300	2.68303800	C	0.79354200	1.94419900	-1.63934000
H	6.95485500	2.56197300	0.98733600	O	-0.08858100	2.78559200	-1.48264600
H	4.25817900	1.61504100	4.19789000	O	0.85172600	1.15441000	-2.74076000
H	6.58835500	1.82843100	3.32289100	C	-0.23642200	1.25145600	-3.68790100

H	-0.24214100	0.28076400	-4.18838400
H	-1.17609100	1.37196000	-3.14272700
C	-0.01831600	2.38643300	-4.67874900
H	-0.81942400	2.38495200	-5.42746500
H	-0.02520400	3.35260100	-4.16646100
H	0.93847200	2.26976900	-5.19935400

TS9a

M06/BSII SCF energy in solution: -2089.433209 a.u.

Solution-phase enthalpy: -2088.947346 a.u.

Solution-phase Gibbs energy: -2089.074714 a.u.

Pd	-1.50808200	-1.48123400	0.74008100
P	0.18683100	-1.59088800	-0.88088100
C	-4.36851200	-0.72750900	0.27028000
C	-5.25295900	0.13541200	-0.40033400
C	-3.40036600	-0.24007400	1.18453200
C	-5.14449100	1.51394300	-0.15949100
C	-3.31203600	1.15330100	1.37039200
H	-3.27606200	-1.01569500	2.28935500
C	-4.17899800	2.02623800	0.70963400
H	-5.82397300	2.19398100	-0.67080500
H	-2.55039600	1.55925300	2.03566100
H	-4.10805700	3.10170300	0.86485400
C	-2.45965600	-2.48611300	3.57187600
O	-1.94717700	-2.68912300	4.72115800
O	-2.06291000	-3.09727100	2.50958500
O	-3.39944800	-1.55076600	3.44312000
Cs	-2.30797800	0.23040800	5.47358500
C	-4.30617300	-2.21994300	0.06434800
C	-2.88739900	-2.60484900	-0.36163000
H	-2.68515500	-2.31611300	-1.39684600
H	-5.02763700	-2.59150600	-0.67478500
Cs	0.61799000	-3.76467300	3.39113300
I	0.33051200	0.03087100	2.52285100
C	1.81597600	-2.33291000	-0.45019100
C	3.10269200	-1.87049000	-0.46828400
O	1.79963400	-3.61472400	0.05807200
C	3.93044400	-2.92128600	0.04100100
H	3.41963900	-0.89910500	-0.81475100
C	3.09317400	-3.95421400	0.33347200
H	5.00547700	-2.90915300	0.15816200
H	3.24884000	-4.96345600	0.68701100
C	-0.10202300	-2.37196200	-2.52424700
C	-0.97036000	-2.05066300	-3.53325300

O	0.60039400	-3.49667600	-2.86276100
C	-0.78883600	-3.03440600	-4.55723200
H	-1.64545900	-1.20615600	-3.54957500
C	0.17035100	-3.88443600	-4.09631700
H	-1.30365500	-3.09505400	-5.50606700
H	0.65070200	-4.76128500	-4.50350100
C	0.67807300	0.07485600	-1.43591000
C	0.12161100	1.29704700	-1.17263600
O	1.69119900	0.22151200	-2.36264600
C	0.82907700	2.25165500	-1.96869200
H	-0.69115700	1.48158700	-0.48528400
C	1.76495800	1.54502900	-2.66247900
H	0.66204900	3.31876700	-2.01328100
H	2.52618700	1.81949800	-3.37797800
C	-6.30091200	-0.37686900	-1.36696100
H	-6.89418500	0.44934400	-1.77388300
H	-5.85250000	-0.90966800	-2.21539500
H	-6.99474500	-1.07654700	-0.88456500
H	-4.53163400	-2.72534300	1.01009000
C	-2.62549400	-4.07343800	-0.19373700
O	-3.43709000	-4.89332100	0.18574100
O	-1.36453800	-4.42602000	-0.58703000
C	-1.04471900	-5.82696300	-0.52613200
H	0.04763300	-5.84996100	-0.47828700
H	-1.46601100	-6.24704100	0.39247600
C	-1.55521800	-6.58586500	-1.74483600
H	-1.21661600	-7.62883900	-1.70670500
H	-2.64801200	-6.57872800	-1.76723800
H	-1.17838800	-6.13166800	-2.66718200

10a

M06/BSII SCF energy in solution: -2089.500037 a.u.

Solution-phase enthalpy: -2089.007868 a.u.

Solution-phase Gibbs energy: -2089.138002 a.u.

Pd	0.54480300	-1.04879900	-0.07595800
P	2.75611800	-0.15068600	0.53377700
C	-1.70475500	-2.73299300	0.79230600
C	-2.81957700	-3.59506600	0.72891400
C	-1.18697900	-2.10949000	-0.36841500
C	-3.44321900	-3.79853800	-0.51127400
C	-1.84177700	-2.32920800	-1.59102500
H	-4.53438000	3.58794800	1.10083600
C	-2.96430100	-3.16416900	-1.66117000
H	-4.29458700	-4.47486600	-0.57653800

H	-1.45746400	-1.87993300	-2.50136200
H	-3.44587900	-3.34519700	-2.62071800
C	-3.50821000	2.92961000	-0.35649800
O	-3.48306600	2.06159700	-1.26216300
O	-2.65804600	3.79315500	-0.04457500
O	-4.66132200	2.87185300	0.45641700
Cs	-4.49543600	-0.33897700	0.21390700
C	-0.97126500	-2.43572600	2.07511300
C	-0.14437000	-1.15361900	1.91987500
H	0.74159200	-1.13912900	2.55679700
H	-0.28722900	-3.26535100	2.30742800
Cs	-0.46914800	2.33371000	-1.68711900
I	1.35807000	-0.93578600	-2.77707400
C	3.54487300	1.25112500	-0.35381600
C	4.81121900	1.48819800	-0.80884500
O	2.74749600	2.34111700	-0.62940100
C	4.80316200	2.79140500	-1.39935000
H	5.64933700	0.81301300	-0.72435700
C	3.53504200	3.26239600	-1.25812100
H	5.63317800	3.30516200	-1.86418400
H	3.05373900	4.19306700	-1.52090000
C	3.09520200	0.34365200	2.27426400
C	3.42047900	-0.36066900	3.40167100
O	2.90774900	1.66255100	2.59315000
C	3.43818200	0.58200700	4.48026100
H	3.63762000	-1.41808500	3.45447800
C	3.12019300	1.78708000	3.93255800
H	3.66565900	0.38434200	5.51858400
H	3.02067000	2.78573300	4.33010900
C	3.98282100	-1.47766600	0.33718000
C	3.85934300	-2.72092300	-0.22298700
O	5.27230200	-1.30797600	0.79980100
C	5.13518700	-3.35480900	-0.10365500
H	2.96532500	-3.11386300	-0.68546300
C	5.94633300	-2.45438900	0.51970200
H	5.40777400	-4.34512800	-0.44024800
H	6.98114100	-2.47362800	0.82853700
C	-3.33049500	-4.30836600	1.96342700
H	-4.17772200	-4.95948300	1.72100400
H	-2.55114400	-4.93416500	2.41654600
H	-3.65670600	-3.60894900	2.74576000
H	-1.65914400	-2.36077600	2.93140500
C	-0.92500000	0.08726600	2.12828600
O	-2.15023600	0.19555000	2.07538400

O	-0.12679500	1.15265600	2.40900900
C	-0.75658900	2.43011800	2.64812000
H	0.04522500	3.15271900	2.47059400
H	-1.55205000	2.60227300	1.91821000
C	-1.27549200	2.54203900	4.07573000
H	-1.65967400	3.55343300	4.25485300
H	-2.08559700	1.82811600	4.24863200
H	-0.47265800	2.34453800	4.79453200

9b

M06/BSII SCF energy in solution: -1060.10224 a.u.

Solution-phase enthalpy: -1059.810869 a.u.

Solution-phase Gibbs energy: -1059.904989 a.u.

Pd	0.32620000	-0.36081000	-0.10662100
C	3.88014900	-1.11841600	-0.11525800
C	4.09150800	-2.28191900	0.65740400
C	4.72102900	-0.86171700	-1.20709200
C	5.12938400	-3.15025600	0.29196400
C	5.75271100	-1.73365800	-1.55282600
H	4.56504300	0.04046100	-1.79265100
C	5.95546000	-2.88962600	-0.80074000
H	5.28922200	-4.04973300	0.88244400
H	6.38999400	-1.50932100	-2.40407500
H	6.75175700	-3.58313100	-1.05820400
C	-1.77912000	1.19068200	-1.47620700
O	-2.85398000	1.09164400	-2.12658400
O	-1.01506100	0.04534000	-1.54038500
O	-1.37109600	2.16593200	-0.78738400
Cs	-0.68623900	2.52985100	1.95911100
C	2.79687300	-0.11047600	0.22944300
C	2.01950600	0.47544500	-0.92746900
H	2.20324100	0.05500000	-1.91328900
H	3.18443200	0.70137100	0.86101700
Cs	-3.31607400	-1.79541600	-1.60737300
I	-1.37647600	-1.52446900	1.84618600
C	3.24103300	-2.61458700	1.86477600
H	3.58866500	-3.53972400	2.33473200
H	3.28134600	-1.82531900	2.62683600
H	2.18308200	-2.75302400	1.60775400
H	2.06745300	-0.62497100	0.93964800
C	1.80261500	1.93764000	-0.92410700
O	1.79854500	2.64443500	0.08616500
O	1.59826300	2.40798800	-2.16463300
C	1.07415600	3.74929200	-2.29753900

H	0.61466300	3.75057400	-3.28892400
H	0.28429900	3.87727600	-1.55554400
C	2.16623000	4.80566700	-2.19791700
H	1.74134100	5.79711000	-2.39816300
H	2.61205000	4.81207100	-1.19984300
H	2.95610100	4.62043700	-2.93462300

TS10b

M06/BSII SCF energy in solution: -1060.098436 a.u.

Solution-phase enthalpy: -1059.811193 a.u.

Solution-phase Gibbs energy: -1059.903228 a.u.

Pd	1.09066400	-0.95581800	-0.47129100
C	3.65080300	-1.74623400	-2.29557400
C	4.30461100	-0.87744600	-3.20184500
C	4.42470000	-2.53598500	-1.43073000
C	5.70388700	-0.84040900	-3.21035200
C	5.81589600	-2.48530400	-1.45359600
H	3.93350100	-3.19992800	-0.72718400
C	6.46174400	-1.63361800	-2.34998200
H	6.20532700	-0.17179400	-3.90624400
H	6.39042500	-3.10996500	-0.77508500
H	7.54697000	-1.58518600	-2.37968500
C	-1.12301100	-2.00436200	1.15883700
O	-1.66963400	-2.15738000	2.28690600
O	0.22559500	-1.80325500	1.18863400
O	-1.71293200	-1.98177700	0.02938800
Cs	-2.13060000	-0.01957800	-1.98270700
C	2.16266300	-1.82930800	-2.29554600
C	1.40873900	-2.77506200	-1.54177300
H	1.88503200	-3.46900100	-0.85940600
H	1.68357300	-1.52821500	-3.22325700
Cs	0.19898900	-0.42848700	3.76272700
I	0.71600300	1.66452100	0.42043200
C	3.53202100	0.02321700	-4.13727200
H	4.21361500	0.65004800	-4.71976900
H	2.91850000	-0.54484200	-4.84891700
H	2.85549300	0.68916200	-3.58487500
H	1.79251800	-0.25201800	-1.73624600
C	0.07476700	-3.19061400	-2.03538500
O	-0.58177300	-2.58803100	-2.88288200
O	-0.30577800	-4.33475700	-1.45436500
C	-1.69070500	-4.73040700	-1.59133200
H	-1.85014000	-5.40387700	-0.74593100
H	-2.30433100	-3.84141700	-1.43741000

11b

M06/BSII SCF energy in solution: -1060.10249 a.u.

Solution-phase enthalpy: -1059.813467 a.u.

Solution-phase Gibbs energy: -1059.907593 a.u.

Pd	-0.42450500	-0.38831500	-0.30100200
C	-2.64790300	-2.48967800	0.21908200
C	-3.17036500	-3.19124200	-0.89706700
C	-2.22951700	-3.21926000	1.34743400
C	-3.24410900	-4.58768700	-0.83902800
C	-2.31344700	-4.60698900	1.38477300
H	-1.83650000	-2.68908800	2.20885500
C	-2.82321300	-5.29852900	0.28427100
H	-3.63980400	-5.12621500	-1.69701300
H	-1.98732400	-5.14503200	2.27092000
H	-2.89650700	-6.38277000	0.30066100
C	1.10067000	1.05051000	1.64949900
O	2.11035500	1.28426600	2.36838100
O	0.80825700	-0.25142800	1.40825600
O	0.35771100	1.93620700	1.09147500
Cs	-0.35150000	3.02031300	-1.45751800
C	-2.57987700	-1.01447900	0.19353200
C	-2.04814700	-0.20163400	1.18879500
H	-1.58486000	-0.60945200	2.07801900
H	-3.19742200	-0.51852200	-0.54681200
Cs	3.61910700	-1.04190300	1.36259700
I	1.68952700	-0.46937000	-2.06773000
C	-3.62113100	-2.47372800	-2.14731500
H	-3.93044600	-3.19117000	-2.91340900
H	-4.47363400	-1.80805500	-1.95766100
H	-2.81378000	-1.85733900	-2.56270600
H	-1.20157600	-0.40057900	-1.66893800
C	-2.37436900	1.24662400	1.27353500
O	-2.74036000	1.96225700	0.34740900
O	-2.26951300	1.65671700	2.54638600
C	-2.33488700	3.07458300	2.79695800
H	-1.77065800	3.20689500	3.72274500
H	-1.80555200	3.58997100	1.99313000
C	-3.77061600	3.56009300	2.94288000
H	-3.77901000	4.62292700	3.21407500

H	-4.31864300	3.43551200	2.00479900	O	-3.95007400	-0.57966200	-1.63593600
H	-4.29045300	3.00384000	3.73041700	C	-3.14019100	-1.83808500	-3.30392700
En-Pro-a				H	-1.06055700	-1.92223900	-2.43483600
M06/BSII SCF energy in solution: -615.8933432 a.u.				C	-4.24423900	-1.22056300	-2.79560100
Solution-phase enthalpy: -615.6433572 a.u.				H	-3.08640300	-2.42366300	-4.21077600
Solution-phase Gibbs energy: -615.7010852 a.u.				H	-5.27071400	-1.14406200	-3.12263600
C	-0.72021300	-1.19413200	-0.15445300	C	-2.77807200	-0.79259300	1.52813800
C	0.09171600	-0.13447100	0.02868800	C	-2.38470700	-1.55645400	2.59433700
H	-0.34358900	-2.19607900	-0.33466800	O	-4.12355800	-0.51917300	1.62437600
C	1.55874400	-0.14565700	0.04924500	C	-3.55024000	-1.76950100	3.39311900
C	2.28052200	1.06804700	-0.09006300	H	-1.38910400	-1.93900500	2.76403700
C	2.27399600	-1.34692700	0.21584600	C	-4.56692000	-1.12104500	2.75665300
C	3.67917600	1.02495000	-0.07221100	H	-3.61857300	-2.33362600	4.31257100
C	3.66413100	-1.36845100	0.23153200	H	-5.61835700	-0.99662300	2.96954500
C	4.37298900	-0.17464600	0.08454500	C	-2.53911500	1.59399100	0.06359100
H	4.23399900	1.95335600	-0.18476800	C	-3.02408100	2.38833100	-0.93977000
H	4.19103200	-2.30902200	0.36578000	O	-2.52184100	2.29999400	1.24102500
H	5.45956300	-0.17540000	0.09782900	C	-3.33090200	3.65525000	-0.34621000
H	1.72721700	-2.27454400	0.35527800	H	-3.17131000	2.09834000	-1.96962400
C	1.58218700	2.39816200	-0.27223800	C	-3.01062000	3.54294100	0.97213100
H	0.94587100	2.64931200	0.58590900	H	-3.74609600	4.52415100	-0.83746200
H	2.31376200	3.20392600	-0.38351200	H	-3.07231200	4.21215900	1.81684800
H	0.94095200	2.40673600	-1.16165800	I	0.29603800	-3.14764300	0.27521200
H	-0.38837800	0.82948400	0.16699000	C	2.72065900	-0.47152500	0.27274500
C	-2.19427600	-1.12327300	-0.14748500	C	3.44257300	-1.49902000	0.88350500
O	-2.91349900	-2.09213300	-0.31213700	C	4.81085400	-1.59565700	0.63510600
O	-2.67345000	0.12949500	0.05888300	C	5.43363600	-0.68547500	-0.22040600
C	-4.11039300	0.25385000	0.07067500	C	4.72794400	0.37208500	-0.80406800
H	-4.51574600	-0.38691600	0.86080300	C	3.35204600	0.51175600	-0.50686800
H	-4.50624900	-0.11160300	-0.88267500	H	1.29345000	0.38385600	1.39466800
C	-4.44079100	1.71736300	0.30025200	H	2.94174200	-2.23584300	1.49960200
H	-4.02610700	2.34227000	-0.49758500	H	5.38646900	-2.39999700	1.08607100
H	-5.52750400	1.85550100	0.31595200	H	6.49481100	-0.79089400	-0.43570500
H	-4.03595600	2.06520600	1.25635600	C	5.45493600	1.32696900	-1.72655300

TS8'

M06/BSII SCF energy in solution: -1712.096555 a.u.

Solution-phase enthalpy: -1711.609235 a.u.

Solution-phase Gibbs energy: -1711.706914 a.u.

Pd	0.67757900	-0.38440100	0.21261600	C	1.01889100	1.52883200	-0.60697800
P	-1.85868700	-0.10692500	0.11948800	H	2.59712500	1.71684800	-2.10613400
C	-2.61214800	-0.79387400	-1.38712300	H	0.34416000	1.40492000	-1.46258700
C	-2.07882900	-1.56389400	-2.38740800	C	2.07456300	3.06205900	0.91022900

H	2.10355700	4.02878000	1.42612900
H	2.36959000	2.27927200	1.61633200
C	2.17734200	4.15313600	-1.21569900
H	2.54955600	5.14651800	-0.94103400
H	2.33618400	4.03431000	-2.29371000
C	0.68003500	3.97728200	-0.80244500
H	0.29365500	4.87581800	-0.30806300
H	0.02094000	3.76876400	-1.65162700
H	3.96888000	3.21065500	-0.28710500
H	-0.15301600	2.73548100	0.85012500

9'

M06/BSII SCF energy in solution: -1712.097598 a.u.

Solution-phase enthalpy: -1711.608604 a.u.

Solution-phase Gibbs energy: -1711.708112 a.u.

Pd	-0.55994600	-0.36053500	-0.39336400
P	1.91895000	0.21634800	-0.19259300
C	2.64349900	0.38445400	1.46595600
C	2.14877100	0.00395800	2.68502300
O	3.92160500	0.87753800	1.62150600
C	3.16805100	0.28499700	3.64750200
H	1.18983500	-0.46452800	2.85682200
C	4.21253700	0.81011800	2.94776800
H	3.12753000	0.10964300	4.71324600
H	5.19093100	1.17078600	3.22878000
C	2.98948300	-0.95331200	-1.08417100
C	2.77965600	-2.25145400	-1.46990600
O	4.25433600	-0.55781000	-1.45318100
C	3.98117800	-2.68241400	-2.11306200
H	1.88383300	-2.82828400	-1.28527000
C	4.83256800	-1.61815500	-2.07339500
H	4.18012600	-3.65334800	-2.54444900
H	5.83878600	-1.45684400	-2.43093800
C	2.34705300	1.81593300	-0.96461600
C	3.06760700	2.91766000	-0.58652900
O	1.80303700	2.02997000	-2.20840600
C	2.96506900	3.86105800	-1.65796000
H	3.61896700	3.02956200	0.33433600
C	2.19365500	3.26805500	-2.61117900
H	3.41104700	4.84455300	-1.70812600
H	1.84383100	3.57298700	-3.58588500
I	-0.33658100	-2.70919800	1.09309200
C	-2.48456100	-0.70505600	-0.90063600

C	-2.81647200	-1.71144800	-1.80465400
C	-4.16469300	-1.96270200	-2.06602900
C	-5.15267800	-1.22840500	-1.40928400
C	-4.82825000	-0.21211800	-0.50259600
C	-3.46467700	0.07504900	-0.27193900
H	-0.69987000	0.71749700	-1.49461800
H	-2.04604200	-2.31617300	-2.27428900
H	-4.44418100	-2.74975200	-2.76208600
H	-6.20076400	-1.45201200	-1.59580600
C	-5.93933200	0.53315400	0.20504200
H	-6.13677100	1.51417600	-0.24652200
H	-6.87346000	-0.03601800	0.16050800
H	-5.70712900	0.70904500	1.26213500
C	-2.97961100	1.14016200	0.68023300
C	-3.29611800	2.62365500	0.29304700
C	-1.03505700	2.59994000	0.45101000
C	-1.42600900	1.16320800	0.77685700
H	-3.38592900	0.92951000	1.68189200
H	-1.01182500	0.77052500	1.70911900
C	-2.09313300	3.00372800	-0.59471500
H	-2.06604400	4.07190800	-0.83851500
H	-2.03025300	2.42535500	-1.52100900
C	-3.04178000	3.49950400	1.54008100
H	-3.38372300	4.52623600	1.36814600
H	-3.56483800	3.12580600	2.42733800
C	-1.48741700	3.44411100	1.68731400
H	-1.03915600	4.44214300	1.62863300
H	-1.16329700	3.00055700	2.63511600
H	-4.28178100	2.75732600	-0.15550200
H	0.01437200	2.74659600	0.19234200

8'

M06/BSII SCF energy in solution: -1984.716736 a.u.

Solution-phase enthalpy: -1984.202623 a.u.

Solution-phase Gibbs energy: -1984.311975 a.u.

Pd	-0.03494200	-0.53125300	0.26551900
P	0.10565800	1.71365500	-0.04920900
C	3.14889900	-1.65952400	-0.76820900
C	4.32017300	-1.44270900	-1.54091900
C	2.10404500	-2.40041700	-1.34370300
C	4.38242300	-1.93994500	-2.85010000
C	2.18728400	-2.89368000	-2.64796000
H	1.20516200	-2.60247300	-0.77147500

C	3.32770900	-2.65878500	-3.41198900
H	5.28297600	-1.76315700	-3.43540300
H	1.35564300	-3.46275700	-3.05621200
H	3.40339100	-3.03428200	-4.42967500
C	-1.78446500	-2.36305900	-0.08159200
O	-2.66222400	-3.24279000	-0.18227700
O	-0.60814400	-2.54906900	0.47070100
O	-1.99248500	-1.10973000	-0.49277000
Cs	-4.90974500	-1.36444700	-0.12126300
C	3.09899500	-1.15917500	0.67283400
C	3.47924900	-2.28888100	1.69398000
C	1.57756400	-1.45142700	2.58033200
C	1.77647100	-0.57423900	1.31535900
C	2.10144300	-2.82768500	2.12576200
H	2.17221800	-3.55085500	2.94905800
H	1.50623200	-3.26534000	1.32388800
C	3.97221200	-1.62142600	3.00141600
H	4.42772800	-2.36700700	3.66427000
H	4.72884000	-0.84967500	2.81438000
C	2.65743500	-1.04521300	3.62123100
H	2.44602000	-1.50540100	4.59514700
H	2.69944100	0.03920200	3.77634000
H	4.17951000	-3.02094700	1.27932300
H	0.56036800	-1.43745800	2.98051000
H	1.97812600	0.45874800	1.61914500
H	3.85339400	-0.37024500	0.74822800
C	-1.30554200	2.34846800	-1.01948500
C	-2.19350300	1.67774500	-1.81877800
O	-1.54752800	3.70116500	-1.08858100
C	-3.03247100	2.67388500	-2.41451200
H	-2.22132600	0.60147700	-1.93063900
C	-2.59515400	3.87370800	-1.93360400
H	-3.84046100	2.52232300	-3.11791800
H	-2.90745400	4.89603500	-2.08843300
C	0.04530400	2.72498300	1.47275200
C	0.86416700	3.66434500	2.03834700
O	-0.99516000	2.44870000	2.32772900
C	0.29593200	3.99057000	3.31126300
H	1.75363300	4.08246500	1.59210800
C	-0.82566900	3.22781500	3.42993800
H	0.67528000	4.69783100	4.03562200
H	-1.57837000	3.12237500	4.19670500
C	1.54497200	2.41910000	-0.90922700
C	2.52755500	1.79711200	-1.63122300

O	1.69170800	3.78697600	-1.01200000
C	3.33219000	2.83232800	-2.20359000
H	2.65515300	0.72901100	-1.73904600
C	2.78075500	4.00928100	-1.79434400
H	4.20141700	2.71051400	-2.83449000
H	3.03111200	5.04675100	-1.96032100
C	5.52261800	-0.69511900	-0.99848700
H	6.32975400	-0.68027000	-1.73856500
H	5.28760200	0.34786600	-0.74730000
H	5.92017400	-1.15769000	-0.08690600

TS9b

M06/BSII SCF energy in solution: -1984.685688 a.u.

Solution-phase enthalpy: -1984.177822 a.u.

Solution-phase Gibbs energy: -1984.284421 a.u.

Pd	0.94586900	0.24177100	-0.11244200
P	2.24948900	-1.60112200	0.29628600
C	0.86719900	3.21093300	0.14926400
C	0.69770500	4.38619300	0.91427500
C	-0.11278100	2.18904900	0.19904000
C	-0.42459800	4.49747500	1.74463000
C	-1.20631400	2.32346700	1.07585200
H	-0.53095100	1.47646000	-0.77622800
C	-1.36577400	3.47074100	1.84569400
H	-0.55605800	5.40596800	2.32999200
H	-1.94158200	1.52489500	1.11254200
H	-2.21952100	3.57875700	2.51071200
C	-1.69164700	-0.39874400	-1.09730300
O	-2.65260500	-1.11392100	-1.47843600
O	-1.36803700	0.72595800	-1.65937500
O	-0.93088000	-0.84343400	-0.07323500
Cs	-1.52157300	-3.69687500	-0.94653400
C	2.13429800	2.96674400	-0.63771200
C	2.11383300	3.36957100	-2.15002500
C	2.80730600	1.21430600	-2.19136100
C	2.54026300	1.45303200	-0.68773200
C	1.69864100	2.06037900	-2.85727200
H	1.81138300	2.12713600	-3.94728500
H	0.68575200	1.71723900	-2.63267300
C	3.58561700	3.49564000	-2.61098500
H	3.63678700	3.91470000	-3.62294200
H	4.17527500	4.14950400	-1.95756500
C	4.08314700	2.01259000	-2.59293700
H	4.43696500	1.69997100	-3.58337100

H	4.90810100	1.85214300	-1.88862600	C	2.08511400	-3.04773700	-0.34039600
H	1.49863800	4.24956900	-2.36143700	H	1.00619700	-1.72698500	1.92265600
H	2.85297900	0.16046700	-2.48389000	C	3.06470700	-3.99716300	-0.63947700
H	3.42328900	1.25400700	-0.07537100	H	5.12852000	-4.33104000	-1.15941500
H	2.94074800	3.52874100	-0.14886100	H	1.06257300	-3.36536500	-0.15869000
C	1.38001700	-2.80225500	1.36613100	H	2.80844200	-5.05459500	-0.67605000
C	0.19763600	-2.68465600	2.04866200	C	-0.81446400	-2.16434500	1.62375000
O	1.96936700	-4.01313400	1.66208900	O	-1.84553800	-2.69677000	2.06436100
C	0.04416100	-3.89224300	2.80436200	O	0.27136100	-2.10749600	2.44473200
H	-0.48139900	-1.84659600	1.95876300	O	-0.68839300	-1.66032000	0.43772900
C	1.14479700	-4.65306500	2.53124300	Cs	-3.56611100	-2.17348600	-0.26575700
H	-0.76487300	-4.14831400	3.47517300	C	4.00408300	0.19700300	-0.47887700
H	1.48023000	-5.62413700	2.86523900	C	4.83500900	0.68004400	0.75683900
C	2.79568800	-2.64898200	-1.10601900	C	2.91799000	1.86922000	0.93307800
C	3.99595700	-2.86289200	-1.72399500	C	2.65295600	0.98996900	-0.31348200
O	1.79164800	-3.25484600	-1.83597400	C	3.74714300	0.91949400	1.82249800
C	3.72878600	-3.64642600	-2.89318100	H	4.13791800	1.40013100	2.72856100
H	4.95755100	-2.51289800	-1.38056000	H	3.20300200	0.01327700	2.10290700
C	2.38615300	-3.85447700	-2.91177500	C	5.30734800	2.12514500	0.47935100
H	4.44630300	-4.00291600	-3.61894000	H	6.02662300	2.45217600	1.23995700
H	1.72279300	-4.37492400	-3.58644800	H	5.79862000	2.22070500	-0.49614400
C	3.81499400	-1.35238700	1.19520600	C	3.98161100	2.94818100	0.57287000
C	4.21144600	-0.30741900	1.98806400	H	4.04267000	3.71345800	1.35710300
O	4.74469300	-2.36553700	1.27557400	H	3.74926800	3.46596000	-0.36622800
C	5.45411400	-0.68906900	2.58255500	H	5.64039400	-0.00120100	1.04384500
H	3.66992900	0.61671600	2.12972800	H	2.01933400	2.28902500	1.39520300
C	5.72690000	-1.93867400	2.11228700	H	2.44326300	1.59513900	-1.20581100
H	6.06097600	-0.10785700	3.26240400	H	4.52935700	0.51466200	-1.39362600
H	6.54422700	-2.62849500	2.26206900	C	-1.94241000	0.89043200	-1.47215100
C	1.70170000	5.51963400	0.87374500	C	-1.67692000	0.10988300	-2.56668500
H	1.33376000	6.38335300	1.43773800	O	-3.24588700	1.33459300	-1.53586800
H	2.66797700	5.23165400	1.31040700	C	-2.87410900	0.07615700	-3.35364200
H	1.90457400	5.85392900	-0.15059700	H	-0.73283000	-0.37686300	-2.77058500

10b

M06/BSII SCF energy in solution: -1984.726542 a.u.

Solution-phase enthalpy: -1984.213481 a.u.

Solution-phase Gibbs energy: -1984.322328 a.u.

Pd	1.01503800	-0.24077700	-0.04548500	O	-2.55377400	0.35136700	1.72472000
P	-0.81794000	1.41972000	-0.11666000	C	-2.97163100	1.89451800	3.28927100
C	3.74299000	-1.28238700	-0.53984700	H	-1.83922100	3.51626500	2.20623000
C	4.73073700	-2.23664700	-0.86821600	C	-3.15927900	0.59796400	2.92212200
C	2.41196700	-1.68389500	-0.28762700	H	-3.33351500	2.36792300	4.19129500
C	4.37184400	-3.58992600	-0.90703700	H	-3.63963400	-0.25257300	3.38138000

C	-0.64668800	3.20019400	-0.48214300	C	2.56457600	-4.97466700	-1.15263700
C	0.46421700	3.96187200	-0.73062600	H	2.01917600	-5.57160000	-1.89501300
O	-1.77397900	3.98581900	-0.60761000	H	3.61042300	-5.30079400	-1.18325300
C	0.00458600	5.28475600	-1.01909400	H	2.15717900	-5.24312200	-0.17091400
H	1.48604400	3.61576800	-0.70778000	C	4.13298100	3.52338200	-0.51828200
C	-1.35428000	5.23650000	-0.92965300	C	2.81149100	3.17899100	-0.84322000
H	0.60697400	6.14982300	-1.25812900	C	2.12698200	3.89027200	-1.84260400
H	-2.13465800	5.97204800	-1.05825400	C	2.76000600	4.93528400	-2.50839000
C	6.15184300	-1.83430700	-1.20087700	C	4.07623600	5.27668500	-2.18191200
H	6.71713700	-2.68736000	-1.59192700	C	4.76037000	4.57148000	-1.18817900
H	6.18347600	-1.03842100	-1.95632300	H	4.65821700	2.96941700	0.25135200
H	6.69459300	-1.45576700	-0.32542100	H	1.10663800	3.60967800	-2.08146600

11b

M06/BSII SCF energy in solution: -2465.004805 a.u.

Solution-phase enthalpy: -2464.304655 a.u.

Solution-phase Gibbs energy: -2464.434155 a.u.

Pd	-0.24727700	-0.31298000	-0.38179700	O	0.93122700	1.79570000	-0.36365800
C	1.32205000	-2.73508300	-1.04907400	O	2.90553200	1.36249600	0.68806400
C	2.45909300	-3.48714000	-1.41855100	C	2.41670400	0.83039300	1.88888900
C	1.29640900	-1.33133500	-1.21993500	O	1.54900800	1.38817300	2.51436700
C	3.52476800	-2.83044900	-2.04911300	C	3.16644400	-0.36750200	2.31481800
C	2.36027200	-0.71806100	-1.90033000	C	3.98176500	-1.09382900	1.43449400
C	3.46475100	-1.46361900	-2.32376700	C	3.02267300	-0.78116300	3.64946400
H	4.40142000	-3.40478400	-2.34478800	C	4.65276800	-2.22511000	1.89556400
H	2.33526100	0.34731600	-2.11567400	H	4.05901100	-0.79733700	0.39506000
H	4.28262900	-0.97901500	-2.85445400	C	3.70466900	-1.90497800	4.10405900
C	0.05634700	-3.34204900	-0.50254300	H	2.37711600	-0.21082400	4.30923700
C	-0.70527100	-4.22914700	-1.54213600	C	4.52104200	-2.62701800	3.22678200
C	-2.18392400	-2.56771000	-1.13035400	H	5.26909900	-2.79747900	1.20892600
C	-1.00166500	-2.21766800	-0.19799800	H	3.59923500	-2.22200400	5.13769600
C	-1.47592400	-3.17133900	-2.35826300	H	5.04927800	-3.50826800	3.58138200
H	-2.17059200	-3.61453700	-3.08341400	P	-2.32303000	0.83896400	0.33335900
H	-0.82254400	-2.45969000	-2.87095200	C	-3.19147500	1.49432900	-1.14178800
C	-1.85429600	-4.96330400	-0.81188500	C	-4.09136900	2.50425600	-1.36483600
H	-2.28368200	-5.74435300	-1.45083900	O	-2.88718200	0.88786500	-2.33810800
H	-1.51116700	-5.45083600	0.10856000	C	-4.35729100	2.51772200	-2.76993700
C	-2.88817000	-3.82241600	-0.54215100	H	-4.50561600	3.15546500	-0.60963700
H	-3.83313700	-4.01228500	-1.06695100	C	-3.60243600	1.51597800	-3.30456600
H	-3.12711200	-3.70261800	0.52033600	H	-5.01841000	3.18421800	-3.30637500
H	-0.05497800	-4.89349800	-2.11615400	H	-3.46318400	1.13915000	-4.30665400
H	-2.87254700	-1.74467900	-1.33003100	C	-3.66542400	-0.15964000	1.08573700
H	-1.30777600	-2.21927000	0.85478000	C	-4.98442200	-0.37517200	0.79144600
H	0.26469000	-3.93585300	0.40111800	O	-3.31568500	-0.89640500	2.19116500
				C	-5.47783800	-1.29441100	1.77177600

H	-5.53472000	0.07241500	-0.02313200	C	3.43171500	5.64547600	-0.74228900
C	-4.42687400	-1.57099400	2.59290600	H	4.45113200	5.55772400	-0.34464200
H	-6.47982200	-1.69280600	1.85076700	H	3.50626200	6.16068000	-1.70608100
H	-4.30452400	-2.19397100	3.46609900	H	2.87560700	6.29472000	-0.05712700
C	-2.31496000	2.29618900	1.43111700	C	-3.41442000	-0.41417500	-1.88587300
C	-1.29476800	2.90268200	2.11137700	C	-2.21866400	-0.72391400	-1.22380700
O	-3.50629200	2.93068900	1.72549900	C	-1.63326900	-1.98405200	-1.40588100
C	-1.88049300	3.97311400	2.85979500	C	-2.23819300	-2.92319300	-2.24033700
H	-0.25752900	2.60178500	2.09698000	C	-3.43054200	-2.61027200	-2.89864200
C	-3.21432100	3.94144500	2.58649700	C	-4.01731000	-1.35443600	-2.72022000
H	-1.37300200	4.66574300	3.51672000	H	-3.85518800	0.56554300	-1.73544500
H	-4.05581400	4.53567800	2.91123100	H	-0.70764800	-2.20972500	-0.88739400

TS12b

M06/BSII SCF energy in solution: -2464.984079 a.u.

Solution-phase enthalpy: -2464.2861 a.u.

Solution-phase Gibbs energy: -2464.412317 a.u.

Pd	0.40865700	1.61013800	1.42587900	O	-0.47807300	-0.03747700	0.24201900
C	2.11789200	3.63845200	0.15865300	O	-2.14043200	1.41470500	-0.19640500
C	2.76340700	4.29724600	-0.91060500	C	-1.37718100	2.77071300	1.24318700
C	1.44539200	2.42672000	-0.08642800	O	-2.00822600	2.56608700	2.23841100
C	2.77211100	3.68439400	-2.17084400	C	-1.40882200	4.01031500	0.41835100
C	1.48939500	1.81069200	-1.33989100	C	-1.16399000	4.05075100	-0.95772900
C	2.17100500	2.44362200	-2.38262100	C	-1.72381000	5.19059100	1.11224900
H	3.26567400	4.19067700	-2.99821500	C	-1.23249800	5.26659900	-1.63369700
H	0.99143700	0.86066800	-1.50296800	H	-0.93380100	3.13589500	-1.48510100
H	2.21284200	1.97915300	-3.36532500	C	-1.77497800	6.40546600	0.43013700
C	2.11178100	4.12926900	1.58477200	H	-1.93021900	5.14487000	2.17652600
C	3.52912200	4.11676500	2.24623300	C	-1.52946000	6.44537500	-0.94366100
C	2.38880800	2.61501900	3.49456100	H	-1.04838400	5.29295600	-2.70384100
C	1.31886000	3.12798000	2.50234300	H	-2.01544500	7.31657700	0.97121800
C	3.67756800	2.63634800	2.64968100	H	-1.57365300	7.39141000	-1.47683600
H	4.58101600	2.44222400	3.24056300	P	-0.32367900	0.03425500	3.44928600
H	3.65447200	1.94886000	1.79832900	C	0.77404700	-1.41675300	3.29761400
C	3.43364100	4.81325200	3.62488100	C	0.68634500	-2.75184900	3.58771000
H	4.43343900	5.01023900	4.02877400	O	1.98709600	-1.15929200	2.69900500
H	2.91372500	5.77630300	3.56277900	C	1.90962500	-3.34976000	3.14772000
C	2.66774500	3.76796500	4.49809000	H	-0.15588400	-3.24049700	4.05503200
H	3.29142500	3.40710400	5.32503300	C	2.65640000	-2.33869700	2.62082800
H	1.74562700	4.16544100	4.93562800	H	2.19011400	-4.39188700	3.21225600
H	4.31658100	4.51877300	1.60540200	H	3.63542800	-2.29087900	2.16858900
H	2.15117000	1.67097800	3.98833500	C	-0.03602300	0.49097400	5.19898100
H	0.48717500	3.60366000	3.03155300	C	0.61901400	-0.09800400	6.24758300
H	1.68314800	5.14022600	1.64234000	O	-0.53207100	1.70959200	5.59475400
				C	0.51507000	0.80365600	7.35375300

H	1.11024300	-1.05999900	6.22777600	C	5.79387900	0.39852700	-1.31162000
C	-0.19392000	1.87563400	6.90095100	H	6.05736200	-0.32445900	-2.09462000
H	0.91415100	0.66859200	8.34941700	H	6.53238200	1.20610500	-1.35870700
H	-0.52832900	2.79547200	7.35663000	H	5.91639500	-0.11182300	-0.35024700
C	-1.98043100	-0.71297700	3.49525100	C	-2.48692700	4.55275500	0.46445300
C	-3.10514000	-0.45449200	2.75977000	C	-2.21736200	3.50090700	-0.42107400
O	-2.25400800	-1.69273700	4.42824000	C	-2.83446100	3.48313700	-1.67905900
C	-4.12673700	-1.32488500	3.25431400	C	-3.71012000	4.50509800	-2.04537200
H	-3.19114800	0.27738100	1.97021200	C	-3.97568200	5.55176800	-1.15835700
C	-3.55572400	-2.04706400	4.25820500	C	-3.36261800	5.57374500	0.09751100
H	-5.14796200	-1.39676800	2.90744300	H	-1.99901500	4.55097600	1.43350500
H	-3.92109700	-2.81479100	4.92414900	H	-2.61666300	2.66348000	-2.35532000

13b

M06/BSII SCF energy in solution: -2464.986853 a.u.

Solution-phase enthalpy: -2464.287631 a.u.

Solution-phase Gibbs energy: -2464.415952 a.u.

Pd	0.41935000	-0.02993200	-0.27417700	O	-1.05661200	1.47981200	-0.87343200
C	3.25382400	0.28237300	-0.98657800	O	-0.72826600	2.46442000	1.12166100
C	4.39399300	0.94846500	-1.48823500	C	0.74513600	0.61852200	1.68804500
C	1.99226200	0.88997400	-1.12136900	O	0.06036700	-0.02114400	2.42569300
C	4.21934300	2.16377000	-2.16338300	C	1.91560000	1.44831500	2.08205700
C	1.82637600	2.08472500	-1.82499600	C	2.23565700	2.68448400	1.51235600
C	2.95304600	2.71490800	-2.35890100	C	2.70631000	0.92155300	3.11764700
H	5.09584600	2.68236700	-2.54702200	C	3.34696900	3.38556900	1.97458700
H	0.83937600	2.51804500	-1.94409000	H	1.60306700	3.09367900	0.73820400
H	2.84410400	3.64755500	-2.90779200	C	3.82844300	1.62137700	3.55817700
C	3.28062800	-1.07767100	-0.33460300	H	2.43579700	-0.02822400	3.56764500
C	3.70804400	-2.21647400	-1.31881400	C	4.15010100	2.85431700	2.98748500
C	1.57680200	-2.77767600	-0.81280500	H	3.58742200	4.35081600	1.53843400
C	1.82743300	-1.52521000	0.06152400	H	4.44273100	1.20734200	4.35303600
C	2.39609900	-2.48099400	-2.08372600	H	5.02128700	3.40322400	3.33508000
H	2.46051100	-3.34070500	-2.76163900	P	-1.75064100	-1.48944400	0.21256000
H	2.03803100	-1.61216400	-2.64486300	C	-2.52973400	-1.79434800	-1.40979700
C	3.87656100	-3.52601400	-0.51172500	C	-3.80781600	-1.97118300	-1.86756200
H	4.37603900	-4.29140300	-1.11672600	O	-1.65819100	-1.80527200	-2.47589300
H	4.48449000	-3.37718800	0.38836100	C	-3.72091100	-2.10159600	-3.28994800
C	2.40423300	-3.93466400	-0.18659400	H	-4.69801200	-1.99828500	-1.25658400
H	2.14123600	-4.88736100	-0.66215700	C	-2.39816500	-1.99449500	-3.59947600
H	2.21412200	-4.04356900	0.88633500	H	-4.53549100	-2.24955000	-3.98520300
H	4.57518400	-1.96448400	-1.93238100	H	-1.84279700	-2.02550900	-4.52463700
H	0.52808700	-3.03858400	-0.96506300	C	-1.60338200	-3.20311000	0.84242100
H	1.72993200	-1.76692700	1.12359800	C	-2.10181500	-4.41343800	0.43972300
H	3.94496300	-1.07265200	0.54159000	O	-0.80660800	-3.38044900	1.94765100
				C	-1.59017200	-5.39094300	1.35050300

H	-2.75828900	-4.57981500	-0.40197300	C	2.71441000	-4.98116400	-1.16131000
C	-0.81758600	-4.70784500	2.24123000	H	2.34902200	-5.25280900	-0.16347500
H	-1.77541100	-6.45604500	1.34145400	H	2.13690500	-5.57626700	-1.88013100
H	-0.23612800	-5.00022700	3.10265000	H	3.75808400	-5.30644500	-1.23662600
C	-3.11784500	-0.81421500	1.20001200	C	4.02977800	3.61307000	-0.43937600
C	-3.21439900	0.32813900	1.94726500	C	2.75016400	3.20934900	-0.85207000
O	-4.28902400	-1.53836000	1.30545100	C	2.11324600	3.87251100	-1.91414900
C	-4.51654300	0.31812800	2.53950000	C	2.75259900	4.92879900	-2.55557800
H	-2.44729500	1.08226500	2.05463500	C	4.02747900	5.32869400	-2.14274500
C	-5.11745700	-0.82911700	2.11758600	C	4.66381600	4.67153900	-1.08623800
H	-4.94180100	1.06708200	3.19267200	H	4.51775400	3.09694600	0.37957300
H	-6.08577700	-1.27237200	2.29744300	H	1.12390800	3.54745800	-2.21807700

11a

M06/BSII SCF energy in solution: -2465.004766 a.u.

Solution-phase enthalpy: -2464.30466 a.u.

Solution-phase Gibbs energy: -2464.435355 a.u.

Pd	-0.18650300	-0.37102000	-0.41039800	O	0.89949900	1.75390200	-0.48977300
C	1.43817900	-2.76262100	-1.06709500	O	2.79213100	1.43719500	0.73544000
C	2.59591500	-3.49304500	-1.41626400	C	2.21941400	0.92048100	1.90553000
C	1.39157900	-1.35835300	-1.22430700	O	1.29131200	1.47114900	2.44570500
C	3.66802000	-2.81230400	-2.00784000	C	2.96023600	-0.25002200	2.41615100
C	2.46448200	-0.72064200	-1.86815100	C	3.83848500	-0.98878900	1.60940000
C	3.59317000	-1.44298100	-2.26617100	C	2.74208400	-0.62546200	3.75181200
H	4.56209800	-3.36836300	-2.28524200	C	4.49563900	-2.09545200	2.14438900
H	2.42819200	0.34540700	-2.07542900	H	3.97577200	-0.72062200	0.56834600
H	4.41785300	-0.93835300	-2.76664600	C	3.41143800	-1.72411100	4.28118100
C	0.17912400	-3.39751100	-0.54305300	H	2.05154000	-0.04462400	4.35461000
C	-0.57950500	-4.26697500	-1.60084500	C	4.28897000	-2.45947100	3.47707000
C	-2.09450500	-2.66683600	-1.08867900	H	5.16044300	-2.67820000	1.51399900
C	-0.88907600	-2.29576000	-0.19740500	H	3.24967300	-2.01061000	5.31647700
C	-1.40760000	-3.20828300	-2.35760200	H	4.80737000	-3.32095600	3.88989500
H	-2.10958500	-3.65019300	-3.07620100	P	-2.28823100	0.75366300	0.30404800
H	-0.79344700	-2.45863700	-2.86462600	C	-3.46639500	0.76599600	-1.09732300
C	-1.68444000	-5.06417000	-0.86963900	C	-4.81173400	0.56470100	-1.25344500
H	-2.11828900	-5.82315600	-1.53173400	O	-2.89601800	1.00695300	-2.32539100
H	-1.29986400	-5.58716100	0.01415400	C	-5.08556500	0.68697000	-2.65232400
C	-2.73343300	-3.96220700	-0.51229200	H	-5.51751700	0.36499300	-0.46186900
H	-3.69784000	-4.16147300	-0.99631200	C	-3.89094000	0.95854200	-3.24854700
H	-2.92196500	-3.88486300	0.56466400	H	-6.04357600	0.58558500	-3.14313500
H	0.07747100	-4.88641500	-2.21626500	H	-3.58821100	1.13217100	-4.27011400
H	-2.82064400	-1.86505000	-1.23749900	C	-3.28386200	0.00305300	1.63904000
H	-1.15709600	-2.32336000	0.86501900	C	-2.91710400	-0.88340900	2.61659900
H	0.39700000	-4.01723400	0.34105700	O	-4.57740700	0.41912300	1.86863400
				C	-4.04241200	-1.03396700	3.48688800

H	-1.95264700	-1.36121300	2.70603600	C	-2.13720900	5.53872000	-0.91995000
C	-5.01522900	-0.22491400	2.98310000	H	-1.81048600	5.66179000	0.11817200
H	-4.11372500	-1.65990100	4.36528400	H	-1.44716300	6.12056000	-1.54483900
H	-6.02928100	-0.00439900	3.28193500	H	-3.12545200	6.00110500	-1.01735300
C	-2.28333400	2.51689100	0.79224100	C	-3.75034500	-3.67207700	-0.39975600
C	-1.33265800	3.27174700	1.42591800	C	-2.76480000	-3.02689100	-1.15895000
O	-3.41769200	3.27186500	0.59610400	C	-2.49030900	-3.47363400	-2.45851200
C	-1.90981100	4.56438600	1.63159500	C	-3.19357000	-4.55346800	-2.99118900
H	-0.35215000	2.92882700	1.72240500	C	-4.17505500	-5.19429400	-2.23025300
C	-3.16647200	4.50468900	1.10651200	C	-4.45222300	-4.75185000	-0.93380600
H	-1.44760700	5.42118100	2.10219800	H	-3.95106700	-3.31371400	0.60435600
H	-3.96862600	5.22158100	1.01095900	H	-1.72493900	-2.96517300	-3.03490200

TS12a

M06/BSII SCF energy in solution: -2464.983239 a.u.

Solution-phase enthalpy: -2464.285059 a.u.

Solution-phase Gibbs energy: -2464.410886 a.u.

Pd	-0.16668500	0.43856500	-0.39156300	O	-2.29590400	-1.49374100	0.59634100
C	-1.26786500	3.12867100	-0.84409700	C	-1.13724400	0.18116200	1.47371200
C	-2.18990700	4.08205500	-1.32987900	O	-0.36598400	-0.35746900	2.21384800
C	-1.42238300	1.77838800	-1.20787300	C	-2.29351900	1.02449700	1.88460300
C	-3.19152900	3.65913900	-2.21391600	C	-3.48003000	1.15329100	1.15600200
C	-2.40543400	1.37455100	-2.11455300	C	-2.13967400	1.70741300	3.10307700
C	-3.28562000	2.33055900	-2.62773900	C	-4.50318900	1.96289800	1.64289700
H	-3.90651900	4.39011300	-2.58664500	H	-3.59764900	0.61306700	0.22785200
H	-2.48955200	0.33271200	-2.40424200	C	-3.16241900	2.52876100	3.57486100
H	-4.05871800	2.03345600	-3.33282900	H	-1.22320800	1.58589400	3.67105700
C	-0.08497400	3.45655900	0.03158200	C	-4.34595800	2.65727800	2.84579100
C	0.97988000	4.35167600	-0.68338200	H	-5.42633400	2.05366100	1.07787600
C	2.12189900	2.43797400	-0.30005800	H	-3.03645900	3.05913600	4.51478400
C	0.74268700	2.15658500	0.34352600	H	-5.14592600	3.29340400	3.21524100
C	1.75950800	3.31387500	-1.51526900	P	1.85714100	-1.22984300	0.08391800
H	2.63874500	3.73848100	-2.01470000	C	2.75159200	-1.39332400	-1.49615900
H	1.14263600	2.79968300	-2.25883100	C	3.73466400	-2.20484200	-1.99471300
C	2.03760200	4.78317800	0.36008700	O	2.35555300	-0.50559500	-2.47464400
H	2.67994500	5.57410900	-0.04382900	C	3.95735100	-1.80064700	-3.34727400
H	1.57569900	5.17592100	1.27349000	H	4.22967200	-2.99584700	-1.45156200
C	2.84646300	3.47016900	0.60806100	C	3.09630600	-0.76922800	-3.58061600
H	3.89111200	3.58172200	0.29292100	H	4.66206400	-2.22262000	-4.05032300
H	2.85618600	3.16155900	1.65865700	H	2.89207900	-0.14716500	-4.43895400
H	0.54989700	5.18510200	-1.24244000	C	3.16995600	-0.73540200	1.25798400
H	2.72769800	1.55372500	-0.50436300	C	3.07655200	-0.09167700	2.46368900
H	0.84223700	1.97028800	1.41711200	O	4.48000700	-1.07656900	1.02123900
H	-0.41633500	3.94420600	0.95974200	C	4.40098100	-0.02988900	3.00046500

H	2.16389700	0.27360900	2.91197400	C	5.83463200	-0.06402100	-1.25571700
C	5.20570900	-0.63722700	2.08345800	H	5.90614400	-0.57812500	-0.29120500
H	4.70978000	0.41141600	3.93783300	H	6.05028600	-0.80853400	-2.03315800
H	6.26815000	-0.82308800	2.03176300	H	6.63411600	0.68363000	-1.29713500
C	1.53847500	-2.95533400	0.56668100	C	-2.14401300	4.71954400	0.43617900
C	0.43324800	-3.53793700	1.12488700	C	-1.93132700	3.65868000	-0.45430600
O	2.55499400	-3.88221500	0.47679000	C	-2.52068600	3.69597000	-1.72508400
C	0.77813200	-4.90243600	1.38294100	C	-3.31340500	4.78091300	-2.09894100
H	-0.50721500	-3.04594100	1.32828200	C	-3.52266100	5.83615500	-1.20701900
C	2.06763500	-5.05188500	0.97079200	C	-2.93642000	5.80365500	0.06134600
H	0.14548900	-5.66583100	1.81355000	H	-1.67934800	4.67467000	1.41556500
H	2.75277600	-5.88650400	0.95511300	H	-2.34828900	2.86848000	-2.40487400

13a

M06/BSII SCF energy in solution: -2464.985004 a.u.

Solution-phase enthalpy: -2464.285846 a.u.

Solution-phase Gibbs energy: -2464.415115 a.u.

Pd	0.43224000	-0.05262900	-0.26692000	O	-0.89999800	1.56742500	-0.90396900
C	3.29052900	0.02433500	-0.95358200	O	-0.57185100	2.49664800	1.11739500
C	4.48416700	0.59255500	-1.45103400	C	0.78663500	0.58602200	1.69183900
C	2.08272700	0.72854800	-1.10584500	O	0.07647400	-0.02002200	2.43807200
C	4.41241800	1.81062000	-2.13985000	C	1.99849300	1.35465800	2.08635400
C	2.01798800	1.92546200	-1.82224400	C	2.39515000	2.56399900	1.50692700
C	3.19553600	2.45811100	-2.35250300	C	2.75186000	0.79377800	3.13200600
H	5.33057800	2.25397300	-2.52028300	C	3.54299800	3.20330400	1.96938200
H	1.06962100	2.43474000	-1.95439800	H	1.79341900	3.00268300	0.72455300
H	3.16527900	3.39049600	-2.91171600	C	3.91059500	1.43036600	3.57315100
C	3.20334700	-1.32650500	-0.28845200	H	2.42427800	-0.13388500	3.58994000
C	3.54446000	-2.50656300	-1.25696500	C	4.30763300	2.63642800	2.99270000
C	1.37391000	-2.89411100	-0.75412900	H	3.84220000	4.14832900	1.52540500
C	1.71597100	-1.65038300	0.10174000	H	4.49481400	0.98870400	4.37576500
C	2.21888800	-2.67934600	-2.02441200	H	5.20748500	3.13678500	3.34043500
H	2.21971200	-3.55053800	-2.69058500	P	-1.85075800	-1.33933500	0.21262700
H	1.93091500	-1.79367100	-2.59954900	C	-2.50126200	-1.77796400	-1.43313400
C	3.60806000	-3.81416800	-0.43157800	C	-3.71593700	-2.13962800	-1.94896600
H	4.04919600	-4.62447700	-1.02319100	O	-1.57449300	-1.71455400	-2.45247300
H	4.22197700	-3.70001000	0.46951900	C	-3.53261700	-2.30826200	-3.35670700
C	2.10716300	-4.10285700	-0.10831800	H	-4.62625300	-2.26595800	-1.38220300
H	1.77327400	-5.03783800	-0.57442800	C	-2.21877500	-2.04006000	-3.60242700
H	1.90451800	-4.18475900	0.96455800	H	-4.27972300	-2.58918700	-4.08597200
H	4.43118600	-2.32921000	-1.86865400	H	-1.61305000	-2.03066400	-4.49594100
H	0.30902800	-3.07525900	-0.90732700	C	-1.80074700	-2.94454200	1.08839300
H	1.59461700	-1.86407700	1.16738400	C	-1.07886000	-3.32641600	2.18857600
H	3.86003000	-1.36677200	0.59257100	O	-2.62242500	-3.97431100	0.69940900
				C	-1.47662500	-4.66542600	2.49630000

H	-0.36500000	-2.71117900	2.71714400
C	-2.40788200	-5.00400300	1.56035000
H	-1.11391200	-5.28986400	3.30085400
H	-2.98083600	-5.89910200	1.36928600
C	-3.25606800	-0.50800300	1.01156600
C	-3.31731200	0.64695300	1.74278400
O	-4.49199100	-1.12112700	1.00758400
C	-4.66618800	0.76408100	2.20577700
H	-2.49604000	1.32674100	1.92227800
C	-5.32707900	-0.32812500	1.73132600
H	-5.08256200	1.55880800	2.80866700
H	-6.34654000	-0.67529000	1.81181800

11d

M06/BSII SCF energy in solution: -1435.642557 a.u.

Solution-phase enthalpy: -1435.142368 a.u.

Solution-phase Gibbs energy: -1435.23448 a.u.

Pd	-0.78674600	-0.00209800	-0.27425500
C	-3.63444600	0.65093400	-0.49303000
C	-4.75935700	1.45904400	-0.76271900
C	-2.33335800	1.19911200	-0.54894600
C	-4.55943600	2.81536500	-1.05213300
C	-2.16469600	2.56004700	-0.83870000
C	-3.27793500	3.36711400	-1.08337200
H	-5.42268900	3.44413300	-1.26335200
H	-1.16572900	2.98885200	-0.88600500
H	-3.14879500	4.42359000	-1.31156400
C	-3.69992100	-0.82048200	-0.18115300
C	-4.28920800	-1.20490900	1.21687400
C	-2.20981800	-2.09761200	1.28377500
C	-2.24619800	-1.41010800	-0.09717700
C	-3.05475800	-1.13153300	2.13981000
H	-3.25965200	-1.50774300	3.15056300
H	-2.61963700	-0.13022400	2.20659500
C	-4.56870000	-2.72627700	1.20901800
H	-5.13668200	-3.02045600	2.09993900
H	-5.15294300	-3.03511700	0.33418500
C	-3.13384800	-3.34791000	1.22822800
H	-2.98674400	-3.97954600	2.11356500
H	-2.92968100	-3.96945300	0.34850200
H	-5.14810400	-0.60033200	1.52018400
H	-1.20275900	-2.32175300	1.64986800
H	-2.02970800	-2.11147500	-0.91478400
H	-4.28528400	-1.33610200	-0.95896200

C	-6.16455800	0.89606100	-0.76500800
H	-6.86981100	1.60826800	-1.20724500
H	-6.22827700	-0.03743500	-1.33820900
H	-6.52253100	0.66754800	0.24708300
O	2.88813500	0.06278800	-0.05698600
C	2.26463600	-1.16859200	-0.16645400
O	1.06699700	-1.34175200	-0.06369700
C	3.24017900	-2.25651400	-0.38703800
C	4.60386900	-2.01387100	-0.61967800
C	2.75572700	-3.57551500	-0.37217400
C	5.47073900	-3.08309000	-0.83257700
H	4.97551200	-0.99611400	-0.64577600
C	3.62892400	-4.63840300	-0.57991700
H	1.69906500	-3.74519900	-0.19539200
C	4.98630400	-4.39374700	-0.80997300
H	6.52424000	-2.89466300	-1.01735000
H	3.25304800	-5.65708400	-0.56485900
H	5.66646500	-5.22496500	-0.97411900
C	2.23401900	1.28676100	-0.04989800
O	1.06939200	1.43733400	-0.35262700
C	3.14277700	2.38616800	0.33799400
C	2.63412700	3.69500900	0.28704500
C	4.46470200	2.16456200	0.75739200
C	3.44296800	4.76898300	0.64459200
H	1.60920000	3.84891500	-0.03288400
C	5.26712700	3.24467600	1.11716400
H	4.85346100	1.15436400	0.81131900
C	4.75954400	4.54543800	1.05883500
H	3.04809200	5.77967400	0.60275500
H	6.28818700	3.07232500	1.44464000
H	5.38947100	5.38526600	1.33880200

12d

M06/BSII SCF energy in solution: -1435.635844 a.u.

Solution-phase enthalpy: -1435.135772 a.u.

Solution-phase Gibbs energy: -1435.230266 a.u.

Pd	0.47907500	-0.44677800	-0.72984700
C	3.35318800	0.00581800	-0.47472200
C	4.61908500	0.52251000	-0.82202000
C	2.24649500	0.19378700	-1.33254600
C	4.75944900	1.18911300	-2.04681600
C	2.41864500	0.86089300	-2.55313100
C	3.67654500	1.35136100	-2.91187000
H	5.73303200	1.59121200	-2.32123900

H	1.57375000	1.00955700	-3.22480800
H	3.81179300	1.87077300	-3.85848200
C	3.06059700	-0.73048900	0.80664400
C	3.65623800	-2.17462700	0.91830200
C	1.43018000	-2.52720000	1.14060900
C	1.52406800	-1.00767900	0.93434600
C	2.57428900	-3.04334200	0.24323300
H	2.76415600	-4.11818200	0.35622000
H	2.42488000	-2.81163900	-0.81526900
C	3.52837100	-2.62589800	2.39241600
H	4.07543100	-3.56139300	2.55931000
H	3.93329400	-1.88322400	3.08987300
C	1.98874900	-2.83853400	2.56183000
H	1.75721300	-3.87281100	2.84423700
H	1.55033400	-2.18745500	3.32631900
H	4.66635700	-2.26861300	0.51172900
H	0.43500200	-2.94588500	0.96665000
H	1.02836600	-0.42907600	1.72107800
H	3.41216600	-0.13705200	1.66541200
C	5.81497200	0.39167300	0.09662000
H	6.63765000	1.03159000	-0.24028500
H	5.56949500	0.67749900	1.12731700
H	6.19687400	-0.63644400	0.13866700
O	-2.77756900	0.76694400	0.25637000
C	-2.71911000	-0.55188800	-0.10633100
O	-1.66297500	-1.14048300	-0.27518400
C	-4.04279200	-1.15969000	-0.34453100
C	-5.23443200	-0.47897900	-0.04802900
C	-4.08982500	-2.45898800	-0.87696800
C	-6.46069800	-1.09664500	-0.28278800
H	-5.19274400	0.52271700	0.36451000
C	-5.31813700	-3.06914200	-1.10991100
H	-3.15905300	-2.97045500	-1.09807300
C	-6.50363700	-2.38872200	-0.81365000
H	-7.38278600	-0.57168400	-0.05111900
H	-5.35400600	-4.07340200	-1.52168300
H	-7.46214400	-2.86693400	-0.99603000
C	-1.86306900	1.28643100	1.20160400
O	-1.45619500	0.60721200	2.10658500
C	-1.59122300	2.71984100	0.97464300
C	-0.78416200	3.38055000	1.91475300
C	-2.09753100	3.41944800	-0.13135200
C	-0.48658500	4.72920800	1.74795900
H	-0.39874700	2.82012800	2.75979500

C	-1.79562400	4.77004000	-0.29220600
H	-2.71817800	2.90569800	-0.85660500
C	-0.99181300	5.42448000	0.64490400
H	0.14116200	5.23883400	2.47294200
H	-2.18403200	5.31153900	-1.14981000
H	-0.75619200	6.47712800	0.51419100

TS13d

M06/BSII SCF energy in solution: -1435.624834 a.u.

Solution-phase enthalpy: -1435.12667 a.u.

Solution-phase Gibbs energy: -1435.216238 a.u.

Pd	-0.09483200	-0.12438800	1.17980600
C	-2.89807000	0.02980400	0.33224400
C	-4.22486900	0.51063800	0.30477000
C	-1.96098300	0.59279900	1.22202100
C	-4.58648300	1.52317300	1.20271000
C	-2.34713800	1.60417600	2.10832800
C	-3.66743700	2.05890700	2.10588900
H	-5.60645600	1.90178000	1.18652800
H	-1.62592400	2.04960900	2.79063300
H	-3.97638400	2.84247000	2.79404000
C	-2.38307700	-1.06573300	-0.56449200
C	-2.92214300	-2.50510700	-0.25241000
C	-0.67897700	-2.74119800	-0.02635800
C	-0.84520800	-1.26242900	-0.37678700
C	-1.93964000	-3.00945300	0.82421400
H	-2.07947400	-4.06925700	1.06685000
H	-1.97224800	-2.42760300	1.75197500
C	-2.55612400	-3.41385600	-1.44830300
H	-3.04375900	-4.39084800	-1.35465700
H	-2.86887000	-2.98380100	-2.40640500
C	-1.00485900	-3.54614900	-1.32313500
H	-0.69837200	-4.59091500	-1.19704400
H	-0.47065900	-3.15478200	-2.19558600
H	-3.97969500	-2.52764300	0.01898300
H	0.28975400	-2.99311700	0.40986300
H	-0.22799000	-0.90328600	-1.20280900
H	-2.59984200	-0.81922600	-1.61451600
C	-5.25057000	-0.02207900	-0.67197700
H	-6.13409300	0.62402900	-0.69875700
H	-4.85008600	-0.08171700	-1.69151300
H	-5.59199500	-1.03063700	-0.40657300
O	2.51657400	0.65568300	-0.07319000
C	2.72503700	-0.44857300	0.51855100

O	1.87451900	-1.02861300	1.26522300	C	1.53797100	-3.00674300	-1.19382300
C	4.06332700	-1.09590800	0.33064100	H	1.44881400	-3.94523800	-1.75236400
C	5.02793400	-0.49741900	-0.49191500	H	1.61185800	-2.17942100	-1.90925900
C	4.35370800	-2.30568300	0.97653600	C	2.23944900	-4.19411100	0.75697500
C	6.27042600	-1.10451900	-0.66593600	H	2.51500000	-5.15736400	0.31326300
H	4.78801800	0.43756800	-0.98644100	H	2.70714700	-4.14451300	1.74647000
C	5.59790100	-2.90927300	0.80158300	C	0.68859000	-4.02530000	0.81270000
H	3.59720000	-2.75692000	1.60944400	H	0.17012600	-4.91198100	0.43138600
C	6.55704800	-2.31012600	-0.01959000	H	0.31304500	-3.84045600	1.82456600
H	7.01533500	-0.63883400	-1.30550200	H	3.68882000	-3.12862200	-0.56091300
H	5.82029500	-3.84689400	1.30394600	H	-0.60912700	-2.76054200	-0.49776000
H	7.52646800	-2.78250400	-0.15610000	H	0.41043200	-1.36619800	1.55289700
C	0.73246600	1.49592200	0.01302400	H	2.78717800	-1.82189000	1.67386200
O	0.37977700	1.63818400	-1.11435700	C	5.46094600	-1.20221200	0.71280300
C	0.94593700	2.51883000	1.07912700	H	6.45328800	-0.75039600	0.81015100
C	0.33408400	3.76661900	0.87817300	H	5.12395400	-1.48568100	1.71757000
C	1.64476500	2.26287400	2.26829800	H	5.58055100	-2.13307800	0.14430800
C	0.43183200	4.75126600	1.85821500	O	-2.28349700	0.46431000	1.21907700
H	-0.20893400	3.94664200	-0.04330900	C	-2.58496600	-0.17601900	0.19868000
C	1.72704500	3.25213300	3.24833400	O	-1.76517000	-0.43155200	-0.77723000
H	2.13224200	1.30599000	2.41905900	C	-3.98606600	-0.70241700	0.02751100
C	1.12338000	4.49547800	3.04592900	C	-4.93764100	-0.45178800	1.02511800
H	-0.03373000	5.71928500	1.69558500	C	-4.35417000	-1.43657000	-1.10797500
H	2.27426100	3.05350700	4.16539900	C	-6.24015000	-0.92943500	0.88977600
H	1.19492600	5.26494900	3.80963100	H	-4.63333100	0.11857400	1.89642700

14d

M06/BSII SCF energy in solution: -1435.63149 a.u.

Solution-phase enthalpy: -1435.132108 a.u.

Solution-phase Gibbs energy: -1435.224223 a.u.

Pd	0.27199500	0.07227200	-0.49481200	H	-7.61854200	-2.03391700	-0.35032900
C	3.10457800	-0.47153800	0.03669200	C	0.11211700	1.35705300	1.10595100
C	4.49729200	-0.24377800	0.04803300	O	0.49159700	1.06964300	2.19352100
C	2.24083900	0.47546800	-0.54628700	C	-0.28015200	2.69783200	0.58928200
C	4.98676800	0.91946500	-0.56025300	C	0.24588800	3.80902100	1.26869100
C	2.75218100	1.63281000	-1.14126800	C	-1.08255000	2.88093500	-0.54652500
C	4.13233600	1.84477700	-1.16119200	C	-0.02756200	5.09419000	0.80707200
H	6.05861400	1.10563500	-0.55275800	H	0.86215400	3.64975500	2.14721400
H	2.08556700	2.37391800	-1.57762100	C	-1.35034200	4.17172900	-0.99972000
H	4.54090300	2.73910500	-1.62563400	H	-1.52503000	2.02490100	-1.04755900
C	2.45142700	-1.69142400	0.63472000	C	-0.82233500	5.27722700	-0.32789700
C	2.67927200	-3.02790300	-0.15745800	H	0.37816700	5.95307400	1.33418100
C	0.42100200	-2.81796300	-0.14281900	H	-1.98257500	4.31363900	-1.87135000
C	0.89831500	-1.57577400	0.60032300	H	-1.03483500	6.28111700	-0.68507300

18a

M06/BSII SCF energy in solution: -1825.045642 a.u.

Solution-phase enthalpy: -1824.531445 a.u.

Solution-phase Gibbs energy: -1824.665286 a.u.

Pd	-0.69741000	-1.32340100	-0.77806500
C	-2.65783900	-1.56589700	-0.41798300
C	-3.31953900	-2.74466200	-0.82222100
C	-3.39023200	-0.55696200	0.25157000
C	-4.71221800	-2.82420500	-0.67203300
C	-4.78723000	-0.68112900	0.40319600
H	5.34501700	2.40807800	0.88367800
C	-5.45216900	-1.79646900	-0.08694900
H	-5.22209800	-3.72483600	-1.00839500
H	-5.34343900	0.10999100	0.89640100
H	-6.53079200	-1.88261600	0.01120600
C	3.45917500	2.64060900	1.03960700
O	2.43500100	2.17041000	1.59270900
O	3.58591400	3.56857300	0.21791200
O	4.65335700	1.95384500	1.39214900
Cs	3.05960200	-0.73380600	1.92926000
C	-1.03489100	-1.37301800	-3.04026500
C	-0.90850100	-0.03881200	-2.73646900
H	-2.00606700	-1.79952300	-3.26312600
Cs	0.58345000	3.17346300	-0.63988500
I	-0.36657800	-2.57102100	1.61544300
C	-2.58273500	-3.95926400	-1.34558200
H	-3.28719300	-4.72444700	-1.68930700
H	-1.90655000	-3.72510600	-2.17282400
H	-1.96442900	-4.39457800	-0.55182800
C	4.69251300	0.26418900	-1.78966500
C	3.72503000	-0.74084800	-1.64905400
C	4.13144600	-2.08018100	-1.55406300
C	5.48693900	-2.41073800	-1.60843100
C	6.44755600	-1.40360100	-1.74425400
C	6.04764400	-0.06695600	-1.83129800
H	4.36496900	1.29760200	-1.84384600
H	3.37277000	-2.84960200	-1.44719700
H	5.79435500	-3.45220300	-1.55094400
H	7.50324800	-1.66027000	-1.78466900
H	6.79332500	0.71757100	-1.93345800
C	2.25706400	-0.35987000	-1.57467500
O	1.48805300	-1.26605000	-1.08500800
O	1.92458000	0.78127200	-1.95469200

C	-2.72333400	0.66218500	0.78613400
O	-1.72162300	1.14630200	0.25021500
C	-3.27489100	1.32972700	2.01277200
C	-3.79052200	0.59052700	3.08878800
C	-3.18778900	2.72636000	2.12258200
C	-4.20965400	1.24001300	4.25071800
H	-3.83537700	-0.49166300	3.02273400
C	-3.62976300	3.37546700	3.27234700
H	-2.78236200	3.29333100	1.28992200
C	-4.13831200	2.63135900	4.34161500
H	-4.59112800	0.65793400	5.08507900
H	-3.57406900	4.45867400	3.34022900
H	-4.47450500	3.13592500	5.24350200
H	-0.15611000	-1.96306100	-3.28348600
C	-2.02457400	0.94516500	-2.75481200
O	-3.23058500	0.38994200	-2.95954700
O	-1.83738600	2.14727100	-2.64195200
C	-4.37300500	1.27794700	-2.99053100
H	-4.20543200	2.08808800	-2.27701400
H	-5.20292400	0.65693700	-2.64709900
C	-4.61184100	1.81655000	-4.39340400
H	-4.73636100	0.99744200	-5.10929500
H	-5.52285100	2.42624700	-4.40718100
H	-3.77421400	2.44251900	-4.71463900
H	0.07537100	0.41960500	-2.67165200

TS19a

M06/BSII SCF energy in solution: -1825.014722 a.u.

Solution-phase enthalpy: -1824.501834 a.u.

Solution-phase Gibbs energy: -1824.632824 a.u.

Pd	-0.33636200	-0.87185800	0.42209600
C	-2.41121900	-1.12484900	0.86280600
C	-2.58601800	-1.93023400	2.01931200
C	-3.32984500	-0.05418200	0.62287000
C	-3.70039500	-1.71590200	2.84317300
C	-4.42761300	0.12271900	1.47345400
H	5.14941800	2.64927700	-2.17939100
C	-4.63230000	-0.72400100	2.56192400
H	-3.82798200	-2.34125200	3.72399600
H	-5.13351000	0.92210300	1.27689500
H	-5.50396800	-0.59330300	3.19668900
C	3.40171200	3.15766800	-1.60973600
O	2.70345500	3.35667600	-0.58578000
O	3.08946400	3.17057800	-2.81742200

O	4.74395100	2.80988300	-1.31166700
Cs	3.69892000	1.33126400	1.37252000
C	-0.70387000	-2.35532400	-1.00644900
C	-2.10487500	-2.15015400	-0.79533900
H	-0.25676200	-3.29855700	-0.70159800
Cs	0.09675700	2.54934300	-1.95556400
I	-0.06232000	1.16503800	2.34660000
C	-1.57368300	-2.96209900	2.46362600
H	-2.06278300	-3.79337200	2.98458900
H	-0.98759800	-3.36553300	1.63660600
H	-0.86861600	-2.49556500	3.16277200
C	4.17900000	-0.29309500	-2.65697800
C	3.56493700	-0.94988600	-1.58113300
C	4.30975300	-1.85500100	-0.81030200
C	5.64844500	-2.10805700	-1.11666200
C	6.25674800	-1.44692300	-2.18787200
C	5.52051400	-0.53784900	-2.95310800
H	3.60157000	0.42609300	-3.22904600
H	3.82215000	-2.36615000	0.01467100
H	6.21432700	-2.82543100	-0.52698000
H	7.29922100	-1.64215000	-2.42668500
H	5.99283200	-0.02081100	-3.78486100
C	2.11093000	-0.66490900	-1.26769600
O	1.76044500	-0.90999900	-0.04730100
O	1.37801900	-0.20501600	-2.16076700
C	-3.15839100	0.92642300	-0.49756000
O	-2.61229400	0.64154900	-1.56649600
C	-3.65736200	2.33455500	-0.32487800
C	-3.51404200	3.04173200	0.88002500
C	-4.17712600	2.99258200	-1.45337400
C	-3.89009200	4.38473800	0.94995200
H	-3.07047900	2.55376900	1.74224300
C	-4.57522400	4.32488900	-1.37132000
H	-4.27350700	2.44088200	-2.38380500
C	-4.42821300	5.02455400	-0.16844600
H	-3.75801500	4.93065600	1.87985600
H	-4.99824300	4.81914300	-2.24181700
H	-4.73008300	6.06669700	-0.10614700
H	-0.24941400	-1.86560400	-1.86524100
C	-3.06397300	-3.29220500	-0.55032500
O	-2.44796100	-4.42039100	-0.14323500
O	-4.25636200	-3.20013100	-0.75454600
C	-3.29372100	-5.57737400	0.07498900
H	-4.23494500	-5.24419800	0.51899600

20a

M06/BSII SCF energy in solution: -1825.044994 a.u.

Solution-phase enthalpy: -1824.529345 a.u.

Solution-phase Gibbs energy: -1824.661087 a.u.

Pd	1.07980900	-0.94451100	-0.73259800
C	3.33907200	-0.24741600	-0.39978300
C	3.71737100	-0.92581100	-1.59347800
C	3.17810600	1.18329100	-0.44856000
C	3.98041300	-0.17799200	-2.75818400
C	3.47338000	1.87680400	-1.62306500
H	-5.76828000	-0.04717900	1.36975100
C	3.89388000	1.20134000	-2.77037300
H	4.27249700	-0.70951800	-3.65958400
H	3.37765800	2.95656000	-1.64522300
H	4.12067300	1.75757000	-3.67463600
C	-4.28169000	1.11807400	1.12975200
O	-3.50818700	1.59408200	0.26396300
O	-4.28104500	1.24874800	2.37262800
O	-5.27461000	0.26475500	0.59359700
Cs	-3.34736600	-0.59394000	-1.82484700
C	1.95096200	-1.83926800	0.86698200
C	3.23561500	-1.02267200	0.93058700
H	2.06785300	-2.89227300	0.59860100
Cs	-1.31073800	2.12206700	2.31165300
I	0.12421500	0.28510400	-3.16381000
C	4.01409600	-2.41009800	-1.66993300
H	5.09563800	-2.57064400	-1.58799900
H	3.53399600	-2.99870000	-0.88915800
H	3.68264900	-2.80670400	-2.63501800
C	-3.40083600	-2.21032100	2.19518400
C	-2.44971700	-2.59136400	1.23777500
C	-2.59426300	-3.81926200	0.57398600
C	-3.66745200	-4.66016900	0.87346900
C	-4.61333900	-4.27443100	1.82784900
C	-4.47982900	-3.04706000	2.48288500
H	-3.30360000	-1.24688100	2.68455300
H	-1.85082500	-4.10727800	-0.16263300

H	-3.76297900	-5.61786500	0.36772100	H	-1.99895300	-1.06162500	5.71712200
H	-5.44983900	-4.92863700	2.06055900	H	-3.50264500	2.92877900	5.32148600
H	-5.21628700	-2.74140600	3.22195300	H	-3.17091900	0.88907300	6.70244700
C	-1.28688500	-1.67054200	0.93000300	C	0.51914700	-1.08072800	-2.71982200
O	-0.74027800	-1.88073400	-0.22447300	O	0.27843800	-0.43941600	-1.66888000
O	-0.96581200	-0.79510200	1.75021900	O	1.37462600	-1.96033300	-2.95184200
C	2.76577300	2.00799500	0.73994700	O	-0.27619800	-0.68443700	-3.82214100
O	3.12503800	1.74814300	1.88685700	Cs	-0.14031800	2.39033400	-2.75599800
C	1.89043700	3.21703400	0.52672400	C	-1.04488900	1.10454000	1.71846600
C	0.95764600	3.31695200	-0.51935000	C	0.30030200	0.75336900	1.41539400
C	1.95746300	4.24081200	1.48963800	H	0.45634500	0.25332000	0.46119200
C	0.10734400	4.42459000	-0.59433900	H	-1.29170600	2.70796900	1.09400300
H	0.86713400	2.52529400	-1.25868800	Cs	3.27084800	-0.87155800	-0.82475300
C	1.12128700	5.35155200	1.40036800	I	-0.31278700	5.31301700	-0.04280500
H	2.67491300	4.14628800	2.29868600	C	-0.90117100	-1.36180300	3.32843200
C	0.18999600	5.44380500	0.35744200	H	0.18839100	-1.36460600	3.44497000
H	-0.61910800	4.48343700	-1.39973800	H	-1.28369500	-2.22604800	3.88073100
H	1.19621700	6.14792900	2.13634800	H	-1.11348800	-1.52649200	2.26781900
H	-0.46439100	6.30885200	0.28725500	C	5.32853600	2.85289300	-1.41217700
H	1.29574600	-1.72024100	1.72722100	C	4.49800400	3.19898300	-0.33709100
C	4.52904100	-1.74937500	1.28155700	C	5.03751800	3.91970000	0.73688700
O	4.30117100	-2.69881800	2.21462300	C	6.38633200	4.27598600	0.74007500
O	5.62563500	-1.48783000	0.83188800	C	7.21077200	3.91677200	-0.32977100
C	5.45855600	-3.41149400	2.71358800	C	6.67838700	3.20619200	-1.40902700
H	6.15263100	-3.57817600	1.88608000	H	4.89129400	2.32301700	-2.25324500
H	5.05841200	-4.37023200	3.05259600	H	4.38176800	4.20026900	1.55360800
C	6.12789300	-2.65212400	3.84958000	H	6.79493000	4.83925000	1.57523900
H	5.41610900	-2.45394600	4.65773500	H	8.26117000	4.19690500	-0.32684000
H	6.95517600	-3.24525200	4.25651700	H	7.31300500	2.93710200	-2.25007200
H	6.53125300	-1.70087600	3.49093600	C	3.03870500	2.78607300	-0.34950800
H	3.13660700	-0.28312800	1.72732400	O	2.37625700	3.10369000	0.69564700

TS22a

M06/BSII SCF energy in solution: -1825.027735 a.u.

Solution-phase enthalpy: -1824.651762 a.u.

Solution-phase Gibbs energy: -1824.5178 a.u.

Pd	0.26611000	2.83673900	0.90192100	C	-2.91245500	3.31030600	2.77983300
C	-1.65812300	1.09738900	3.09935600	O	-3.40787400	3.05396500	1.68558200
C	-1.54221300	-0.09353600	3.85775100	C	-2.88080400	4.70575600	3.30415600
C	-2.41582200	2.16856300	3.62929200	C	-2.02257100	5.10027900	4.34267900
C	-2.09259600	-0.14087600	5.14632100	C	-3.70544200	5.66311800	2.69096900
C	-2.92989600	2.09343800	4.93178600	C	-1.99610600	6.42930700	4.76431600
H	0.00633900	-1.27617800	-4.53938700	H	-1.36313100	4.37236300	4.80429200
C	-2.75806900	0.94668900	5.69921200	C	-3.68787300	6.98477600	3.12289400
				H	-4.34451100	5.34703500	1.87341900
				C	-2.83239600	7.37020900	4.16048200
				H	-1.31952100	6.73105400	5.55903400
				H	-4.33167400	7.71954000	2.64738500

H	-2.81277400	8.40522100	4.49166500	C	-1.71745400	0.64610600	2.52252000
H	-1.74831400	0.82346000	0.93506800	C	-0.87886700	0.93294800	3.60928000
C	1.42978300	0.58307500	2.35832100	C	-1.41823200	1.23715900	4.85933000
O	1.27898700	1.21877100	3.53220100	C	-2.80433000	1.26126500	5.03721900
O	2.42183300	-0.07991300	2.07221300	C	-3.64697000	0.97205900	3.96073500
C	2.38578700	1.16988300	4.46456000	H	-3.76941400	0.42328000	1.88208800
H	1.91218600	1.23652600	5.44704200	H	0.19435700	0.90145700	3.45409400
H	2.88622100	0.20380800	4.36599300	H	-0.75852600	1.45133800	5.69666200
C	3.34668800	2.32439700	4.22405500	H	-3.22528900	1.49846300	6.01119400
H	4.15835800	2.28888200	4.96062400	H	-4.72602900	0.98268900	4.09304100
H	3.77736600	2.26621100	3.22105700	C	-1.12956000	0.32100700	1.16144400
H	2.83066500	3.28488900	4.31943300	O	0.13502000	0.44422900	1.05664800

23a

M06/BSII SCF energy in solution: -1825.044329 a.u.

Solution-phase enthalpy: -1824.532059 a.u.

Solution-phase Gibbs energy: -1824.664437 a.u.

Pd	1.07865100	-0.35342500	-0.77860100
C	3.52662400	1.90869800	-1.27718300
C	3.75111400	3.30489400	-1.33346300
C	4.52628900	1.07755700	-0.71025200
C	4.90601100	3.83351900	-0.73760100
C	5.65133000	1.64394200	-0.10041200
H	-6.16564900	-1.70598700	0.96910100
C	5.83760400	3.02410300	-0.09955800
H	5.07330400	4.90688600	-0.79235600
H	6.40032500	0.99319600	0.33911500
H	6.72015500	3.45850700	0.36173000
C	-5.48526200	-0.64077100	-0.45067300
O	-4.89716800	-0.68852500	-1.55606200
O	-5.85683800	0.34360300	0.22768800
O	-5.70214400	-1.90909900	0.13950900
Cs	-2.77933200	-2.74240600	-0.81882500
C	2.31886200	1.31339100	-1.92676100
C	0.98066100	1.65691400	-1.76493000
H	0.29112100	1.39786300	-2.56482900
H	1.63870100	-1.10027300	-1.99053600
Cs	-3.73126600	2.12397600	-1.04956200
I	1.04774900	-2.92759100	-0.01575500
C	2.84729900	4.27580200	-2.06551200
H	2.13844100	4.76244400	-1.38641100
H	3.44882200	5.06611200	-2.52705700
H	2.26741700	3.79542000	-2.85730900
C	-3.10829200	0.66116500	2.71060600

O	-1.91342100	-0.02145500	0.23881700
C	4.54066800	-0.41685900	-0.92684900
O	4.33717900	-0.84921400	-2.05625700
C	4.90493200	-1.33075100	0.19584300
C	4.78451900	-0.95622400	1.54296500
C	5.33926900	-2.62776700	-0.12209300
C	5.10419900	-1.86182500	2.55427200
H	4.42280700	0.03445000	1.79870200
C	5.67109200	-3.52454500	0.88768800
H	5.40306800	-2.90926500	-1.16779700
C	5.55463200	-3.14240800	2.22837700
H	4.99608400	-1.56977600	3.59513800
H	6.01320600	-4.52432100	0.63467200
H	5.80737600	-3.84594600	3.01740500
H	2.54910300	0.72173000	-2.80733400
C	0.37827700	2.61951500	-0.80220400
O	1.18244900	2.98242200	0.19782200
O	-0.76334300	3.04280100	-0.94164600
C	0.60183500	3.79081700	1.24597900
H	0.26564700	4.73997600	0.81389100
H	-0.26737900	3.26229000	1.64494200
C	1.67006600	3.98967300	2.30427400
H	1.27539600	4.61125600	3.11557100
H	1.97529200	3.02553700	2.72156000
H	2.55415100	4.48181500	1.88629600

3b

M06/BSII SCF energy in solution: -1439.509141 a.u.

Solution-phase enthalpy: -1439.181545 a.u.

Solution-phase Gibbs energy: -1439.267314 a.u.

Pd	0.62974700	-0.19220300	-0.07380100
P	-1.65457000	0.00984900	0.01396800

C	-2.39073900	1.05627900	-1.28763400	Pd	-3.61990300	1.79761500	-0.12173800
C	-1.77682400	1.79001500	-2.26862400	P	-5.25423500	3.44075500	0.18754800
O	-3.75322700	1.20811200	-1.38893400	C	-6.69307300	3.30591200	-0.92321400
C	-2.81456100	2.42971300	-3.01622400	C	-6.97215800	2.36277200	-1.87728300
H	-0.70966900	1.85890900	-2.42617400	O	-7.71307800	4.22635700	-0.87547600
C	-3.98541200	2.03891200	-2.43721700	C	-8.23186100	2.72015800	-2.45177000
H	-2.70294200	3.08803000	-3.86644700	H	-6.34822900	1.51551900	-2.12582900
H	-5.02402100	2.25234400	-2.64265500	C	-8.62870200	3.85342200	-1.80586900
C	-2.56942700	-1.56181200	-0.14087500	H	-8.76678400	2.20304700	-3.23605000
C	-2.09020700	-2.83301200	-0.32027400	H	-9.49761000	4.48974500	-1.88670100
O	-3.94255100	-1.59499600	-0.08333500	C	-5.99977900	3.49793100	1.85053200
C	-3.22750700	-3.69819700	-0.37701200	C	-5.77949100	2.69238100	2.93669100
H	-1.04692300	-3.10378000	-0.40197600	O	-6.94144400	4.44691500	2.16870900
C	-4.31678600	-2.89179300	-0.22768500	C	-6.63046600	3.16826600	3.98259300
H	-3.23249000	-4.77111100	-0.50981800	H	-5.09125200	1.85971800	2.97330200
H	-5.38064000	-3.07640900	-0.20207300	C	-7.30693200	4.22946400	3.45802900
C	-2.31967000	0.73068700	1.55451100	H	-6.72433300	2.77422200	4.98485300
C	-1.65606500	1.16576000	2.67156100	H	-8.04924200	4.90694900	3.85342300
O	-3.67098400	0.91283600	1.72749300	C	-4.66618700	5.14680800	-0.07671000
C	-2.64921500	1.64125200	3.58397600	C	-3.40691300	5.59969500	-0.37265700
H	-0.58471500	1.14571700	2.81349500	O	-5.52560800	6.21527300	0.01429100
C	-3.84629800	1.46222800	2.95652700	C	-3.49261200	7.02370300	-0.46989600
H	-2.49249900	2.05893300	4.56869700	H	-2.52927900	4.98170500	-0.50237300
H	-4.86966400	1.66555500	3.23548200	C	-4.79743700	7.33519000	-0.22622400
I	3.24104300	1.57350300	-0.17517200	H	-2.69345100	7.71735400	-0.69075900
C	2.50148600	-1.15010700	-1.45355400	H	-5.34543800	8.26510600	-0.18940000
C	2.53013000	-2.54734300	-1.58405400	I	-3.75021400	-0.85275400	-1.04718900
C	2.83010400	-3.34047300	-0.48205500	C	-1.59959300	0.34036300	1.02246200
C	3.08306400	-2.74705900	0.76044000	C	-0.31150000	0.69803500	1.43035000
C	3.07073000	-1.35965300	0.94522900	C	0.59723700	1.18959300	0.49519000
C	2.77074000	-0.55567400	-0.19391300	C	0.21834700	1.32880100	-0.84298600
H	2.37210100	-0.52561700	-2.33028100	C	-1.06192800	0.98672800	-1.29833800
H	2.33623800	-2.99369500	-2.55547400	C	-1.98169900	0.51675900	-0.32427700
H	2.86780100	-4.42184500	-0.57915500	H	-2.29655400	-0.09737300	1.72863000
H	3.31044400	-3.37700500	1.61714200	H	-0.02397700	0.57404200	2.47095000
C	3.44320800	-0.77209300	2.28473200	H	1.60459900	1.45908200	0.80008500
H	2.73482400	-0.00512600	2.61035300	H	0.93786700	1.70728300	-1.56576900
H	3.47880000	-1.55387200	3.04950500	C	-1.38979400	1.07729400	-2.77016200
H	4.43190100	-0.29643900	2.23987500	H	-2.34426400	1.57806700	-2.95274100
				H	-0.60609400	1.62232500	-3.30567100
				H	-1.46632800	0.07381700	-3.20915100

TS4b

M06/BSII SCF energy in solution: -1439.503228 a.u.

Solution-phase enthalpy: -1439.175597 a.u.

Solution-phase Gibbs energy: -1439.262896 a.u.

5b

M06/BSII SCF energy in solution: -1439.509514 a.u.

Solution-phase enthalpy: -1439.180675 a.u.

Solution-phase Gibbs energy: -1439.271187 a.u.

Pd	-0.91957100	0.31737000	-0.06672200
P	1.55607900	0.26739300	-0.00961700
C	2.29623800	-0.57333800	1.42004000
C	1.70373600	-1.34085000	2.38834400
O	3.65280400	-0.52227400	1.63609600
C	2.75137800	-1.78648100	3.25288700
H	0.64958200	-1.57107700	2.45384400
C	3.90333600	-1.26002500	2.74792600
H	2.65723200	-2.41424600	4.12776200
H	4.93891600	-1.31074500	3.05002500
C	2.33986900	-0.49362600	-1.46090700
C	1.77529500	-1.18973100	-2.49761600
O	3.70398300	-0.44788400	-1.62365100
C	2.84923600	-1.59378300	-3.35021700
H	0.72181100	-1.40035400	-2.61799900
C	3.98746900	-1.11673600	-2.77061700
H	2.78051700	-2.16324100	-4.26637900
H	5.03300000	-1.16283300	-3.03707300
C	2.24377900	1.95206500	0.04726900
C	1.59472500	3.15996500	0.05984100
O	3.59978500	2.16363400	0.08240400
C	2.60414400	4.17110400	0.10523600
H	0.52333800	3.30954600	0.03809200
C	3.79438400	3.50625000	0.11700400
H	2.46116700	5.24223600	0.12600900
H	4.82484000	3.82777500	0.14754600
I	-1.73190700	-2.18792100	-0.08710400
C	-3.31295300	1.03703700	-1.45855600
C	-4.48796100	1.78031200	-1.61782100
C	-5.21281700	2.16481000	-0.49084000
C	-4.76896800	1.80667200	0.78472800
C	-3.59236800	1.06761200	0.97833700
C	-2.84985500	0.74038300	-0.17236400
H	-2.76600500	0.69215200	-2.33179200
H	-4.83994100	2.03066000	-2.61520700
H	-6.13718600	2.72568300	-0.60126100
H	-5.35127000	2.09744800	1.65680900
C	-3.16115000	0.66949000	2.37267900
H	-2.24009500	1.18086000	2.67903300
H	-3.93726500	0.91833200	3.10387900
H	-2.96621200	-0.40686500	2.42577000

2d

M06/BSII SCF energy in solution: -2951.554067 a.u.

Solution-phase enthalpy: -2950.93191 a.u.

Solution-phase Gibbs energy: -2951.070928 a.u.

O	-3.02152600	-0.85428300	0.80623900
C	-2.88551000	-1.72558600	-0.24908400
O	-1.80313300	-1.94262000	-0.81920700
C	-4.17708500	-2.32338800	-0.66174900
C	-5.36583400	-2.08465900	0.04985800
C	-4.19431800	-3.15517900	-1.79555600
C	-6.55966700	-2.67287900	-0.37464600
H	-5.34010500	-1.44768600	0.92495900
C	-5.38972600	-3.74008200	-2.21509400
H	-3.26647600	-3.33190100	-2.32752600
C	-6.57418500	-3.49939300	-1.50557800
H	-7.47629700	-2.48997100	0.17646200
H	-5.40023200	-4.38243600	-3.08952700
H	-7.50354500	-3.95609100	-1.83135200
C	-1.88580600	-0.43664000	1.63636000
O	-1.07658100	-1.34697600	2.04909000
C	-2.26456900	0.75653600	2.43104500
C	-1.63954400	0.95925100	3.67678900
C	-3.22969100	1.67628000	1.98452400
C	-1.97112400	2.07022100	4.45598300
H	-0.91066700	0.23320100	4.01908400
C	-3.55550200	2.78589800	2.76852600
H	-3.71237400	1.51887500	1.02784300
C	-2.92831000	2.98896500	4.00454100
H	-1.49027500	2.21412100	5.41873600
H	-4.29861700	3.49337500	2.41414000
H	-3.18593600	3.85130500	4.61150700
P	2.23679800	-1.29636400	0.39032400
C	2.80514200	-2.23063000	1.85558900
C	3.86859500	-2.13373700	2.71985400
O	1.94319200	-3.24003100	2.31594100
C	3.67399100	-3.11533900	3.75466200
H	4.69716900	-1.45052300	2.62852700
C	2.50549800	-3.76418700	3.47514600
H	4.32882900	-3.30501900	4.59086000
H	1.95343500	-4.56029300	3.94218000
C	2.28945800	-2.56481000	-0.90439400
C	1.28644600	-3.06257700	-1.69685400
O	3.48488000	-3.26484400	-1.19101200
C	1.85669500	-4.10218100	-2.51236000

H	0.25830000	-2.73330400	-1.68020000	C	-3.01332900	1.32379800	-0.39818500
C	3.17852000	-4.19304200	-2.18189400	O	-2.34745500	0.32046400	-0.80722300
H	1.33800000	-4.70041500	-3.24507900	C	-4.46217700	1.44771300	-0.68639100
H	3.99521000	-4.81013700	-2.51422400	C	-5.18427800	2.58096200	-0.27447600
C	3.74411500	-0.32103300	0.07903000	C	-5.11364900	0.41283300	-1.37951400
C	5.01382600	-0.58762300	-0.37225100	C	-6.54801000	2.67845800	-0.56071400
O	3.64085100	1.06371500	0.32472500	H	-4.66816600	3.36537800	0.26564600
C	5.73054800	0.65822600	-0.41695700	C	-6.47754400	0.51478900	-1.66040400
H	5.38272600	-1.56214500	-0.64784800	H	-4.53992800	-0.45662400	-1.67823400
C	4.86929300	1.62926200	0.01098500	C	-7.19582100	1.64748400	-1.25379900
H	6.75266900	0.80154300	-0.73121000	H	-7.10510700	3.55381700	-0.24275200
H	4.94164700	2.69374400	0.14662700	H	-6.98087400	-0.28561100	-2.19317000
Pd	0.05806300	-0.21360100	0.52247300	H	-8.25613700	1.72508000	-1.47402300
P	0.10406900	1.70429900	-0.79756700	C	-0.89191500	2.15439400	0.93815400
C	-1.39673100	2.10300600	-1.75926000	O	-0.94158900	1.65387500	2.08695200
C	-2.39099700	1.29524000	-2.25620200	C	-0.25401000	3.45873100	0.59612200
O	-1.63401100	3.42267900	-2.19635900	C	0.70458300	3.97807500	1.48514700
C	-3.28315300	2.12241800	-3.02362700	C	-0.59142300	4.18993200	-0.55452600
H	-2.46047200	0.22986900	-2.11093600	C	1.32046800	5.20377300	1.22023600
C	-2.79621100	3.39689400	-2.96024100	H	0.95261600	3.42013400	2.37987000
H	-4.17010600	1.79915900	-3.54575700	C	0.01891500	5.42066800	-0.80939000
H	-3.11865300	4.34524800	-3.35319000	H	-1.34378900	3.80166000	-1.22886100
C	0.38746900	3.23221100	0.14299800	C	0.97929900	5.93033800	0.07355300
C	0.31464300	3.47678200	1.49169600	H	2.05870600	5.59444500	1.91348300
O	0.72224900	4.43775600	-0.51191000	H	-0.25853900	5.98427600	-1.69499800
C	0.60570000	4.86942100	1.69950000	H	1.45300100	6.88605500	-0.12804600
H	0.07537800	2.74832500	2.24958900	P	-0.59814100	-2.26109100	0.07324600
C	0.84821800	5.41289000	0.47049700	C	-1.87745000	-2.72383800	1.29510000
H	0.63012500	5.38564400	2.64622600	C	-1.95782000	-3.64452800	2.31178100
H	1.10784600	6.39734100	0.12217400	O	-3.04704000	-1.94087800	1.30863000
C	1.37459800	1.82352400	-2.10483600	C	-3.21369100	-3.44125700	2.98301200
C	1.86726700	2.82257700	-2.90821600	H	-1.21156900	-4.38360100	2.55351700
O	1.99555500	0.61158800	-2.46979000	C	-3.84290000	-2.40901800	2.34815700
C	2.83102300	2.23092700	-3.79581200	H	-3.58772700	-3.99770100	3.82817100
H	1.57377000	3.85793400	-2.86008200	H	-4.78224800	-1.90209300	2.48055000
C	2.87981500	0.89721400	-3.50211500	C	-1.24807000	-2.96794900	-1.46836300
H	3.40725700	2.74172300	-4.55159300	C	-1.55826000	-2.35793500	-2.65740800
H	3.43832400	0.06059000	-3.88236800	O	-1.57443900	-4.34100900	-1.57116600
				C	-2.08878900	-3.36258000	-3.53994600
				H	-1.43964900	-1.30625100	-2.86191200
				C	-2.08162700	-4.54192200	-2.85155800
				H	-2.43017300	-3.21385700	-4.55238900
				H	-2.37628800	-5.55003800	-3.08601300
O	-2.45943900	2.31704000	0.27402500	C	0.68053600	-3.47200800	0.54128800

TS3d

M06/BSII SCF energy in solution: -2951.537087 a.u.

Solution-phase enthalpy: -2950.90992 a.u.

Solution-phase Gibbs energy: -2951.05356 a.u

C	0.90169200	-4.81270100	0.33803200	C	6.66000300	1.04046100	-1.09627000
O	1.74335000	-2.95777300	1.31277200	H	4.91825300	1.80223000	-2.13871500
C	2.13479400	-5.15448900	0.99493600	C	6.18567100	-0.30084800	0.85949000
H	0.25423600	-5.47199500	-0.21644000	H	4.09014100	-0.56892900	1.32057800
C	2.61048500	-4.01077700	1.57177900	C	7.10979900	0.27945900	-0.01356700
H	2.59825900	-6.12826700	1.02556700	H	7.37584800	1.49313700	-1.77816900
H	3.48069900	-3.76606800	2.15439700	H	6.53243500	-0.89717300	1.70018000
Pd	-0.25360700	0.30295700	-0.02887000	H	8.17581000	0.13830200	0.14840400
P	2.06122600	0.61482900	-0.11871800	C	0.15411300	2.44023900	-0.79187300
C	2.81498100	2.01133000	-1.01369300	O	-0.36023000	2.66924300	-1.86065900
C	2.30721000	2.85041900	-1.97414200	C	0.86924600	3.48371300	0.00827000
O	4.19197300	2.28386300	-0.86610600	C	1.07008700	4.74327900	-0.58086100
C	3.38287500	3.68151100	-2.44255400	C	1.30518100	3.25253300	1.31862700
H	1.28021700	2.88286000	-2.29707200	C	1.70301600	5.75517700	0.13460900
C	4.50025000	3.31144100	-1.75014700	H	0.72708000	4.90159200	-1.59797500
H	3.31864800	4.45458000	-3.19201300	C	1.93329400	4.27200500	2.03541100
H	5.52363200	3.64382000	-1.74250700	H	1.16505300	2.27065100	1.75779800
C	2.81658200	0.69067600	1.53047500	C	2.13417200	5.52151700	1.44489100
C	2.22690200	0.76712800	2.76933000	H	1.86268500	6.72661500	-0.32591800
O	4.21744400	0.63453300	1.70171900	H	2.27307100	4.08858000	3.05112800
C	3.27865400	0.76622000	3.75040800	H	2.62869000	6.31255400	2.00289100
H	1.16381600	0.82450500	2.95084100	P	0.28658000	-2.06051500	0.07440300
C	4.45994400	0.68346100	3.06978500	C	1.42027900	-2.74683500	-1.18960000
H	3.15699300	0.81798700	4.82099200	C	1.27784600	-3.69943600	-2.16477000
H	5.49502900	0.65194300	3.36243900	O	2.66051500	-2.17460200	-1.28617300
C	2.97194200	-0.76825800	-0.89041500	C	2.50544900	-3.71425500	-2.90006500
C	4.28642300	-1.16253000	-0.92718500	H	0.40705900	-4.31628900	-2.33172700
O	2.22011800	-1.64370400	-1.70134500	C	3.30337000	-2.77299500	-2.32141100
C	4.36912500	-2.32120500	-1.77445100	H	2.75542700	-4.34221400	-3.74381800
H	5.09431200	-0.67493600	-0.40696000	H	4.30448800	-2.41717300	-2.51165100
C	3.10498500	-2.58072000	-2.22270300	C	1.05096900	-2.57285400	1.64508200
H	5.26022400	-2.88092700	-2.01284200	C	1.51203100	-1.80868600	2.68209300
H	2.67010000	-3.32773400	-2.86255700	O	1.29858500	-3.90236800	1.90918800

4d

M06/BSII SCF energy in solution: -2951.557127 a.u.

Solution-phase enthalpy: -2950.935357 a.u.

Solution-phase Gibbs energy: -2951.074961 a.u

O	2.52280800	1.44282500	-1.71504600	C	-1.10480600	-3.23254400	-0.11021300
C	2.88807900	0.86174200	-0.68715800	C	-1.32722500	-4.54281500	0.22310600
O	2.09722200	0.40723200	0.23974400	O	-2.22564600	-2.72568800	-0.72474800
C	4.36151700	0.64510800	-0.42806800	C	-2.65512500	-4.85749800	-0.20557200
C	5.29266200	1.21958800	-1.30341500	H	-0.62201800	-5.19488900	0.71683700
C	4.81752600	-0.11808300	0.65466600	C	-3.14810900	-3.71916400	-0.77139800

H	-3.17071400	-5.80223500	-0.10253200
H	-4.09026700	-3.45574000	-1.22693900
Pd	0.01511600	0.53061900	-0.11582500
P	-2.31343300	0.74678700	-0.01195600
C	-3.06223100	2.35121800	0.43293000
C	-2.57637200	3.45787100	1.07469400
O	-4.40231900	2.52321000	0.17024500
C	-3.67354100	4.36588300	1.21307800
H	-1.55824100	3.61300500	1.39976100
C	-4.74792000	3.74862700	0.64777700
H	-3.65605200	5.34791100	1.66448700
H	-5.77862200	4.03405300	0.49884800
C	-3.10861500	0.34780700	-1.59929600
C	-2.63819600	0.51162300	-2.87373200
O	-4.38691800	-0.15583500	-1.63272900
C	-3.68538800	0.08276000	-3.74858800
H	-1.67039600	0.91457600	-3.13682400
C	-4.71337900	-0.31043700	-2.94523100
H	-3.66929100	0.06803000	-4.82940400
H	-5.69887700	-0.70869900	-3.13623800
C	-3.12627800	-0.35684800	1.19598900
C	-4.43128600	-0.59004900	1.53973700
O	-2.30137200	-1.10076300	2.00438700
C	-4.41030700	-1.53795300	2.60930700
H	-5.29566400	-0.13700000	1.07716100
C	-3.09553000	-1.81041000	2.84638400
H	-5.25956800	-1.95788800	3.13021000
H	-2.57846200	-2.45224100	3.54320100

Norbornene

M06/BSII SCF energy in solution: -272.5834586 a.u.

Solution-phase enthalpy: -272.4235986 a.u.

Solution-phase Gibbs energy: -272.4582606 a.u

C	1.19093700	0.78133500	-0.51631400
C	-0.08824700	1.12849800	0.32317800
C	-0.08735900	-1.12863000	0.32289800
C	1.19175400	-0.78043300	-0.51620000
H	1.14595200	1.20720100	-1.52310800
H	2.08833000	1.17862100	-0.02798200
H	1.14743700	-1.20647000	-1.52295100
H	2.08939700	-1.17678400	-0.02756400
C	-0.04151100	-0.00016900	1.38071400
H	-0.91301300	-0.00058600	2.04297700
H	0.87774900	0.00012500	1.98008900

C	-1.27944100	0.67002100	-0.50761300
H	-1.92083700	1.32818200	-1.08598600
C	-1.27855700	-0.67074300	-0.50825000
H	-1.92080700	-1.32932800	-1.08519700
H	-0.12056600	2.15753500	0.68987400
H	-0.11909700	-2.15776500	0.68937200

TFP

M06/BSII SCF energy in solution: -1029.330729 a.u.

Solution-phase enthalpy: -1029.133252 a.u.

Solution-phase Gibbs energy: -1029.191112 a.u

P	0.00000500	0.00038100	-1.09373800
C	-1.11406100	1.17272600	-0.22214700
C	-1.01757000	1.95169200	0.90074000
O	-2.31571600	1.42298700	-0.84574600
C	-2.22654900	2.71344700	0.98109100
H	-0.17895600	1.97675200	1.58190300
C	-2.97330100	2.34780100	-0.09868500
H	-2.49894100	3.43528600	1.73864100
H	-3.94665400	2.63893400	-0.46459800
C	-0.45835400	-1.55029300	-0.22157600
C	-1.17323500	-1.85561900	0.90652900
O	-0.08248700	-2.71640900	-0.84966700
C	-1.23244100	-3.28340400	0.98532900
H	-1.60660600	-1.14142000	1.59198500
C	-0.55241100	-3.74776800	-0.10063500
H	-1.71745800	-3.87962900	1.74587700
H	-0.32402800	-4.73647900	-0.46987600
C	1.57217100	0.37924700	-0.22156100
C	2.19522300	-0.08989400	0.90474800
O	2.39389300	1.28850500	-0.84894700
C	3.46184000	0.57178200	0.98321800
H	1.79345600	-0.82364100	1.58880100
C	3.52312800	1.39509900	-0.10107600
H	4.22171800	0.44756400	1.74235300
H	4.26523900	2.08735700	-0.46999800

Benzoic Anhydride

M06/BSII SCF energy in solution: -764.9012827 a.u.

Solution-phase enthalpy: -764.6804247 a.u.

Solution-phase Gibbs energy: -764.7380317 a.u

C	-3.54902100	-1.76024600	-0.76971200
C	-2.35787400	-1.07005100	-0.55029900
C	-2.37844700	0.16283900	0.11815000

C	-3.59792600	0.69649000	0.56245700
C	-4.78434200	0.00305200	0.34148900
C	-4.76085900	-1.22639300	-0.32428800
H	-3.53232000	-2.71413600	-1.28930800
H	-1.41499100	-1.47817800	-0.89616400
H	-3.59161700	1.65283000	1.07487100
H	-5.72701400	0.41844200	0.68622400
H	-5.68737800	-1.76749300	-0.49696100
C	-1.14893800	0.95383500	0.37929100
O	-1.11152100	2.03600900	0.90549900
O	-0.00000100	0.26083800	-0.00001900
C	1.14894400	0.95384100	-0.37929900
O	1.11153400	2.03601900	-0.90549600
C	2.37844800	0.16284000	-0.11815200
C	2.35786400	-1.07005700	0.55028500
C	3.59793300	0.69649200	-0.56244100
C	3.54900800	-1.76025700	0.76970400
H	1.41497700	-1.47818400	0.89613600
C	4.78434500	0.00304800	-0.34146700
H	3.59163300	1.65283600	-1.07484700
C	4.76085200	-1.22640300	0.32429900
H	3.53229800	-2.71415200	1.28929200
H	5.72702200	0.41843900	-0.68618800
H	5.68736800	-1.76750600	0.49697700

CsICsHCO₃

M06/BSII SCF energy in solution: -316.2725544 a.u.

Solution-phase enthalpy: -316.2328204 a.u.

Solution-phase Gibbs energy: -316.2876694 a.u

C	-0.14595300	-2.56343900	0.31708800
O	0.02127600	-1.91133400	-0.74213200
O	1.06696800	-2.98076100	0.92319000
O	-1.19267300	-2.84835300	0.93266300
Cs	-2.55076200	-0.33941200	-0.21637300
H	0.77963700	-3.46326200	1.71623800
Cs	2.52710300	-0.37542800	-0.23274100
I	0.03149100	2.44979300	0.21132000

CsHCO₃

M06/BSII SCF energy in solution: -284.6098568 a.u.

Solution-phase enthalpy: -284.5756998 a.u.

Solution-phase Gibbs energy: -284.6139568 a.u

C	2.02175900	0.04247200	0.00016000
O	3.40999200	0.07511300	0.00023900

O	1.45049700	1.15736500	0.00004800
O	1.49568100	-1.11009000	0.00019200
Cs	-1.21166000	-0.00674000	-0.00009300
H	3.66137800	-0.86326600	0.00031200

CsOCOPh

M06/BSII SCF energy in solution: -440.2907834 a.u.

Solution-phase enthalpy: -440.1769934 a.u.

Solution-phase Gibbs energy: -440.2254024 a.u

O	-0.01041600	1.12939700	-0.00400800
C	0.56419000	0.00004000	-0.00388500
O	-0.01039800	-1.12932700	-0.00400900
C	2.08687900	0.00001500	-0.00153600
C	2.79676100	1.20688000	-0.00045500
C	2.79672300	-1.20687400	-0.00045500
C	4.19208800	1.20905900	0.00165900
H	2.22851200	2.13170500	-0.00131900
C	4.19204900	-1.20909600	0.00166000
H	2.22844400	-2.13168100	-0.00131900
C	4.89371600	-0.00003000	0.00272200
H	4.73494900	2.15195600	0.00248100
H	4.73488000	-2.15201100	0.00248200
H	5.98149400	-0.00004700	0.00437000
Cs	-2.70684000	-0.00000800	0.00107600

11c1

M06/BSII SCF energy in solution: -2045.77672 a.u.

Solution-phase enthalpy: -2045.163979 a.u.

Solution-phase Gibbs energy: -2045.278243 a.u

Pd	-0.62055100	0.34627400	-0.55797000
P	1.64461200	-0.74099300	-0.25089700
C	-3.54215400	-0.24883500	-0.42884000
C	-4.87663100	-0.32385100	-0.88513100
C	-2.56395900	0.44561300	-1.17522200
C	-5.21491000	0.30605100	-2.08886300
C	-2.93650900	1.05247200	-2.38419700
C	-4.25587400	0.98585700	-2.83809100
H	-6.24079300	0.24928700	-2.44756000
H	-2.20309000	1.56858800	-3.00035600
H	-4.53354600	1.45709300	-3.77869600
C	-3.05364900	-0.93569800	0.81188600
C	-3.44873900	-0.26627400	2.17292400
C	-1.18865500	-0.33466900	2.26901800
C	-1.48716000	-0.91289000	0.86903300

C	-2.29716500	0.73051100	2.41523800	H	1.58605800	1.85819200	-1.86046700
H	-2.33582600	1.18103000	3.41514000	H	0.19256800	1.64725700	-3.06448600
H	-2.23491800	1.52722500	1.66866900	C	0.10908800	3.29499400	0.02866800
C	-3.19018000	-1.29960700	3.29298700	O	-0.62547400	4.02750500	0.66189300
H	-3.59172800	-0.94303800	4.24906300	O	1.37976700	3.00308500	0.38283200
H	-3.66102200	-2.26704700	3.08228700	C	1.85562300	3.58571400	1.61830700
C	-1.62983000	-1.38207300	3.33466400	H	2.63424300	2.89738800	1.95295000
H	-1.24217600	-1.10951700	4.32404200	H	1.03625100	3.59160900	2.34123200
H	-1.25148800	-2.38325000	3.10239800	C	2.40126600	4.98887800	1.39484200
H	-4.45691300	0.15692400	2.18081200	H	1.60428500	5.66468300	1.07251500
H	-0.16064200	0.01089700	2.41245500	H	2.82449300	5.37709500	2.32874800
H	-1.05500900	-1.90740300	0.72403200	H	3.18991300	4.98395900	0.63466900
H	-3.42022500	-1.97395200	0.82178900				
C	1.62149300	-2.06730100	-1.49723800				
C	0.62343500	-2.45183600	-2.35414400				
O	2.70093800	-2.91115100	-1.64200300				
C	1.11199100	-3.58827300	-3.07123000				
H	-0.34544500	-1.97888600	-2.44007600				
C	2.36921900	-3.81811000	-2.59675400				
H	0.59396000	-4.15687200	-3.83058100				
H	3.12605100	-4.55471500	-2.82317600				
C	3.24472700	0.06835300	-0.64964000				
C	4.06362600	0.03049400	-1.74582500				
O	3.72245200	0.99645000	0.24508900				
C	5.10848400	0.98219000	-1.51261800				
H	3.94753700	-0.61188000	-2.60609800				
C	4.85473100	1.53159900	-0.29409000				
H	5.93798200	1.21525200	-2.16546800				
H	5.35283200	2.27507600	0.30948800				
C	2.13614800	-1.65149200	1.26853300				
C	3.13059700	-1.48769900	2.19496200				
O	1.32063900	-2.68762000	1.64739800				
C	2.92103200	-2.48744200	3.19850400				
H	3.91653000	-0.74826700	2.16282800				
C	1.81663700	-3.18431300	2.81457400				
H	3.51917100	-2.66201000	4.08194800				
H	1.27792400	-4.02189900	3.23061800				
C	-5.93388000	-1.09263200	-0.12254700				
H	-6.87493500	-1.12248900	-0.68197700				
H	-5.62490800	-2.12916200	0.06577300				
H	-6.14621000	-0.64661500	0.85682700				
C	-0.30587800	2.63458400	-1.24266300				
H	-1.31959700	2.88465400	-1.52989300				
C	0.53178400	1.96750100	-2.08388800				

TS12c1

M06/BSII SCF energy in solution: -2045.712525 a.u.

Solution-phase enthalpy: -2045.101433 a.u.

Solution-phase Gibbs energy: -2045.210045 a.u

Pd	4.93869200	3.20864600	0.88153600
P	2.69760600	2.79029900	0.95501100
C	7.32205600	4.92335800	0.68320800
C	8.26115400	5.66502100	-0.07860100
C	7.05439400	3.57432400	0.29086400
C	8.78476100	5.13905400	-1.26477200
C	7.52646800	3.12564800	-0.95887700
C	8.36781600	3.90070300	-1.74649800
H	9.49907400	5.72962300	-1.83429500
H	7.28569200	2.11621600	-1.28381300
H	8.73501500	3.52190700	-2.69658900
C	6.40539400	5.68344500	1.62407800
C	6.58311500	5.70146500	3.18632500
C	4.34713700	5.47957900	2.87147100
C	4.89778700	5.26866500	1.44627600
C	5.44453300	4.79886500	3.71356300
H	5.30348400	4.90954100	4.79738400
H	5.54259800	3.73760500	3.48173900
C	6.04068300	7.07940100	3.64074800
H	6.19748000	7.21675500	4.71780500
H	6.53142500	7.91643100	3.13042400
C	4.51447800	6.96939700	3.30571900
H	3.89756700	7.19845000	4.18380500
H	4.20975600	7.65804600	2.50910800
H	7.59287200	5.46864300	3.53331800
H	3.33036200	5.10514000	3.02332200
H	4.39489700	5.88960600	0.69656000

H	6.50378400	6.72896300	1.31022000
C	2.13088100	1.76881200	-0.44441400
C	2.82492400	1.18174100	-1.46733900
O	0.78358200	1.52708500	-0.60689700
C	1.86071200	0.53735400	-2.30435400
H	3.89668800	1.21632200	-1.59537800
C	0.64694500	0.77959600	-1.73448200
H	2.04785800	-0.02498700	-3.20841800
H	-0.36547800	0.50855100	-1.99509200
C	2.07401200	1.85353600	2.39663500
C	1.14059400	0.86493800	2.56429900
O	2.64794100	2.15055000	3.60882300
C	1.13791000	0.53555500	3.95657600
H	0.52809600	0.43470800	1.78574200
C	2.06683800	1.34706400	4.53655000
H	0.52799800	-0.20585800	4.45368400
H	2.41916800	1.47281800	5.54922800
C	1.50257100	4.17683400	0.92801300
C	0.38599200	4.48060800	1.66030700
O	1.73637700	5.17135600	0.01225100
C	-0.09783900	5.73310400	1.16580900
H	-0.03954100	3.87933400	2.45056300
C	0.75659100	6.09960300	0.16958000
H	-0.96276600	6.28350400	1.50893500
H	0.80908500	6.95009500	-0.49330100
C	8.68021200	7.06543200	0.32503400
H	9.60694000	7.34508500	-0.18789400
H	7.92366800	7.81663000	0.06056600
H	8.85548200	7.14789500	1.40220300
C	6.94359800	1.94659200	1.26491000
H	7.84588400	1.60653600	0.76567800
C	5.72434800	1.19948000	0.92188700
H	5.21810600	0.69733700	1.74110200
H	5.79057900	0.59535300	0.01713500
C	7.36095200	2.15292800	2.70991800
O	8.34476100	2.78203500	3.04107500
O	6.56998700	1.48782300	3.57965500
C	6.93784200	1.56702500	4.97708200
H	5.99857400	1.40059600	5.51014800
H	7.30288000	2.57441500	5.18891700
C	7.97750700	0.51499200	5.33542700
H	8.91450400	0.70481300	4.80456400
H	8.18053900	0.54509400	6.41238300
H	7.62117800	-0.48859300	5.08030100

13c1

M06/BSII SCF energy in solution: -2045.735996 a.u.

Solution-phase enthalpy: -2045.123312 a.u.

Solution-phase Gibbs energy: -2045.233962 a.u

Pd	-0.21234200	-0.47731900	-0.31062400
P	1.97331000	-0.09494300	-0.20205800
C	-2.59717700	-1.44864400	-0.30196300
C	-2.88947400	-2.83081600	-0.55897300
C	-2.90150400	-0.51696800	-1.35978700
C	-3.56589300	-3.23237500	-1.71308000
C	-3.61587200	-0.97733800	-2.48077400
C	-3.97714800	-2.30365000	-2.65855900
H	-3.78766400	-4.28732000	-1.85329700
H	-3.85939200	-0.26135800	-3.26104300
H	-4.53605700	-2.61128200	-3.53831000
C	-2.15445200	-1.21890400	1.21876100
C	-2.63131600	0.00989800	2.05703700
C	-0.47904600	-0.29238200	2.71931700
C	-0.62434600	-1.29239100	1.56426200
C	-1.36318600	0.87478100	2.22678900
H	-1.49770900	1.66738800	2.97426800
H	-0.98800700	1.33049100	1.30574800
C	-2.77848300	-0.51706900	3.51090900
H	-3.23288300	0.25532300	4.14238600
H	-3.41948300	-1.40405200	3.57556700
C	-1.30046400	-0.79576200	3.94321200
H	-1.03847300	-0.23730400	4.85087800
H	-1.11288900	-1.85559100	4.15080400
H	-3.51879900	0.50913700	1.67105100
H	0.55849700	-0.04094300	2.96125300
H	-0.25316300	-2.29794600	1.78380100
H	-2.62943900	-2.08128200	1.68594400
C	2.84671900	-0.50912200	-1.74334500
C	2.37501600	-0.93717500	-2.95470700
O	4.22324600	-0.44783500	-1.77953800
C	3.51751000	-1.14869800	-3.78819200
H	1.33356400	-1.07585200	-3.20478600
C	4.60327300	-0.83719200	-3.02526600
H	3.52656300	-1.48925000	-4.81412900
H	5.66774100	-0.84236200	-3.20786100
C	2.45773000	1.64474200	0.07179700
C	3.31053000	2.50241900	-0.56962200
O	1.82592000	2.30491900	1.09647500

C	3.19893700	3.76368700	0.09743900	C	4.47466000	1.62320100	-2.16629500
H	3.94455600	2.25874800	-1.40930900	H	6.45917700	1.28495700	-1.40443500
C	2.28927600	3.58290000	1.09582100	H	2.40563500	1.87961500	-2.65552400
H	3.72628000	4.67764200	-0.13771100	H	4.81893800	2.18343400	-3.03309200
H	1.88364500	4.22623500	1.86208300	C	3.02323200	-0.78110800	1.08398300
C	2.99003800	-0.92082800	1.07498700	C	3.41624300	-2.28407600	0.91039100
C	3.94197800	-0.48011500	1.95536700	C	1.16260200	-2.32816000	0.72430000
O	2.78469700	-2.26532200	1.25480500	C	1.45494400	-0.82939100	0.96271700
C	4.35029900	-1.61911100	2.71907800	C	2.37512800	-2.76970900	-0.11829700
H	4.31060700	0.53192300	2.03979900	H	2.41309300	-3.85338100	-0.28619500
C	3.61938700	-2.66865000	2.24870500	H	2.44060500	-2.25320000	-1.08055500
H	5.08639700	-1.64877400	3.51033200	C	2.98357600	-3.05012100	2.18157500
H	3.57241700	-3.71742100	2.50065700	H	3.40365500	-4.06293300	2.18683900
C	-2.52968600	-3.93930800	0.41394800	H	3.32413800	-2.55365600	3.09797700
H	-2.61385400	-4.90999500	-0.08434500	C	1.42677400	-3.08649100	2.05523300
H	-1.51002100	-3.85014900	0.79812600	H	1.05858000	-4.11798500	1.98672000
H	-3.20378600	-3.96664300	1.28201600	H	0.91831800	-2.61883300	2.90589100
C	-2.27989900	0.87404400	-1.61257700	H	4.46266900	-2.43930900	0.63927900
H	-2.80470600	1.25849600	-2.50501500	H	0.18232000	-2.55108000	0.30125300
C	-0.78160900	0.68664900	-1.99649700	H	0.97707100	-0.47401900	1.88461000
H	-0.28679500	1.65232000	-2.12613200	H	3.32305800	-0.44046800	2.08751700
H	-0.75045900	0.14410500	-2.94949200	C	-3.27524900	0.42527200	-0.83515500
C	-2.64711900	1.97839700	-0.62851000	C	-3.72636700	1.71795400	-0.75730500
O	-3.70558300	2.04892100	-0.03516100	O	-4.24949500	-0.35951800	-1.40598700
O	-1.71350200	2.95770800	-0.59473300	C	-5.04519900	1.73039800	-1.31115800
C	-2.02903200	4.12819900	0.19145300	H	-3.17477500	2.55283100	-0.35162300
H	-1.05334900	4.53662300	0.46748500	C	-5.30499100	0.44684200	-1.68704500
H	-2.56196300	3.81629000	1.09283300	H	-5.70338300	2.58124500	-1.41924800
C	-2.84602700	5.13154300	-0.61040300	H	-6.14873600	-0.03585100	-2.15742000
H	-3.82409300	4.71325800	-0.86447300	C	-1.67740600	-1.83544000	-1.37427300
H	-3.00465600	6.04167100	-0.01983000	C	-2.28787100	-3.06043100	-1.41479500
H	-2.32652500	5.40700800	-1.53430200	O	-0.82769600	-1.71289600	-2.44841900

11c2

M06/BSII SCF energy in solution: -2045.76991 a.u.

Solution-phase enthalpy: -2045.156956 a.u.

Solution-phase Gibbs energy: -2045.268765 a.u

Pd	0.67096200	0.56569800	-0.39181200	C	-2.31784500	-1.12267600	1.31159900
P	-1.72934600	-0.38762500	-0.25439100	C	-1.86356400	-0.97481000	2.59546800
C	3.59515600	0.12117300	0.02736000	O	-3.46198000	-1.89042700	1.32306300
C	4.97702900	0.34936300	-0.15599300	C	-2.76351600	-1.69599700	3.44226900
C	2.65175600	0.72748400	-0.83020000	H	-0.98598600	-0.42229700	2.89655800
C	5.39563700	1.10670300	-1.25712200	C	-3.70680300	-2.22863800	2.61706900
C	3.10668100	1.44570500	-1.94570500	H	-2.71027800	-1.80207400	4.51661800

H	-4.57888100	-2.84376200	2.78206900	H	9.76225600	4.64549600	-1.42243800
C	6.01931100	-0.19436400	0.79926900	H	8.77243100	3.55821700	-2.39450400
H	5.66175000	-0.20376300	1.83470600	C	7.59854900	4.89032800	-1.04820500
H	6.31283500	-1.22346200	0.55361800	H	7.88372800	5.91695100	-0.78024600
H	6.92871400	0.41569300	0.76374800	H	6.88353200	4.95704500	-1.87714100
C	0.48714500	2.95083300	-0.86502100	H	9.93533900	2.62041000	-0.11741900
H	1.53484800	3.15338900	-1.04774000	H	6.29456300	4.70455300	0.74479000
C	-0.29622800	2.39088300	-1.82649300	H	6.01427100	2.87329600	-1.28832600
H	-1.37010800	2.30720600	-1.72356200	H	7.91041500	1.51305200	-1.55075100
H	0.12602300	2.11914300	-2.78918200	C	1.65138300	2.34375400	0.25010800
C	0.02275500	3.57103600	0.40813700	C	1.42012500	1.43634800	-0.74911200
O	0.75713500	4.22492700	1.12029700	O	0.46411500	2.94877300	0.60044600
O	-1.29321300	3.37350400	0.67300500	C	0.01593400	1.47158100	-1.02220800
C	-1.80008200	3.99455900	1.88139200	H	2.17173600	0.82754200	-1.23013000
H	-2.86988400	4.11558300	1.69266700	C	-0.50882000	2.40033000	-0.17522000
H	-1.33646600	4.97802500	1.98707400	H	-0.52617500	0.88251300	-1.74871300
C	-1.54694200	3.12924400	3.10627300	H	-1.50833700	2.77013100	-0.00090200
H	-0.47361800	3.02516100	3.28730800	C	2.81357500	3.03093400	2.76187800
H	-2.00133000	3.59649900	3.98784100	C	1.68021700	2.85894800	3.50952400
H	-1.98737900	2.13511400	2.97772000	O	3.87830800	3.28196600	3.59292900

TS12c2

M06/BSII SCF energy in solution: -2045.705621 a.u.

Solution-phase enthalpy: -2045.09481 a.u.

Solution-phase Gibbs energy: -2045.202647 a.u

Pd	5.06255700	1.58595800	0.71983800	C	3.18747000	4.69155900	0.47608900
P	3.21827800	2.93187900	0.98300600	C	3.83982500	5.36260800	-0.52358900
C	7.92971700	0.72114900	0.47024700	O	2.30027800	5.54151100	1.09399700
C	9.15614300	0.24187100	0.98952600	C	3.33167600	6.69953500	-0.52206600
C	6.72795300	0.19224800	1.05436500	H	4.59729800	4.95027200	-1.17287500
C	9.17448900	-0.43969800	2.21682700	C	2.40778400	6.74755100	0.47884800
C	6.79033900	-0.41454300	2.32578600	H	3.62399000	7.51294200	-1.17136700
C	8.00888200	-0.68054500	2.93800800	H	1.77620500	7.53026200	0.87211400
H	10.13269000	-0.76987700	2.61363900	C	10.48661400	0.37124800	0.26676200
H	5.87441700	-0.76731500	2.78874000	H	10.36380500	0.59882200	-0.79406000
H	8.04612900	-1.15179500	3.91621700	H	11.14457300	1.13101100	0.70608700
C	7.83868900	1.88688800	-0.51943100	H	11.01680400	-0.58634300	0.33709100
C	8.92353600	2.98649300	-0.26696000	C	5.40863300	-0.67340400	0.19406500
C	7.02479600	4.12838900	0.17195900	H	5.83208200	-1.65393800	0.41692500
C	6.50994200	2.75199000	-0.31332200	C	4.12204900	-0.35087600	0.86764100
C	8.31870100	3.76438800	0.91896700	H	3.23618400	-0.37183500	0.24334900
H	8.91548700	4.63950400	1.20656000	H	3.96775400	-0.84011200	1.82849700
H	8.14978400	3.14290500	1.80458200	C	5.51330600	-0.55715300	-1.32136000
C	8.85259900	4.03374800	-1.40978200	O	6.52453100	-0.82350300	-1.93769500

O	4.35056700	-0.20830700	-1.92220500	C	-3.84511600	3.13446100	-1.16624200
C	4.36287600	-0.16592200	-3.37106800	H	-1.62318400	2.71972700	-1.19140900
H	3.32484400	-0.36057300	-3.65286300	C	-4.85456300	2.29969300	-0.79128400
H	4.99713300	-0.97612500	-3.73795700	H	-3.94718700	4.15183000	-1.51729800
C	4.83693700	1.18335600	-3.88888000	H	-5.92866000	2.40237000	-0.74637300
H	5.87750900	1.36054200	-3.60450500	C	-2.76103400	-1.67313700	-0.83092800
H	4.76950500	1.20289900	-4.98302600	C	-3.82285400	-1.81066000	-1.68322900
H	4.21896900	1.99436300	-3.49023400	O	-2.14131800	-2.88609600	-0.66605900

13c2

M06/BSII SCF energy in solution: -2045.707582 a.u.

Solution-phase enthalpy: -2045.094453 a.u.

Solution-phase Gibbs energy: -2045.204583 a.u

Pd	0.20157600	-0.13070800	-0.44898200	C	-2.58002500	-0.46730900	1.73832900
P	-1.98321400	-0.25934000	0.01958600	C	-2.10875900	0.01230600	2.93141800
C	3.07602300	-0.68960000	-0.43866400	O	-3.76057700	-1.13915600	1.94846200
C	3.97100900	-1.81267500	-0.45404500	C	-3.04811900	-0.38574700	3.93350100
C	2.33473400	-0.46308900	-1.65802400	H	-1.19969900	0.57702500	3.07297300
C	3.91533500	-2.75547300	-1.48679900	C	-4.02108000	-1.08190800	3.28021200
C	2.31146800	-1.46491400	-2.65597300	H	-2.99713800	-0.18824500	4.99515700
C	3.04897500	-2.62684200	-2.56381000	H	-4.91876600	-1.58827400	3.60246800
H	4.58877400	-3.60770700	-1.44439200	C	5.10842000	-2.06394700	0.52929900
H	1.72331700	-1.28792700	-3.55087000	H	5.73826000	-1.17848200	0.65470400
H	3.00710600	-3.37960100	-3.34575400	H	4.78459600	-2.38946500	1.52030900
C	2.82491400	0.19638000	0.82373600	H	5.75161800	-2.85237500	0.12630000
C	3.53270700	-0.19349700	2.15180800	C	1.59922900	0.82976600	-2.25426200
C	1.37247100	-0.56143600	2.70793800	H	2.08362200	0.92548100	-3.23912800
C	1.30570100	0.13501500	1.32862900	C	0.09500500	0.51935800	-2.44129900
C	2.67043500	-1.38376700	2.63246700	H	-0.51455500	1.40313400	-2.61976300
H	2.98257000	-1.78587800	3.60486800	H	-0.06936500	-0.21691500	-3.22974400
H	2.60789300	-2.20359300	1.91120600	C	1.97984600	2.17175300	-1.63179300
C	3.21569500	0.88500700	3.23093800	O	3.12714900	2.51197000	-1.42676600
H	3.95144600	0.83287300	4.04155800	O	0.92148700	2.99227300	-1.42891300
H	3.26985100	1.89795300	2.81495600	C	1.22328900	4.33205400	-0.96481300
C	1.78516000	0.51803600	3.73461400	H	0.40256800	4.94180400	-1.35165300
H	1.81448500	0.11307200	4.75577600	H	2.16264100	4.65531000	-1.41880000
H	1.10635200	1.37977500	3.74288500	C	1.29448200	4.39327400	0.55328000
H	4.60482500	-0.34953700	2.08110400	H	2.12443200	3.78629600	0.92552900
H	0.47540500	-1.12451500	2.97867100	H	1.45468000	5.42922100	0.87445200
H	0.96953000	1.17206600	1.48937000	H	0.36418700	4.03244700	1.00403000
H	3.09851500	1.22256000	0.55937500				
C	-2.99336100	1.15131000	-0.54321300				
C	-2.63431300	2.39008400	-1.00220900				
O	-4.36309700	1.09311600	-0.40308600				

11c3

M06/BSII SCF energy in solution: -2045.770467 a.u.

Solution-phase enthalpy: -2045.157704 a.u.

Solution-phase Gibbs energy: -2045.269829 a.u

Pd	0.62224400	-0.80119000	-0.38886100
P	-1.46127400	0.78805100	-0.28609700
C	3.49948200	0.06069900	-0.48085100
C	4.76042500	0.27519400	-1.07895600
C	2.50076600	-0.66275100	-1.16667500
C	4.99720700	-0.24302900	-2.35840800
C	2.76290000	-1.16238900	-2.44946600
C	4.01001800	-0.95080600	-3.04352500
H	5.96502600	-0.07632600	-2.82685700
H	1.99805000	-1.70403200	-3.00313500
H	4.20842800	-1.33294000	-4.04252300
C	3.08885500	0.62248900	0.84857800
C	3.68252800	-0.07651500	2.11751800
C	1.44807900	-0.34066000	2.38669800
C	1.55063800	0.41415700	1.04799700
C	2.70043200	-1.24345200	2.34716700
H	2.88242700	-1.77211800	3.29117800
H	2.68867500	-1.96758200	1.52784500
C	3.37536600	0.82352100	3.33756000
H	3.91698800	0.47196500	4.22345000
H	3.67152900	1.86509900	3.16688500
C	1.83143000	0.65675900	3.51998700
H	1.59192400	0.22796100	4.50087800
H	1.28492900	1.60239300	3.43747600
H	4.73691400	-0.34874400	2.01968300
H	0.48743900	-0.83418800	2.55857900
H	1.00355300	1.36094100	1.05540000
H	3.34240600	1.69289700	0.88976000
C	-3.14124700	0.62755600	-0.98795100
C	-3.70926600	-0.33036100	-1.78699200
O	-4.05317300	1.63450600	-0.75846500
C	-5.04202900	0.10874300	-2.06598300
H	-3.25127200	-1.25387500	-2.11084000
C	-5.19063900	1.29829200	-1.41792800
H	-5.78550200	-0.40122200	-2.66238500
H	-6.00871500	1.99711300	-1.32318200
C	-1.81129200	1.46088800	1.38241700
C	-1.95656900	2.71571900	1.90933500
O	-1.94412700	0.52703600	2.38602100
C	-2.19455200	2.55004600	3.31064200
H	-1.91236300	3.64145200	1.35545000
C	-2.17976800	1.20755800	3.54022300
H	-2.35593400	3.32760500	4.04432100

H	-2.31031900	0.59967300	4.42272300
C	-0.83677700	2.27350000	-1.14637400
C	0.32786800	2.47917200	-1.83847600
O	-1.61788100	3.40741900	-1.22064300
C	0.26710400	3.80857100	-2.36306000
H	1.12997200	1.76272400	-1.94933600
C	-0.92908200	4.31871800	-1.95736700
H	1.01385400	4.31038200	-2.96227700
H	-1.42189000	5.26856200	-2.10367400
C	5.83992700	1.07399100	-0.38171900
H	6.69099400	1.24699800	-1.04858600
H	5.46972200	2.05274300	-0.05044000
H	6.21920800	0.56320600	0.51194700
C	-1.71678100	-3.19219700	-0.74417800
O	-2.73911100	-3.31258000	-1.40209100
O	-1.66373000	-3.39592300	0.59404800
C	-2.88786400	-3.81993700	1.23776900
H	-2.54814700	-4.37106000	2.11869800
H	-3.41889000	-4.50049200	0.56747300
C	-3.76252300	-2.63723700	1.62659500
H	-4.12417300	-2.11445000	0.73715300
H	-4.63009300	-2.99260600	2.19566000
H	-3.20667200	-1.92653000	2.24580500
C	-0.40458000	-2.87243400	-1.33918700
H	-0.43796700	-2.71688600	-2.41337500
C	0.79185500	-3.06809100	-0.68662500
H	1.71986900	-3.15726300	-1.23698000
H	0.79863700	-3.42538400	0.33876700

TS12c3

M06/BSII SCF energy in solution: -2045.739175 a.u.

Solution-phase enthalpy: -2045.127404 a.u.

Solution-phase Gibbs energy: -2045.234695 a.u

Pd	4.74341400	3.02323800	1.43012500
P	3.56161400	5.00365200	1.07938400
C	7.40597200	1.91897500	0.72432800
C	8.36494000	1.43624600	-0.19994200
C	6.05701600	1.48409000	0.60247800
C	7.95868700	0.63352400	-1.27180400
C	5.67357000	0.74859700	-0.53433900
C	6.61179200	0.33294300	-1.47273900
H	8.70534200	0.27041600	-1.97450000
H	4.63581200	0.44599700	-0.64951800
H	6.30092200	-0.25249500	-2.33423700

C	7.74711700	3.09204900	1.61398300	H	10.20118200	1.74210600	0.93150500
C	8.21688400	2.88598900	3.09673600	C	2.62306100	1.47059800	2.95904300
C	6.64006000	4.51015800	3.24307300	O	1.39621900	1.46603700	2.93728200
C	6.54716300	4.09333200	1.76111300	O	3.32557600	1.73953100	4.10597000
C	6.95317400	3.16825800	3.93795500	C	2.54602000	2.04523400	5.27876500
H	7.18801600	3.28100500	5.00409900	H	3.20572400	1.79595100	6.11494000
H	6.15098700	2.43531500	3.84429900	H	1.67059300	1.39098000	5.30289400
C	9.05555800	4.13749300	3.45585300	C	2.13057600	3.50956400	5.32107200
H	9.51365200	4.02066500	4.44510200	H	1.44616900	3.73701500	4.49952800
H	9.86577100	4.32027600	2.74073000	H	1.61940100	3.72493000	6.26755100
C	7.98144900	5.27675400	3.46550600	H	3.00243900	4.16666400	5.23954500
H	7.97104300	5.80522100	4.42631800	C	3.47508600	1.18408200	1.81240000
H	8.15457300	6.02672400	2.68580800	H	2.91902400	0.76796600	0.97727200
H	8.72649500	1.93454900	3.27853200	C	4.86491600	0.77004300	1.98032400
H	5.76916900	5.05006900	3.61955700	H	5.12924000	-0.21549100	1.61487300
H	6.64121200	4.94132100	1.07522100	H	5.28646100	0.93019500	2.96750600
H	8.56456900	3.61641500	1.10316900				
C	1.74244500	5.04436200	1.05306600				
C	0.79784900	4.07072000	1.24729700				
O	1.12423900	6.24929900	0.79540900				
C	-0.47367600	4.70910400	1.09708000				
H	0.97561200	3.03506700	1.50551600				
C	-0.21261900	6.01904300	0.82614300				
H	-1.44731400	4.24827600	1.18762300				
H	-0.83793900	6.88006800	0.64090900				
C	3.95322500	6.48444100	2.07801400				
C	4.60259500	7.66184700	1.82614700				
O	3.58302300	6.43638400	3.39996900				
C	4.63026400	8.38547300	3.06152600				
H	4.99415100	7.98267800	0.87239700				
C	3.99789400	7.59885600	3.97520200				
H	5.05876100	9.36216800	3.23811400				
H	3.76444900	7.70958100	5.02328200				
C	4.04012600	5.57118800	-0.58680300				
C	4.85415100	4.99574600	-1.52713500				
O	3.50133200	6.73137700	-1.09639100				
C	4.81846900	5.84477300	-2.67715800				
H	5.40688700	4.07540200	-1.40154400				
C	3.98586000	6.87538600	-2.35677900				
H	5.34146100	5.70392800	-3.61263700				
H	3.64747300	7.75219500	-2.88891700				
C	9.82579600	1.82395900	-0.09400200				
H	10.44140400	1.17877300	-0.72951800				
H	9.99916300	2.85972500	-0.41696200				

13c3

M06/BSII SCF energy in solution: -2045.765771 a.u.

Solution-phase enthalpy: -2045.151976 a.u.

Solution-phase Gibbs energy: -2045.26159 a.u.

Pd	-0.39166500	0.36941500	-0.13115000
P	1.60488400	-0.63986700	-0.16463700
C	-3.06608800	-0.63316800	-0.38509000
C	-3.56023200	-1.86961200	-0.90124800
C	-3.07130600	0.49812300	-1.25041800
C	-4.06508600	-1.94390700	-2.20303100
C	-3.60405400	0.37699800	-2.54499400
C	-4.10379700	-0.82308300	-3.02705700
H	-4.44431500	-2.89566200	-2.56714000
H	-3.60501000	1.25743900	-3.18306300
H	-4.51231200	-0.88908700	-4.03193400
C	-2.59790700	-0.66942700	1.09726200
C	-3.01827000	0.44215600	2.12895500
C	-0.90490300	-0.11211500	2.74938200
C	-1.06680300	-0.84300700	1.41147500
C	-1.70658500	1.18320900	2.48738900
H	-1.82037100	1.80605000	3.38307300
H	-1.27735200	1.81623300	1.70337900
C	-3.24384700	-0.31084500	3.46653000
H	-3.62426300	0.37647600	4.23083400
H	-3.96709800	-1.12869100	3.37516800
C	-1.80180300	-0.80449400	3.82536500
H	-1.50889800	-0.48513700	4.83210400

H	-1.70816200	-1.89589800	3.79292500
H	-3.86489700	1.05737400	1.81370300
H	0.13390900	0.01575600	3.06171600
H	-0.72432000	-1.88155700	1.40654300
H	-3.05887100	-1.58488100	1.47079300
C	2.91653800	0.22359400	-1.07034600
C	2.91040100	1.38072800	-1.80441100
O	4.18125800	-0.32638000	-1.06245800
C	4.24840100	1.55334100	-2.28057800
H	2.06941800	2.04371600	-1.97716500
C	4.96595500	0.49722500	-1.80306800
H	4.61885800	2.36288800	-2.89371700
H	6.00005400	0.19819200	-1.89256400
C	2.40874700	-1.04412300	1.42393000
C	2.73235200	-2.20943500	2.06500600
O	2.73326400	0.02569200	2.22119800
C	3.29735200	-1.83730900	3.32662700
H	2.60578700	-3.20829400	1.67513800
C	3.27532000	-0.47607200	3.36443000
H	3.67399800	-2.49787600	4.09506500
H	3.59316100	0.25688300	4.09042600
C	1.47050300	-2.28098000	-0.94104900
C	0.41016100	-2.89366700	-1.55566200
O	2.58395800	-3.08503900	-1.03640500
C	0.89190400	-4.14448200	-2.05369000
H	-0.58902000	-2.49080000	-1.64671800
C	2.20961200	-4.20365700	-1.71018600
H	0.33217100	-4.89310300	-2.59650100
H	2.98678700	-4.93779600	-1.86295700
C	-3.57847600	-3.15264100	-0.08835600
H	-3.90328200	-3.98876100	-0.71533300
H	-2.59289100	-3.41189100	0.31567500
H	-4.27345700	-3.10130400	0.76049100
C	-0.26765000	3.19708100	-1.26785800
O	0.66258400	3.63658400	-1.94265800
O	-0.69326300	3.85974000	-0.13152600
C	0.03126800	5.04986100	0.21985200
H	-0.67604500	5.64301700	0.80788300
H	0.28762500	5.59496100	-0.69239800
C	1.28534700	4.73292800	1.02551800
H	1.98634900	4.15203400	0.41974500
H	1.78117900	5.66130600	1.33497800
H	1.03735900	4.15904000	1.92551500
C	-0.99718000	1.96401500	-1.50603300

H	-0.92553300	1.66512700	-2.55131800
C	-2.44622800	1.85733600	-0.94681200
H	-3.08135700	2.63515600	-1.39990800
H	-2.47014400	2.08180100	0.12177500

11c4

M06/BSII SCF energy in solution: -2045.775461 a.u.

Solution-phase enthalpy: -2045.162551 a.u.

Solution-phase Gibbs energy: -2045.275754 a.u.

Pd	-0.55965600	0.02603100	0.06728100
P	1.94998100	0.26360900	-0.13354700
C	-2.91871200	-1.71805500	-0.47453500
C	-4.25347200	-2.03297700	-0.81193500
C	-2.54888900	-0.39569600	-0.13392200
C	-5.21750200	-1.01923500	-0.76694200
C	-3.54500900	0.59139800	-0.09351900
C	-4.87140700	0.28041900	-0.40286700
H	-6.24777400	-1.25400200	-1.02800400
H	-3.30095700	1.61535700	0.16484200
H	-5.63411200	1.05670600	-0.37320800
C	-1.81128900	-2.73041900	-0.48494300
C	-1.84177400	-3.76624800	0.68944200
C	0.16152800	-2.74918100	0.95912700
C	-0.43044400	-2.02672000	-0.27147500
C	-1.09636900	-3.01530400	1.81111700
H	-0.90097000	-3.64563100	2.68800200
H	-1.60165200	-2.09897600	2.12992200
C	-0.83948800	-4.89473400	0.35610100
H	-0.94747200	-5.72965900	1.05875300
H	-0.99162300	-5.29691700	-0.65239100
C	0.54689500	-4.19319400	0.52461500
H	1.14607300	-4.67925000	1.30482400
H	1.14458800	-4.20084300	-0.39318400
H	-2.84481700	-4.12223400	0.93843200
H	0.97908800	-2.22198300	1.45749500
H	0.21131000	-2.10150200	-1.15381800
H	-1.81706400	-3.27967100	-1.43917700
C	2.82896500	0.57736000	1.44473900
C	4.02339000	1.15752800	1.78236400
O	2.17688400	0.18323300	2.59373900
C	4.11639700	1.11627600	3.20879100
H	4.74518100	1.56052100	1.08696700
C	2.97384700	0.51396500	3.64379000
H	4.92400500	1.48705400	3.82448400

H	2.58967900	0.25916000	4.62006300	C	9.11859200	3.26486000	-0.16849000
C	2.90544900	-1.17561500	-0.74432200	C	7.17995300	1.81313900	0.19180900
C	3.90989400	-1.94342000	-0.22128700	C	9.35966600	2.61328400	-1.38377900
O	2.55912600	-1.65213600	-1.98434200	C	7.40393100	1.25202400	-1.08023000
C	4.20414100	-2.94961100	-1.19668700	C	8.47594200	1.65262200	-1.87032900
H	4.38771700	-1.80153700	0.73697900	H	10.23281400	2.89338100	-1.96938300
C	3.36057300	-2.72214000	-2.24135900	H	6.76935000	0.43652500	-1.41087200
H	4.94653900	-3.73228800	-1.12617700	H	8.64580400	1.18839900	-2.83854600
H	3.20790300	-3.19990400	-3.19728100	C	7.49555100	3.88441300	1.66224900
C	2.60801700	1.58904100	-1.19822000	C	7.83301800	3.68625800	3.18204200
C	1.99613500	2.62291700	-1.85635600	C	5.61862600	4.17499000	3.16677600
O	3.96411300	1.61548300	-1.45725400	C	5.93212400	4.02975300	1.66255700
C	3.02671400	3.32895300	-2.55411900	C	6.53786900	3.09642100	3.78252400
H	0.94603900	2.88079100	-1.82396400	H	6.54910800	3.10571200	4.87988200
C	4.18921900	2.67535300	-2.27825200	H	6.29741000	2.08394100	3.44795700
H	2.90816000	4.20333200	-3.17840900	C	7.79670200	5.09767100	3.81670200
H	5.21629600	2.82281300	-2.57809300	H	8.12017000	5.05583100	4.86363300
C	-4.66000200	-3.42539000	-1.24498700	H	8.45252800	5.80791400	3.30036700
H	-5.68863100	-3.43089200	-1.62114500	C	6.28219800	5.47802000	3.71174800
H	-4.01142500	-3.80852200	-2.04321500	H	5.87014200	5.74514600	4.69242400
H	-4.60756700	-4.15094600	-0.42368200	H	6.10736100	6.32924900	3.04435400
C	-0.45134300	2.55073700	0.90276100	H	8.75763400	3.13130500	3.37020900
H	0.61825700	2.68393400	0.77994300	H	4.55738900	4.10196100	3.42105100
C	-0.94575900	1.66533600	1.81167500	H	5.59163900	4.87835800	1.06275400
H	-2.00804000	1.59595200	2.01452700	H	7.92221700	4.85469200	1.38058900
H	-0.27748800	1.13514400	2.48281800	C	2.11462600	1.73324000	2.63287600
C	-1.24846000	3.49101100	0.07926200	C	1.79254900	0.40548700	2.72179300
O	-0.81954700	4.04100500	-0.92182800	O	1.93561400	2.34246600	3.85186900
O	-2.48525500	3.71754900	0.57151300	C	1.36961100	0.18630300	4.07238800
C	-3.32718300	4.59731400	-0.21111400	H	1.89690800	-0.32864000	1.93248100
H	-3.50270800	4.13398000	-1.18752400	C	1.47594600	1.38530800	4.70835600
H	-2.79101600	5.53629600	-0.37779700	H	1.03315600	-0.74525300	4.50572000
C	-4.61593200	4.80267900	0.56283400	H	1.27107800	1.72173900	5.71348100
H	-5.28099400	5.46867400	0.00215200	C	2.29898600	4.35862200	1.54305800
H	-5.13573800	3.85244900	0.72230600	C	1.36156300	4.94488900	2.35169100
H	-4.41768000	5.25587500	1.53956300	O	2.86503300	5.31280100	0.73197000

TS12c4

M06/BSII SCF energy in solution: -2045.734654 a.u.

Solution-phase enthalpy: -2045.122945 a.u.

Solution-phase Gibbs energy: -2045.23246 a.u.

Pd	5.14575900	2.19966100	0.95461600	C	1.96848900	2.11023900	-0.18364500
P	2.91013000	2.65913600	1.27084000	C	2.37915100	1.54888500	-1.36295200
C	7.98811200	2.91461900	0.60884500	O	0.60334000	2.27670400	-0.20224200

C	1.20514500	1.35573000	-2.15466700	C	0.04067000	2.66352700	-2.06899800
H	3.39858500	1.30045300	-1.62107400	H	0.39812300	3.17105200	-2.97332100
C	0.16549700	1.81270300	-1.40003900	H	-0.00576500	1.59046000	-2.27458000
H	1.14451800	0.93092900	-3.14672100	C	-0.77822800	4.74911500	-1.32705100
H	-0.90023900	1.87503000	-1.56338600	H	-0.74156300	5.27162600	-2.28978100
C	10.05499000	4.38163200	0.24848600	H	-1.43640000	5.32702600	-0.66883500
H	10.98718300	4.33162800	-0.32438600	C	0.66057100	4.55593500	-0.73977600
H	9.61779300	5.37366000	0.07016900	H	1.41170900	5.07694300	-1.34528100
H	10.31293200	4.33135800	1.31162700	H	0.75231500	4.93254600	0.28509200
C	5.14809800	-0.02631100	1.18761100	H	-2.15617700	3.20246900	-2.15927100
H	4.60582500	-0.00768700	2.12933500	H	1.92239400	2.71347000	-0.82556200
C	6.57194700	0.30163800	1.22761700	H	0.33956600	2.62429900	1.32113700
H	7.21890600	-0.36926100	0.67477200	H	-1.74018000	3.55257700	0.53319500
H	6.97567700	0.50346000	2.21661400	C	2.56380100	-1.09140000	-1.29748300
C	4.53277700	-0.94294100	0.24124700	C	2.20471600	-2.14612200	-2.09334500
O	3.40251400	-1.40854800	0.34870200	O	3.60329500	-0.39787000	-1.87127700
O	5.32643900	-1.26042000	-0.83493100	C	3.09002200	-2.11439400	-3.21729400
C	4.75250100	-2.18469700	-1.77649700	H	1.37445000	-2.81959600	-1.90902700
H	3.84363100	-1.74756300	-2.20465500	C	3.90976200	-1.04242000	-3.03341000
H	4.45451800	-3.09608400	-1.24787500	H	3.10621900	-2.80111400	-4.05217300
C	5.79648700	-2.46936800	-2.84237700	H	4.72556800	-0.61703700	-3.59835700
H	5.40029300	-3.18536900	-3.57134800	C	3.05302100	0.53055600	1.01029600
H	6.07476700	-1.55534700	-3.37830800	C	4.38250700	0.77737500	0.78954400
H	6.70193200	-2.89636100	-2.39849000	O	2.64629400	1.19857900	2.14173400

13c4

M06/BSII SCF energy in solution: -2045.757231 a.u.

Solution-phase enthalpy: -2045.143344 a.u.

Solution-phase Gibbs energy: -2045.252701 a.u

Pd	-0.31088900	0.35175700	-0.09603900	C	1.64694800	-1.94128400	1.27565600
P	1.74978700	-0.47264500	0.21427300	C	0.57270600	-2.60497400	1.80364700
C	-2.51198400	1.62192700	0.27617300	O	2.81218000	-2.56796400	1.65269700
C	-3.07827800	1.80534400	1.58152100	C	1.10085700	-3.70166500	2.55240900
C	-3.07313900	0.59686200	-0.55316500	H	-0.46462000	-2.34254400	1.65594500
C	-4.20758500	1.08818100	1.97503600	C	2.45608500	-3.62783800	2.42242500
C	-4.23430100	-0.06798000	-0.11864600	H	0.54542800	-4.44619600	3.10510400
C	-4.81489900	0.17861700	1.11391000	H	3.27282500	-4.22475000	2.80059000
H	-4.62855400	1.26724200	2.96137100	C	-2.52995400	2.81029300	2.57678300
H	-4.65542700	-0.82654500	-0.76761900	H	-2.99078500	2.65352800	3.55678400
H	-5.71672600	-0.34891500	1.41393600	H	-1.44617900	2.73023000	2.70429400
C	-1.42889900	2.70818700	-0.08552200	H	-2.74652900	3.84762400	2.28405900
C	-1.26643800	3.28907500	-1.52985500	C	-1.30543400	-0.97759100	-1.56311400
C	0.86972600	3.01098700	-0.81028500	H	-0.55704600	-0.96426700	-2.35847600
C	0.04303100	2.35720500	0.30502700	C	-2.45457000	0.02914600	-1.83727600

H	-3.26185900	-0.42982300	-2.42591000
H	-2.05180200	0.83353600	-2.46036200
C	-1.55596300	-2.36748800	-1.21234400
O	-0.74534100	-3.28918000	-1.32384100
O	-2.80452000	-2.61170300	-0.69185000
C	-3.05768000	-3.96738700	-0.29406100
H	-2.33698200	-4.26210500	0.47736000
H	-2.90166400	-4.63436700	-1.14889700
C	-4.48543800	-4.04057900	0.22140500
H	-4.71586500	-5.06173800	0.54654100
H	-4.62939900	-3.36609300	1.07211300
H	-5.19933400	-3.76195000	-0.56149700

11c5

M06/BSII SCF energy in solution: -2045.775369 a.u.

Solution-phase enthalpy: -2045.162539 a.u.

Solution-phase Gibbs energy: -2045.274643 a.u

Pd	0.51406800	-0.78731100	-0.42936800
P	-1.30645300	0.91787900	0.06702100
C	2.98817000	-0.40051900	1.22620200
C	3.73308600	-0.24329000	2.41670000
C	1.57857500	-0.42828800	1.26203700
C	3.04593700	-0.12517000	3.63028700
C	0.91848800	-0.32740500	2.49620800
C	1.65266500	-0.17757300	3.67477200
H	3.61265100	-0.00964500	4.55212800
H	-0.16573400	-0.37071900	2.55125100
H	1.13593200	-0.09966700	4.62901500
C	3.60610000	-0.64960300	-0.11618100
C	4.25355800	0.57730000	-0.84419400
C	2.72970200	-0.17207000	-2.34073300
C	2.50606300	-1.10664900	-1.13346100
C	3.07585000	1.16340400	-1.64852700
H	3.39193100	1.94594100	-2.34972900
H	2.26066600	1.54721400	-1.02943100
C	5.14191700	0.02531800	-1.98304300
H	5.73351400	0.82956100	-2.43622900
H	5.84484700	-0.73807400	-1.63021100
C	4.09441500	-0.53882200	-2.99797600
H	4.19164300	-0.05833800	-3.97933800
H	4.19684500	-1.61880200	-3.15438700
H	4.76869700	1.27071700	-0.17353000
H	1.90587800	-0.13708000	-3.06078600
H	2.61518700	-2.16369400	-1.39063300

H	4.37638100	-1.43000400	-0.01443400
C	-2.05860700	1.57416000	-1.47340400
C	-3.17076800	1.24715400	-2.20264800
O	-1.31887700	2.51083500	-2.15197600
C	-3.12012400	2.04076200	-3.39449600
H	-3.90732200	0.50503000	-1.93233600
C	-1.98182700	2.78365300	-3.30960600
H	-3.84069400	2.05422300	-4.20050800
H	-1.52161100	3.52430400	-3.94602100
C	-2.81889500	0.58486700	1.04260000
C	-4.02427300	1.21563100	1.19797400
O	-2.76461400	-0.50656700	1.87902000
C	-4.75495100	0.47414800	2.17655900
H	-4.34238600	2.10601200	0.67566000
C	-3.94265500	-0.55299700	2.55462300
H	-5.74985700	0.67881300	2.54693500
H	-4.04546300	-1.36343900	3.26044300
C	-0.69703000	2.47655400	0.79801000
C	0.52884600	2.87414100	1.26031300
O	-1.59191800	3.51808900	0.91792200
C	0.38596200	4.23175600	1.68725000
H	1.41734500	2.26285800	1.30034600
C	-0.91502200	4.56434200	1.45671000
H	1.15039600	4.86746700	2.11155700
H	-1.49259800	5.46325700	1.61427100
C	5.24637200	-0.24601100	2.40903900
H	5.64201200	-0.18264300	3.42814600
H	5.64678600	-1.16118300	1.95314100
H	5.66183200	0.59455200	1.83973400
C	-1.10646400	-1.79589700	-1.96821300
H	-1.39619000	-0.99407900	-2.63863500
C	0.10574200	-2.42171000	-2.08025600
H	0.31019500	-3.33928700	-1.54015800
H	0.79562600	-2.14731700	-2.86913100
C	-2.21907900	-2.32265700	-1.13660000
O	-3.35780900	-1.88806100	-1.17379000
O	-1.84479300	-3.35916700	-0.35720300
C	-2.87710500	-3.94365500	0.46538500
H	-3.67927400	-4.31019400	-0.18410600
H	-3.29695800	-3.16324300	1.10619700
C	-2.23847100	-5.06090500	1.26945300
H	-2.99027500	-5.53381400	1.91125300
H	-1.81837800	-5.82787800	0.61052900
H	-1.43491400	-4.67358500	1.90412900

TS12c5

M06/BSII SCF energy in solution: -2045.735124 a.u.

Solution-phase enthalpy: -2045.122387 a.u.

Solution-phase Gibbs energy: -2045.231402 a.u

Pd	4.85480800	2.94572400	0.89198800
P	3.04181400	1.73974300	1.59191900
C	7.50801300	1.82809500	0.46317900
C	8.50915200	0.99577200	-0.09985300
C	6.15128700	1.44172500	0.41278200
C	8.13053300	-0.20742100	-0.70473700
C	5.81191300	0.22877800	-0.20725900
C	6.79190200	-0.59161500	-0.76559100
H	8.89799400	-0.84490200	-1.13933100
H	4.77204900	-0.07899000	-0.27100300
H	6.51417200	-1.52554000	-1.25007100
C	7.91633100	3.11604700	1.13672600
C	8.36763600	2.89787600	2.62722100
C	6.88547500	4.58582500	2.84462700
C	6.90158900	4.35328200	1.30929300
C	7.07437200	3.16764800	3.41576900
H	7.22388900	3.16142700	4.50242600
H	6.25770900	2.48581100	3.16143900
C	9.25731200	4.08378700	3.07126400
H	9.75988900	3.85680100	4.01850900
H	10.03831800	4.31194300	2.33705300
C	8.23041200	5.24911100	3.24494800
H	8.19158200	5.59111100	4.28612600
H	8.46685800	6.12287600	2.62672900
H	8.82639400	1.91689700	2.77887900
H	6.00964100	5.13200100	3.20554900
H	7.42171300	5.17187400	0.81236400
H	8.77120500	3.51905300	0.58138300
C	1.98980200	2.57202700	2.83702000
C	1.11444200	3.62429800	2.77185400
O	2.14426700	2.17291000	4.14253500
C	0.69360700	3.87801800	4.11574900
H	0.85106800	4.16629700	1.87318300
C	1.34836500	2.97485000	4.89893800
H	-0.00363100	4.63436300	4.44876100
H	1.35672700	2.77125800	5.95917600
C	1.81431100	1.33540600	0.30696900
C	0.45375000	1.18498800	0.29972300
O	2.31211400	1.08587000	-0.94876900

C	0.09054400	0.82220000	-1.03376800
H	-0.20332600	1.32394100	1.14532400
C	1.25437100	0.77468300	-1.74253200
H	-0.90334400	0.62812900	-1.41218200
H	1.49407300	0.54578800	-2.77003300
C	3.36295900	0.15407000	2.42701300
C	4.51282400	-0.45896000	2.84574000
O	2.27506400	-0.60883800	2.78720200
C	4.11603500	-1.66590700	3.50119600
H	5.51582700	-0.09597400	2.68106400
C	2.75497300	-1.70143800	3.43297100
H	4.75993000	-2.40700100	3.95352000
H	2.01121500	-2.40642500	3.77388700
C	9.97653300	1.37401400	-0.08308300
H	10.58322500	0.58449500	-0.53876100
H	10.16911400	2.29861200	-0.64427000
H	10.35706200	1.53684500	0.93281100
C	3.93194500	4.89375500	0.83941600
H	3.49303300	5.20568100	1.78300100
C	5.32147900	5.27013000	0.57812800
H	5.57556200	5.37790700	-0.47280300
H	5.65326100	6.12269500	1.16467200
C	2.95301200	4.83872800	-0.25315100
O	1.73491200	4.85544500	-0.11891200
O	3.53496000	4.74562900	-1.48481500
C	2.63636400	4.60811800	-2.60003000
H	1.95113400	5.46231900	-2.61585800
H	2.03359000	3.70412900	-2.46331400
C	3.48243600	4.53678900	-3.85902200
H	2.83720000	4.43121400	-4.73863500
H	4.08123000	5.44579800	-3.97979800
H	4.16293900	3.67960900	-3.82331700

13c5

M06/BSII SCF energy in solution: -2045.76374 a.u.

Solution-phase enthalpy: -2045.150034 a.u.

Solution-phase Gibbs energy: -2045.2585 a.u

Pd	-0.22980600	0.44431400	0.33407700
P	1.63678300	-0.73236200	-0.22491800
C	-2.77300900	-0.88301400	0.95762300
C	-3.67810600	-1.72246600	1.67573000
C	-1.39358400	-0.96383900	1.27925200
C	-3.19514300	-2.57945100	2.67057700
C	-0.94668000	-1.82808200	2.28795600

C	-1.84036400	-2.63602800	2.98566100	H	2.80440200	-5.30422300	-1.15502800
H	-3.90029500	-3.21154900	3.20603800	C	-5.17279500	-1.74714100	1.40894600
H	0.11073400	-1.87130700	2.53005100	H	-5.65581100	-2.49975400	2.04031900
H	-1.48575500	-3.30602500	3.76615000	H	-5.65535400	-0.78538000	1.62873800
C	-3.41024000	-0.03006400	-0.16630100	H	-5.41063000	-1.99381900	0.36714900
C	-3.42677000	-0.76119900	-1.55895200	C	-0.45467900	2.37361100	-0.65085000
C	-2.91182800	1.36261700	-2.13151900	H	-0.43845700	2.19843700	-1.72003700
C	-2.97691600	1.46762400	-0.58220900	C	-1.74300400	2.12988000	0.09724200
C	-2.31835700	-0.04417300	-2.35149600	H	-1.54244700	1.50778600	1.07009000
H	-2.28732400	-0.33867100	-3.40781500	H	-2.02886300	3.03800500	0.64028100
H	-1.31878600	-0.17389200	-1.92253100	C	0.44365300	3.45135400	-0.25490300
C	-4.68566500	-0.30466700	-2.33218200	O	1.38245100	3.86972700	-0.92623300
H	-4.81871400	-0.90457200	-3.24019700	O	0.17035100	3.95348900	0.98778900
H	-5.60200000	-0.40505900	-1.73999900	C	1.06019200	4.98067500	1.45954700
C	-4.34897300	1.18029500	-2.68426800	H	1.05555300	5.81489600	0.74973600
H	-4.36499000	1.34438900	-3.76750700	H	2.08071500	4.58394400	1.49082400
H	-5.05359100	1.89247500	-2.23984300	C	0.57907000	5.40691700	2.83539300
H	-3.33155800	-1.84666000	-1.46784000	H	1.23033400	6.19365500	3.23258700
H	-2.38223700	2.19718900	-2.59773900	H	-0.44298600	5.79781100	2.78870900
H	-3.82286700	2.11051400	-0.31450000	H	0.59249200	4.56307100	3.53326800
H	-4.45069900	0.08223200	0.13844500				
C	2.59737600	-0.10418600	-1.63871700				
C	2.69492500	1.14771400	-2.18858900				
O	3.44954500	-0.96894500	-2.29121700				
C	3.65784600	1.04793700	-3.24189400				
H	2.17111200	2.04208600	-1.87145400				
C	4.07316100	-0.25033400	-3.25891300				
H	3.98746000	1.84141100	-3.89791600				
H	4.76863800	-0.80270900	-3.87356100				
C	2.90765100	-0.72743400	1.08620600				
C	4.18217400	-0.23155300	1.13946400				
O	2.56217400	-1.24641800	2.30858600				
C	4.65315000	-0.46420100	2.47048400				
H	4.71644100	0.24018500	0.32769600				
C	3.63351800	-1.08082500	3.13056900				
H	5.62170700	-0.20734700	2.87610000				
H	3.51147600	-1.45341700	4.13636700				
C	1.39710300	-2.49516800	-0.59465400				
C	0.25896500	-3.23363500	-0.78127200				
O	2.50109600	-3.30333200	-0.73661100				
C	0.68174300	-4.56923100	-1.06275300				
H	-0.75185400	-2.86413600	-0.69603600				
C	2.04459600	-4.54885400	-1.01906400				
H	0.05448100	-5.42724000	-1.25954000				

11c6

M06/BSII SCF energy in solution: -2045.77858 a.u.

Solution-phase enthalpy: -2045.165668 a.u.

Solution-phase Gibbs energy: -2045.278738 a.u

Pd	-0.40672400	-0.01704400	-0.22233000
P	2.13352800	-0.22048000	0.05659500
C	-1.76995300	2.61692700	-0.45620400
C	-1.88747900	4.00645600	-0.68380000
C	-0.51078500	2.02935700	-0.17833700
C	-0.74849300	4.80968300	-0.55698500
C	0.59796900	2.87705900	-0.02163200
C	0.48002200	4.25673300	-0.20123100
H	-0.83104400	5.88058400	-0.73359400
H	1.57464400	2.48046200	0.23425600
H	1.35186900	4.89659100	-0.08102300
C	-2.94964900	1.68794100	-0.45147200
C	-3.87663200	1.87993400	0.79658500
C	-3.14365100	-0.24772200	1.03280900
C	-2.47071100	0.20637600	-0.28508600
C	-3.14746500	1.04689600	1.86936100
H	-3.72053100	0.95647100	2.80077400
H	-2.14370900	1.41463900	2.09924500
C	-5.16326200	1.05132100	0.58078200

H	-5.91633100	1.29980200	1.33791100	O	-2.73506000	-3.22867200	-0.66954600
H	-5.61545400	1.23820600	-0.40050700	C	-3.90693000	-3.93532700	-0.20321000
C	-4.66352400	-0.42033500	0.74479500	H	-4.32696200	-3.39651600	0.65144500
H	-5.16156200	-0.91603800	1.58797700	H	-3.60131800	-4.92656900	0.14566200
H	-4.84678900	-1.02776400	-0.14803500	C	-4.88459600	-4.01538000	-1.36090800
H	-4.06368500	2.92614300	1.05097000	H	-4.44457100	-4.55101100	-2.20851000
H	-2.69395300	-1.12149900	1.51037700	H	-5.78770800	-4.55002200	-1.04635100
H	-2.78093100	-0.42263100	-1.12658200	H	-5.17794700	-3.01615300	-1.69892800
H	-3.54658400	1.81079400	-1.36797500				
C	3.14459800	0.59699100	-1.21848300				
C	2.77311200	1.35766400	-2.29492600				
O	4.51527300	0.44795700	-1.21264800				
C	3.97464300	1.70350800	-2.98891900				
H	1.76168900	1.65025200	-2.53888100				
C	4.99213700	1.12685700	-2.28940800				
H	4.06476400	2.29990500	-3.88590200				
H	6.06372900	1.10005800	-2.42114100				
C	2.76705800	0.47076800	1.62309200				
C	3.97184700	0.97805200	2.03604400				
O	1.86022900	0.55193500	2.65261400				
C	3.79749500	1.39439500	3.39191500				
H	4.86811800	1.04327500	1.43599600				
C	2.50131600	1.10972700	3.70889100				
H	4.53504400	1.84787400	4.03925800				
H	1.90656500	1.23823800	4.60060800				
C	2.92489400	-1.87612600	0.10115300				
C	3.54721800	-2.60802200	1.07513400				
O	2.81863600	-2.63184700	-1.04374400				
C	3.85180900	-3.88334600	0.49793700				
H	3.76930000	-2.27393100	2.07810600				
C	3.39246900	-3.84041100	-0.78236000				
H	4.34962500	-4.71504700	0.97651300				
H	3.39484700	-4.54297200	-1.60190000				
C	-3.20354500	4.64571100	-1.07434900				
H	-3.71302400	4.08024800	-1.86418500				
H	-3.90424500	4.70998900	-0.23235700				
H	-3.04417200	5.66475000	-1.44311900				
C	-0.48180300	-2.55351700	-0.38754400				
H	0.41259600	-2.75552200	0.19081600				
C	-0.42331600	-1.95846000	-1.61274000				
H	-1.30829500	-1.88344000	-2.23495700				
H	0.52908000	-1.74005900	-2.08370700				
C	-1.68884200	-3.19865200	0.18666900				
O	-1.71187600	-3.70165200	1.29464200				

TS12c6

M06/BSII SCF energy in solution: -2045.73377 a.u.

Solution-phase enthalpy: -2045.120854 a.u.

Solution-phase Gibbs energy: -2045.229559 a.u

Pd	4.70796800	2.14977800	1.37157300
P	2.94647200	0.70945700	1.56873800
C	7.40409500	1.26616800	0.70691600
C	8.43036700	0.45406200	0.15592500
C	6.15968400	0.70412900	1.07404100
C	8.22690200	-0.92553900	0.05729700
C	6.01948000	-0.69154800	0.99403800
C	7.04045900	-1.50413200	0.50288400
H	9.01371400	-1.54927500	-0.36246500
H	5.09667800	-1.17152900	1.30567700
H	6.90380100	-2.58238900	0.44881100
C	7.72221800	2.71248900	1.00237800
C	8.56611200	2.80704600	2.32775900
C	6.84904200	4.18621000	2.81579000
C	6.59584200	3.81404400	1.32539200
C	7.46587400	2.90345100	3.39903900
H	7.86243700	3.04316100	4.41223700
H	6.78512200	2.04697300	3.39532700
C	9.24601700	4.19510100	2.43305900
H	10.03254100	4.18268500	3.19615400
H	9.71818900	4.49418400	1.48974000
C	8.07062800	5.13909600	2.84668200
H	8.22060300	5.53836300	3.85728600
H	7.95268900	5.99717200	2.17429100
H	9.25816100	1.96757000	2.43083200
H	5.96895900	4.57538500	3.32562100
H	6.92387800	4.64426500	0.70142300
H	8.31768600	3.11465000	0.17418900
C	2.70036400	-0.30261600	0.07577800
C	3.37909300	-0.36198900	-1.11073100
O	1.61373500	-1.14938200	0.02853600

C	2.68144400	-1.29868900	-1.93550700	Solution-phase Gibbs energy: -2045.233579 a.u			
H	4.28127700	0.18318900	-1.34572600	Pd	0.27538400	-0.19085800	-0.36377900
C	1.62710000	-1.74179500	-1.19446900	P	-1.90066400	-0.04274900	0.13694000
H	2.93399100	-1.59932600	-2.94258500	C	1.99359600	-2.29024600	-0.30657500
H	0.82660100	-2.44183900	-1.38257400	C	2.45408800	-3.59308100	-0.64889700
C	3.09490700	-0.49763600	2.92964100	C	0.63838400	-2.13667800	0.08943000
C	2.57080800	-1.74436200	3.15274900	C	1.59308700	-4.68847800	-0.49717300
O	3.90061700	-0.14378100	3.98271200	C	-0.17823500	-3.25442500	0.27274900
C	3.08505200	-2.18375000	4.41154900	C	0.29844400	-4.53517500	-0.00776400
H	1.90169500	-2.27575100	2.49147400	H	1.95867000	-5.68133500	-0.75016000
C	3.88201100	-1.17359600	4.86478100	H	-1.20445300	-3.13052900	0.60944200
H	2.89158300	-3.12492900	4.90689500	H	-0.34212200	-5.40451700	0.12632100
H	4.48040300	-1.03762900	5.75291600	C	3.05022100	-1.16883600	-0.17925900
C	1.25459700	1.32331200	1.84740000	C	3.26587900	-0.72826000	1.32044500
C	0.36507000	1.19624600	2.87962200	C	3.65471500	1.17767400	0.16815500
O	0.70273500	2.08121700	0.84872900	C	3.16442300	0.25091700	-0.97593200
C	-0.80460900	1.92212900	2.49537300	C	2.77376200	0.72794400	1.34810400
H	0.52396600	0.64678800	3.79594400	H	2.99987300	1.23978300	2.29211200
C	-0.53960300	2.43929600	1.26403500	H	1.69548600	0.84587400	1.15698100
H	-1.71375900	2.04772100	3.06629500	C	4.78215600	-0.52137800	1.52840000
H	-1.10058800	3.05599800	0.57862400	H	5.00206100	-0.31852400	2.58373700
C	9.74373800	1.03074300	-0.33493600	H	5.37285800	-1.39717700	1.23655300
H	9.59198700	1.79534700	-1.10850200	C	5.06596000	0.73505200	0.64355300
H	10.32449300	1.50501000	0.46569900	H	5.54134800	1.53172300	1.22719900
H	10.36879400	0.24424600	-0.77082600	H	5.73211100	0.51702200	-0.19966000
C	3.55441600	3.95577800	1.19654600	H	2.80153300	-1.41304200	2.03338600
H	2.85040300	3.72594000	0.40057800	H	3.59575500	2.23062900	-0.09721600
C	4.85619200	4.48865200	0.79283800	H	3.99312400	0.09423400	-1.67765300
H	5.11732800	5.41918900	1.28948300	H	3.97457300	-1.65708800	-0.48107500
H	4.98938100	4.55198500	-0.28570800	C	-2.92668300	-1.18162900	-0.84040100
C	2.85988100	4.44382700	2.39634000	C	-2.61527500	-2.05343500	-1.84769600
O	1.66679300	4.31213200	2.61946000	O	-4.29008900	-1.17784100	-0.63840600
O	3.68249900	5.08932600	3.28244800	C	-3.84842800	-2.62602300	-2.29013100
C	3.04042100	5.58993600	4.46941200	H	-1.62067600	-2.26559900	-2.21084000
H	2.63325700	4.74719900	5.03886500	C	-4.82301500	-2.06103000	-1.52341500
H	2.19637200	6.22403600	4.17922500	H	-3.98657400	-3.35746900	-3.07384200
C	4.07604200	6.36153000	5.26865200	H	-5.89668700	-2.17014500	-1.48418700
H	4.48091700	7.19378500	4.68313700	C	-2.27131600	-0.46590200	1.87113100
H	3.61751200	6.77090300	6.17599800	C	-3.33140200	-1.07290400	2.49169200
H	4.90776500	5.71471900	5.56747200	O	-1.31169200	-0.15270600	2.80106300
				C	-3.00595700	-1.13915800	3.88198200
				H	-4.23210300	-1.42129300	2.00779200
				C	-1.77478200	-0.56632100	4.00779400
				H	-3.60613900	-1.56008800	4.67646400

13c6

M06/BSII SCF energy in solution: -2045.736825 a.u.

Solution-phase enthalpy: -2045.122771 a.u.

H	-1.11880100	-0.38501800	4.84575300	C	-2.98664200	1.76449400	-0.10626700
C	-2.79506100	1.52569500	-0.06106800	C	-3.52323500	1.64779700	1.35959200
C	-3.27366200	2.45033100	0.82893000	C	-2.90008800	-0.47096100	0.87229000
O	-3.02707500	1.94705700	-1.34140000	C	-2.55538300	0.29433600	-0.42541300
C	-3.83529000	3.50536400	0.04685300	C	-2.59616600	0.57548200	1.96455200
H	-3.23329300	2.38229400	1.90658500	H	-2.91133400	0.25789300	2.96682900
C	-3.64997000	3.14834000	-1.25523700	H	-1.54550500	0.87828100	1.99475200
H	-4.30503900	4.40941800	0.40776900	C	-4.87446400	0.89639500	1.31355600
H	-3.89254700	3.61637600	-2.19691000	H	-5.37835000	0.94428600	2.28626800
C	3.86235800	-3.87328700	-1.14318800	H	-5.55863600	1.32349400	0.57123400
H	4.14859400	-3.22957500	-1.98344100	C	-4.45114100	-0.56919900	0.97025500
H	4.61839200	-3.73672100	-0.35854300	H	-4.74163500	-1.26074600	1.77208700
H	3.94065600	-4.91014500	-1.48631700	H	-4.89502800	-0.93951200	0.04092200
C	0.71552300	1.49844900	-1.55541500	H	-2.40340800	-1.43944900	0.98327700
H	0.01590900	1.40789100	-2.38930500	H	-3.08180900	-0.10611900	-1.29404600
C	2.09909000	0.91288900	-1.95058400	H	-3.81715200	2.07252100	-0.75971900
H	2.68198700	1.71925100	-2.42171600	C	3.26243300	-0.23052800	-1.14616800
H	1.91504600	0.18334800	-2.75030900	C	3.26165600	0.07194500	-2.48391100
C	0.55735800	2.86235900	-1.02572300	O	4.53775000	-0.55795300	-0.75436300
O	-0.49623900	3.48418600	-1.00450500	C	4.60686300	-0.08033100	-2.94289200
O	1.70722600	3.42438400	-0.53356500	H	2.40347300	0.38533900	-3.06260400
C	1.56135700	4.74911000	0.00683300	C	5.32959000	-0.46360600	-1.85224900
H	0.85239500	4.72149500	0.84170400	H	4.98131900	0.07523800	-3.94481400
H	1.13264100	5.40461200	-0.75850900	H	6.37139300	-0.70312800	-1.69845400
C	2.93343300	5.22737700	0.45054500	C	2.50011100	1.04734600	1.26452200
H	3.63323400	5.24587000	-0.39192500	C	2.19734800	1.25663800	2.58202300
H	2.86156300	6.24214300	0.85858200	O	3.35532000	2.02272400	0.82524400
H	3.34733900	4.57483900	1.22663700	C	2.91285800	2.42980600	2.98159500

11c7

M06/BSII SCF energy in solution: -2045.775171 a.u.

Solution-phase enthalpy: -2045.162353 a.u.

Solution-phase Gibbs energy: -2045.275681 a.u

Pd	-0.47568200	0.04199500	-0.77333900	C	1.16257300	-2.65681700	1.41281800
P	1.88550900	-0.18166600	0.04804700	O	3.29110900	-1.98909500	1.61684300
C	-1.82331500	2.68857900	-0.30248100	C	1.85400800	-3.58426300	2.25344000
C	-1.93665100	4.09632700	-0.31884000	H	0.12451700	-2.69478100	1.11392900
C	-0.58037700	2.06501600	-0.54684700	C	3.13571800	-3.12739800	2.33727700
C	-0.79443200	4.86298300	-0.57544400	H	1.45027600	-4.46776800	2.72759500
C	0.54214000	2.86264400	-0.81142800	H	4.02004500	-3.48302900	2.84510100
C	0.43486000	4.25501600	-0.82403100	C	-3.26629200	4.78678600	-0.10497800
H	-0.87602700	5.94806100	-0.59474700	H	-3.17889300	5.86402500	-0.28203600
H	1.50892200	2.41779400	-1.02641100	H	-4.03828300	4.39938900	-0.78238500
H	1.31172300	4.86386900	-1.03420900	C	-1.17765100	-1.87693200	-2.19490900

C	0.15143300	-2.05617200	-1.95223000	H	6.67887000	5.73323200	3.34989300
H	0.50034800	-2.78999000	-1.23592800	H	5.03442300	3.60341400	3.55561200
H	0.89711400	-1.61329200	-2.60279300	H	6.18869800	4.83338600	1.31225200
C	-2.25894100	-2.68364700	-1.57727600	H	8.02581400	3.98462500	0.66086200
O	-3.41604000	-2.63720200	-1.94740600	C	2.12167600	-0.02390800	-0.42388800
O	-1.82630500	-3.50271100	-0.58617100	C	2.02685500	0.73768200	-1.55837600
C	-2.83511500	-4.36592900	-0.01019200	O	1.08506900	-0.92452000	-0.38643000
H	-3.28543800	-4.95908200	-0.81224500	C	0.86477500	0.28736200	-2.25835500
H	-3.62293100	-3.74441700	0.42578600	H	2.71553900	1.51524900	-1.85640000
C	-2.15730600	-5.23953900	1.02887400	C	0.33785500	-0.71592100	-1.50028600
H	-2.88889500	-5.92796200	1.46596200	H	0.47758100	0.66064500	-3.19593200
H	-1.35339700	-5.83155500	0.57938300	H	-0.52872200	-1.35149100	-1.60651700
H	-1.73381300	-4.63513300	1.83818300	C	3.97660800	-1.77150600	0.79824800
H	-3.56284900	2.60136200	1.89303100	C	4.45845900	-2.63116400	1.74759600
H	-3.64711700	4.65079800	0.91478400	O	4.04408900	-2.36282300	-0.43708700
H	-1.52183100	-1.26707400	-3.02319000	C	4.84056100	-3.82544300	1.05923300

TS12c7

M06/BSII SCF energy in solution: -2045.71634 a.u.

Solution-phase enthalpy: -2045.103945 a.u.

Solution-phase Gibbs energy: -2045.214328 a.u

Pd	4.76409600	1.75558400	0.82595000	C	2.55166500	0.62954300	3.60266800
P	3.38140500	-0.04179000	0.88938200	O	1.52957700	-1.11865500	2.64359000
C	7.62622100	1.93419400	0.27644500	C	1.61886500	0.07816300	4.53483100
C	8.86145500	1.71206400	-0.38508500	H	3.20904500	1.47372700	3.74997300
C	6.57268500	0.99583100	0.17617000	C	1.03008200	-0.97299200	3.89611700
C	9.03299400	0.53432900	-1.11989600	H	1.41569000	0.41933900	5.54017400
C	6.79591900	-0.17433600	-0.56696800	H	0.26978900	-1.68509700	4.18113500
C	8.01176900	-0.40980500	-1.20845300	C	10.00183900	2.70957600	-0.33483000
H	9.97924700	0.36149000	-1.62923000	H	10.85815100	2.34346700	-0.91107900
H	6.00690300	-0.91226200	-0.67077300	H	9.71677500	3.68286800	-0.75702300
H	8.16148300	-1.32061400	-1.78534700	C	4.20843100	4.12932000	0.91489600
C	7.48546100	3.16282800	1.14400900	C	3.16674100	3.11372500	1.07502700
C	8.10805900	2.92468200	2.56877200	H	2.62109800	3.13203900	2.01433300
C	6.03709400	3.62393800	3.12398700	H	2.51399300	2.97788600	0.21254800
C	6.06161000	3.78727000	1.57833800	C	4.05117100	5.42158100	1.69384800
C	6.91108800	2.37865000	3.36457900	O	4.52302500	6.48274300	1.33460300
H	7.13663900	2.21734800	4.42606300	O	3.31043700	5.28767600	2.81274200
H	6.49781900	1.45931700	2.93895600	C	3.11162100	6.49509800	3.58420600
C	8.37034700	4.28087700	3.26992800	H	2.62063200	7.23872600	2.94877500
H	9.03193100	4.14744600	4.13341600	H	4.08919200	6.89660900	3.86922600
H	8.85310000	5.00270200	2.60123000	C	2.26906400	6.13044300	4.79220400
C	6.94335600	4.73592100	3.71701000	H	2.09052600	7.02285200	5.40203000
H	6.85880600	4.75367000	4.81069700	H	1.30026100	5.72291200	4.48573100

H	2.77657700	5.38562000	5.41396300	C	3.27828000	1.02731600	0.23290300
H	8.98415500	2.27278900	2.51981700	C	3.76988800	1.72537800	1.30244800
H	10.35195700	2.90067300	0.68729600	O	3.66177200	1.63864300	-0.93295400
H	4.43280300	4.40063300	-0.11506100	C	4.50325200	2.83000000	0.76476100

13c7

M06/BSII SCF energy in solution: -2045.740018 a.u.

Solution-phase enthalpy: -2045.12676 a.u.

Solution-phase Gibbs energy: -2045.238202 a.u

Pd	-0.01425800	-0.16196300	-0.41640800
P	2.16508800	-0.41339700	0.08821200
C	-1.59904200	2.28761500	-0.45615000
C	-2.03012000	3.58167900	-0.87471200
C	-0.31625600	1.83483700	-0.86835200
C	-1.19272700	4.36825800	-1.67403600
C	0.48733700	2.65271200	-1.67350600
C	0.06030700	3.91557900	-2.07658400
H	-1.53593000	5.35371900	-1.98231900
H	1.46345600	2.29818400	-1.99112200
H	0.69416900	4.54232200	-2.70100800
C	-2.56170600	1.54821700	0.50809400
C	-2.22577100	1.81050100	2.02134500
C	-2.76460800	-0.38468200	2.02482300
C	-2.90268100	-0.03462400	0.51765600
C	-1.57685200	0.49135700	2.47462900
H	-1.39427300	0.45080600	3.55613100
H	-0.63866700	0.27297300	1.95085700
C	-3.54553600	1.78517600	2.82796500
H	-3.37729500	2.12841100	3.85567900
H	-4.31479200	2.43229700	2.39207200
C	-3.93692500	0.27205200	2.79823900
H	-4.00292200	-0.13953700	3.81195000
H	-4.90233600	0.08954200	2.31300300
H	-2.68781700	-1.45881400	2.21134800
H	-3.95875200	-0.11280800	0.24855200
H	-3.53348000	2.00452200	0.32209400
C	2.97966700	-1.40973900	-1.19638500
C	2.47082700	-2.04677500	-2.29673000
O	4.33788600	-1.61065900	-1.13199700
C	3.57492300	-2.67862600	-2.94849700
H	1.43313400	-2.05394000	-2.59876600
C	4.67416700	-2.37948600	-2.19896600
H	3.55110400	-3.27083700	-3.85243200
H	5.72241800	-2.62443200	-2.28549000

H	3.63435700	1.47752200	2.34513600
C	4.40386600	2.72609100	-0.58950400
H	5.03523200	3.59269500	1.31599200
H	4.78609400	3.30865900	-1.41383300
C	2.53364800	-1.25844800	1.66146500
C	1.71240900	-1.83578200	2.59349300
O	3.84585400	-1.42998000	2.04087100
C	2.55911800	-2.39175300	3.60191600
H	0.63395900	-1.85870400	2.55563900
C	3.83597900	-2.11597800	3.21160400
H	2.25639700	-2.92303300	4.49328100
H	4.80603800	-2.32800200	3.63635900
C	-3.37148200	4.17971600	-0.48615200
H	-3.46789100	5.18900600	-0.89952500
H	-4.22004900	3.59509800	-0.86613100
C	-2.16200300	-0.98256000	-0.48125600
C	-1.05508600	-1.94049700	0.00582100
H	-1.11513800	-2.23116200	1.05142300
H	-0.91621200	-2.80380100	-0.64524400
C	-3.07629900	-1.80139500	-1.39866400
O	-2.83224000	-2.06458800	-2.55626700
O	-4.16134600	-2.25466800	-0.73820500
C	-5.05555600	-3.09717700	-1.50375300
H	-4.49434900	-3.96489500	-1.86468500
H	-5.40114000	-2.53850400	-2.37921700
C	-6.19934900	-3.49465600	-0.58975000
H	-6.90151300	-4.13685400	-1.13267700
H	-5.83096500	-4.04568500	0.28154000
H	-6.74268400	-2.61259600	-0.23555100
H	-1.62971200	2.71454300	2.16756400
H	-3.49939600	4.26070900	0.60053100
H	-1.71692600	-0.29195700	-1.28612900

11c8

M06/BSII SCF energy in solution: -2045.776315 a.u.

Solution-phase enthalpy: -2045.163033 a.u.

Solution-phase Gibbs energy: -2045.275003 a.u

Pd	0.57706500	0.47969300	0.22045200
P	-1.76881500	-0.52802300	0.17452100
C	2.73831400	-1.00523400	-1.23230600

C	3.33251200	-1.72097700	-2.29500700	H	-0.15616600	-1.09032500	2.91127000
C	1.36331500	-0.68130800	-1.25953700	C	-3.25718900	-1.96132100	3.52995700
C	2.53491600	-2.10311700	-3.37928100	H	-1.62733900	-2.13430500	4.98064300
C	0.59847700	-1.06335600	-2.37126900	H	-4.18296500	-2.30613000	3.96627300
C	1.18165500	-1.77148400	-3.42423300	C	4.81109200	-2.04398400	-2.30421200
H	2.98674300	-2.65053400	-4.20434300	H	5.10432600	-2.50238900	-3.25462000
H	-0.45283600	-0.80628100	-2.44110700	H	5.42423400	-1.14371600	-2.16605900
H	0.57868500	-2.06064700	-4.28244400	C	0.59541400	2.62082200	1.29448500
C	3.51566100	-0.45540000	-0.07496300	C	-0.59377700	2.09332600	1.70325100
C	3.97778100	-1.47533800	1.02006600	H	-0.67173200	1.58747900	2.65982100
C	2.75613100	0.02738900	2.19025300	H	-1.52006300	2.30872600	1.18635900
C	2.62615400	0.53847600	0.74034500	C	0.79258000	3.53114900	0.13428500
C	2.77696200	-1.50452900	1.98646500	O	1.83313900	4.12848500	-0.06130300
H	2.98676500	-2.06468100	2.90676600	O	-0.29910200	3.63516700	-0.66251800
H	1.86267100	-1.89223300	1.52710900	C	-0.15429900	4.47295100	-1.83652200
C	5.04607100	-0.77422800	1.89100600	H	-0.88039500	4.06931600	-2.54648900
H	5.51729500	-1.48801200	2.57717500	H	0.85362800	4.34040500	-2.23586700
H	5.84342100	-0.32677500	1.28682100	C	-0.43611900	5.93356900	-1.51653000
C	4.21319300	0.29101900	2.67535000	H	0.30936500	6.32506900	-0.81903300
H	4.29234200	0.13992900	3.75912200	H	-0.39317900	6.52889800	-2.43602700
H	4.53373700	1.31765000	2.46574500	H	-1.43190500	6.05315100	-1.07631000
H	2.00357400	0.41371400	2.88722200	H	4.29273400	-2.44311000	0.62105300
H	2.95981800	1.57212600	0.61679800	H	5.09091600	-2.73935400	-1.50305100
H	4.40880100	0.06365800	-0.45571200	H	1.46991400	2.56275700	1.93077100
C	-3.22847700	0.48546500	-0.24123900	TS12c8 M06/BSII SCF energy in solution: -2045.720582 a.u. Solution-phase enthalpy: -2045.107924 a.u. Solution-phase Gibbs energy: -2045.216342 a.u.			
C	-3.30072400	1.74912400	-0.76903200				
O	-4.49735900	-0.02728200	-0.10845700				
C	-4.68811400	2.03484600	-0.96355400				
H	-2.45855000	2.39268900	-0.98311200	Pd	4.73005800	2.11834300	0.87709800
C	-5.35951100	0.92377300	-0.54689100	P	3.30425200	0.36097700	0.85906500
H	-5.12308000	2.94116300	-1.36088700	C	7.61812800	2.19471200	0.44311300
H	-6.40643900	0.66279100	-0.49907200	C	8.87382500	1.95764700	-0.17384500
C	-2.16188400	-2.07108100	-0.73693200	C	6.51477400	1.34920900	0.17972900
C	-1.99937700	-3.39416000	-0.43157000	C	9.00798200	0.86918100	-1.04201400
O	-2.63061000	-1.94592900	-2.01939900	C	6.70020700	0.26588800	-0.69348200
C	-2.39656700	-4.13112100	-1.59306900	C	7.93129400	0.02371800	-1.30281700
H	-1.64328700	-3.79442600	0.50692700	H	9.96987900	0.68774100	-1.51789900
C	-2.76762600	-3.20597800	-2.52005100	H	5.87045400	-0.39651200	-0.92071300
H	-2.40555800	-5.20529100	-1.71442600	H	8.05229300	-0.81765700	-1.98276900
H	-3.14268000	-3.26772000	-3.53030600	C	7.51189500	3.33200200	1.43553200
C	-2.08122800	-1.11544600	1.87625700	C	7.98514600	2.89572000	2.87148400
C	-1.21527100	-1.30664200	2.92204700	C	6.00015200	3.86156900	3.33440300
O	-3.34002700	-1.52425000	2.24794400	C	6.13229400	4.07349200	1.80338600
C	-1.98071400	-1.85698600	3.99747300				

C	6.66780100	2.49011300	3.55392700	O	5.12226900	6.21775100	-0.30950500
H	6.79136100	2.23863300	4.61457600	O	4.15151400	4.39173900	-1.22941900
H	6.15615800	1.66763100	3.04274500	C	4.43291200	4.91181000	-2.55262200
C	8.39142500	4.14645000	3.68730000	H	4.48039600	4.02233700	-3.18503400
H	8.92629800	3.85599600	4.59887400	H	5.41134600	5.39698600	-2.53449300
H	9.05282500	4.81226400	3.12164900	C	3.34789600	5.87407600	-3.01282700
C	7.01728000	4.80687800	4.02935100	H	3.32705100	6.76306400	-2.37640800
H	6.84244000	4.82252300	5.11183800	H	3.54718800	6.19232300	-4.04276600
H	6.93691400	5.83985200	3.67267500	H	2.36272600	5.39600200	-2.98635900
H	4.98123700	3.97122800	3.71713100	H	8.75646000	2.12259100	2.82716000
H	6.33224100	5.11850400	1.57739100	H	10.36340400	2.89195900	1.12554900
H	8.17133000	4.13510500	1.08892500	H	4.33986000	5.26841700	1.91244200
C	2.00563600	0.51803500	-0.40444100				
C	1.83243600	1.44791700	-1.39542800				
O	1.01275200	-0.42908700	-0.48057700				
C	0.66444900	1.05660100	-2.12119700				
H	2.47018900	2.30191100	-1.57507100				
C	0.21421100	-0.08228500	-1.52140800				
H	0.22271000	1.55511800	-2.97260000				
H	-0.62419900	-0.73779400	-1.70492600				
C	3.84635900	-1.36999800	0.61024900				
C	4.27057200	-2.33798800	1.47930100				
O	3.92919100	-1.83634900	-0.67657300				
C	4.63211600	-3.47027100	0.68302400				
H	4.31308800	-2.25572300	2.55605200				
C	4.40516600	-3.11040800	-0.61078100				
H	5.00581200	-4.42289100	1.03154200				
H	4.51810700	-3.61487700	-1.55829100				
C	2.43055300	0.17263300	2.44906200				
C	2.58355600	0.81471700	3.64970000				
O	1.44908000	-0.78413000	2.56560500				
C	1.64487100	0.22789400	4.55419900				
H	3.28712600	1.60782700	3.85489900				
C	0.98675800	-0.72902800	3.83978300				
H	1.48297200	0.48582600	5.59134900				
H	0.19648100	-1.42474900	4.08016300				
C	10.07902700	2.84547500	0.06674200				
H	10.94682200	2.47452700	-0.48891100				
H	9.90213900	3.87996900	-0.25807100				
C	4.32849100	4.49097500	1.15324100				
C	3.22605700	3.52894300	1.29914100				
H	2.76246900	3.51662200	2.28533500				
H	2.49310000	3.51525600	0.49548700				
C	4.57525800	5.13896200	-0.18418300				

13c8

M06/BSII SCF energy in solution: -2045.735096 a.u.

Solution-phase enthalpy: -2045.121079 a.u.

Solution-phase Gibbs energy: -2045.230145 a.u

Pd	0.18249600	-0.29625500	-0.43793900
P	-1.95395200	0.12825600	0.03997500
C	2.42363700	-0.39061500	1.26152200
C	3.37148400	-0.93124900	2.18039000
C	1.09019600	-0.87893600	1.30389200
C	2.96689400	-1.90853700	3.09978700
C	0.72310500	-1.84596900	2.24614700
C	1.65316200	-2.36558700	3.14591400
H	3.70224500	-2.30910600	3.79451900
H	-0.30169100	-2.20651800	2.26836900
H	1.36220600	-3.12374000	3.87067200
C	2.96348200	0.78722000	0.39237700
C	2.76694300	2.13744000	1.16859300
C	2.09017800	2.75181600	-0.89491700
C	2.61941500	1.29953100	-1.12941700
C	1.48881500	2.69606800	0.52312100
H	1.20156400	3.68377600	0.90583700
H	0.63836300	2.01340200	0.62189400
C	3.83133800	3.17848000	0.73150100
H	3.88056100	4.00467100	1.44994400
H	4.83490800	2.74155400	0.67527000
C	3.31134000	3.66896600	-0.65817000
H	3.00107800	4.71995900	-0.61464600
H	4.06111000	3.58347400	-1.45254900
H	1.42982400	3.10291200	-1.69398500
H	3.62396100	1.38959900	-1.55718900
H	4.03358700	0.59206600	0.32730100

C	-3.03591600	-0.93045100	-0.97555600
C	-2.77000300	-1.71178100	-2.06866500
O	-4.37545300	-0.99893900	-0.67558100
C	-4.01295500	-2.29481600	-2.46678100
H	-1.80010100	-1.84328400	-2.52547600
C	-4.94460400	-1.82769200	-1.58742800
H	-4.18654800	-2.97048000	-3.29257400
H	-6.00723000	-1.98489400	-1.47610200
C	-2.61507500	-0.16506200	1.71809000
C	-2.99160800	0.66766700	2.73669900
O	-2.71088000	-1.47005400	2.12971500
C	-3.34475700	-0.17231300	3.84007300
H	-3.02527600	1.74678200	2.70169500
C	-3.15798300	-1.45249300	3.41536400
H	-3.69532600	0.13975500	4.81388900
H	-3.29159200	-2.41961900	3.87567000
C	-2.57886600	1.81869200	-0.25033800
C	-1.97082400	2.96157300	-0.69749900
O	-3.91812200	2.06645500	-0.04473600
C	-2.98351500	3.96797900	-0.76980100
H	-0.92558100	3.06794400	-0.94236900
C	-4.13797800	3.36672100	-0.36548400
H	-2.86470600	4.99605100	-1.08186000
H	-5.15618800	3.70910500	-0.25455900
C	4.82482400	-0.49232200	2.23905500
H	5.34750000	-1.02730900	3.03861400
H	5.36570200	-0.69946500	1.30587900
C	1.87163400	0.55066400	-2.31663400
C	0.31629100	0.51312500	-2.35524600
H	-0.09054800	1.51748500	-2.49919100
H	-0.02197700	-0.11072300	-3.19105200
C	2.46056900	-0.84215500	-2.42711400
O	3.37721800	-1.20470500	-3.12694500
O	1.82297900	-1.66676100	-1.54227700
C	2.30876100	-3.02269600	-1.35830900
H	2.12528500	-3.23212100	-0.30337400
H	3.38263800	-3.02143100	-1.55639300
C	1.57193200	-3.98511300	-2.27481800
H	1.76877800	-3.74855900	-3.32501100
H	1.91156200	-5.00973700	-2.08359500
H	0.49215300	-3.94372600	-2.09626000
H	2.72505400	1.98354400	2.24941500
H	4.93515900	0.58052000	2.43986200
H	2.23254400	1.08510600	-3.20656500

11c9

M06/BSII SCF energy in solution: -1332.708982 a.u.

Solution-phase enthalpy: -1332.255014 a.u.

Solution-phase Gibbs energy: -1332.367537 a.u

Pd	-1.54129100	0.48467700	-0.10515400
C	-4.51896100	0.62469200	-0.06111700
C	-5.78278800	1.25015900	0.01068000
C	-3.34430100	1.35442900	0.22651800
C	-5.84811300	2.59594500	0.39035100
C	-3.43825600	2.70183100	0.60065600
H	3.51630600	0.50538300	3.07089000
C	-4.69096600	3.31597100	0.68340100
H	-6.81899700	3.08525100	0.44383600
H	-2.54797800	3.28602600	0.81158200
H	-4.76026500	4.36398400	0.96791800
C	3.67385600	-0.95790900	1.85982000
O	4.10341700	-1.28479100	0.72646800
O	3.03535400	-1.62105500	2.70286500
O	3.91390600	0.39782000	2.19066500
Cs	3.84188700	1.29159600	-0.82992000
C	-4.31659000	-0.79708700	-0.49806400
C	-4.73803200	-1.90174400	0.52745700
C	-2.53634400	-2.30645500	0.20983300
C	-2.78957100	-1.07490600	-0.68021900
C	-3.47683900	-2.04260100	1.40429100
H	-3.53950200	-2.88395300	2.10701300
H	-3.22807400	-1.13007000	1.95392000
C	-4.74457100	-3.25847000	-0.21538100
H	-5.19194500	-4.04135500	0.40871300
H	-5.31917800	-3.21646800	-1.14778500
C	-3.22403300	-3.53378400	-0.45759500
H	-2.91041800	-4.46823900	0.02795300
H	-2.97009400	-3.61547600	-1.52007700
H	-5.66706100	-1.68418200	1.06058600
H	-1.48113400	-2.47960800	0.44611800
H	-2.50075400	-1.23886300	-1.72262400
H	-4.85668100	-0.97279900	-1.44135500
Cs	1.92898000	-3.45651100	0.57214700
I	0.64493400	-0.68536500	-1.81106900
C	-7.05658500	0.51110200	-0.33943100
H	-7.90572400	1.20116700	-0.38817000
H	-6.98085100	0.00690200	-1.31136400
H	-7.30604700	-0.26311700	0.39733100

C	-0.79043400	1.19418500	1.89785200	H	4.71324000	-1.00885900	4.31571400
C	0.26152900	1.70742100	1.16314400	H	4.32558500	0.49646600	5.15549800
C	0.36692500	3.12594200	0.82128200	C	2.54609900	-0.76305100	4.67545000
O	-0.41878000	4.01392700	1.10119400	H	2.58064600	-1.83698700	4.90221900
O	1.53418000	3.38674800	0.12721200	H	2.06308400	-0.27132300	5.52671400
C	1.72712500	4.76550800	-0.26011500	H	4.71906200	0.75650400	2.50555100
H	2.35392100	4.72056800	-1.15778300	H	0.91452100	-1.16055900	3.21656600
H	0.75946200	5.19530700	-0.52651700	H	0.75372700	1.33561600	4.07298400
C	2.39638500	5.57296300	0.84390100	H	3.00633100	2.02107200	4.28908900
H	2.58756200	6.59520700	0.49652700	Cs	0.21337300	-3.34631700	1.06528700
H	1.74755100	5.62366200	1.72221800	I	-1.79384400	-0.00892000	1.94502300
H	3.35360000	5.12703300	1.13914400	C	4.40151000	4.05902300	4.08642600
H	-0.69468000	0.22418900	2.37824400	H	4.95882900	4.99930000	4.15651100
H	1.11714100	1.08286800	0.94223600	H	3.89499600	3.91119500	5.05040100
H	-1.55716500	1.85178500	2.29188400	H	5.12945100	3.24768400	3.97794300

TS12c9

M06/BSII SCF energy in solution: -1332.664177 a.u.

Solution-phase enthalpy: -1332.211634 a.u.

Solution-phase Gibbs energy: -1332.320232 a.u

Pd	0.46339500	1.48264100	1.43698800
C	2.80595900	2.94265800	2.42780800
C	3.42106600	4.11040800	2.93178000
C	1.92330000	3.04699600	1.30950900
C	3.07503700	5.35958900	2.40116600
C	1.52637600	4.32856000	0.87417200
H	0.22952700	-2.24727600	-3.79800400
C	2.09165600	5.47569600	1.41984100
H	3.55771400	6.25245600	2.79333400
H	0.85094000	4.41440800	0.03068600
H	1.79782300	6.45483700	1.05052500
C	-0.44126200	-2.92028900	-2.15043300
O	-1.46927200	-2.98117200	-1.43011500
O	0.71708200	-3.33148400	-1.92833100
O	-0.63988300	-2.22963000	-3.36403100
Cs	-2.77682900	-0.32023200	-1.83907400
C	2.80346300	1.68273300	3.26511400
C	3.78670000	0.48429900	3.00923600
C	1.77022200	-0.49364000	3.34649300
C	1.39757600	0.99725300	3.25507200
C	2.91436800	-0.58751700	2.31100400
H	3.42056400	-1.56408300	2.28825800
H	2.59999700	-0.32875300	1.29672900
C	3.97658300	-0.19899200	4.38448600

C	2.02914000	2.01221200	-0.26555100
C	0.75156600	1.68215000	-0.90279700
C	0.17819000	2.61644900	-1.83168800
O	0.52707800	3.77499900	-2.04595000
O	-0.90029300	2.07324800	-2.54335300
C	-1.46738800	2.93918200	-3.54250800
H	-2.50522500	2.60128800	-3.66232200
H	-1.47238800	3.96448000	-3.16608100
C	-0.71517000	2.85227400	-4.86424600
H	-1.21049700	3.47044200	-5.62292000
H	0.30748200	3.21674900	-4.73609700
H	-0.67852500	1.81973400	-5.23049200
H	2.68649600	1.17203000	-0.05700000
H	0.50645700	0.63511900	-1.05373700
H	2.57959600	2.79849100	-0.77452900

13c9

M06/BSII SCF energy in solution: -1332.726677 a.u.

Solution-phase enthalpy: -1332.270596 a.u.

Solution-phase Gibbs energy: -1332.379088 a.u

Pd	-0.91621700	0.39099700	-0.26318700
C	-3.69803200	-1.59281800	0.19589100
C	-4.49335600	-2.22727200	-0.79537400
C	-4.17305600	-0.39202700	0.76917100
C	-5.72153500	-1.66840100	-1.17087200
C	-5.40754400	0.13672700	0.37161500
H	2.78202800	-0.12088500	3.69742700
C	-6.18668100	-0.49312800	-0.59163300
H	-6.31738900	-2.16858000	-1.93099800

H	-5.74018600	1.06914100	0.81774500
H	-7.14178800	-0.06976800	-0.89204000
C	3.56400400	-0.30250300	1.97184700
O	3.95040700	0.34168900	0.96672500
O	3.52386300	-1.53592300	2.16973900
O	3.04108700	0.50979800	3.00481300
Cs	1.92920300	2.56468500	0.83039300
C	-2.37587300	-2.26032600	0.58219500
C	-2.11091900	-2.70843600	2.07304700
C	-0.07842200	-2.04889800	1.32487400
C	-1.01486600	-1.60245600	0.18192300
C	-0.94907400	-1.81537100	2.57030600
H	-0.49658900	-2.20926400	3.48926700
H	-1.18791500	-0.76543900	2.72409100
C	-1.34922900	-4.05310300	1.96530600
H	-1.18410300	-4.48587700	2.95923100
H	-1.88479900	-4.79854000	1.36723400
C	0.00865300	-3.61146400	1.31953200
H	0.86443700	-3.94746700	1.91733100
H	0.13448100	-4.01358800	0.30509900
H	-3.00672800	-2.75103400	2.69880100
H	0.90464900	-1.57175100	1.34032200
H	-0.68388000	-1.97697200	-0.79567900
H	-2.38778900	-3.19494300	0.01908900
Cs	3.47855700	-2.11218700	-0.81372900
I	0.94452300	0.38881700	-2.41678000
C	-4.07718200	-3.50874700	-1.49674600
H	-4.82429200	-3.78425500	-2.24783700
H	-3.11751600	-3.40684500	-2.01850400
H	-3.98494500	-4.35833500	-0.80759600
C	-3.38959800	0.38455300	1.81128800
C	-2.16642100	1.12110800	1.26193600
C	-2.51226000	2.36414800	0.53781400
O	-3.59949800	2.84780000	0.30439100
O	-1.33578900	2.95268500	0.02722000
C	-1.53573200	4.05078200	-0.89504700
H	-0.66197200	4.02588900	-1.55326200
H	-2.43036300	3.84834700	-1.48762000
C	-1.65951100	5.38249500	-0.16684400
H	-1.75688000	6.19783700	-0.89354700
H	-2.54444100	5.38438600	0.47479700
H	-0.77663500	5.58609600	0.45251100
H	-3.07598800	-0.28158400	2.61685800
H	-1.43362800	1.34040600	2.05050900

4a

M06/BSII SCF energy in solution: -2468.857807 a.u.

Solution-phase enthalpy: -2468.328985 a.u.

Solution-phase Gibbs energy: -2468.463967 a.u.

Pd	2.61991200	1.03562700	-0.34250800
C	1.44298900	0.68908700	1.23716700
C	1.95372100	0.99100100	2.49729300
C	0.14693300	0.19063800	1.04665100
C	1.15629700	0.77945200	3.62848200
H	2.95707300	1.38742700	2.60603400
C	-0.62453100	-0.01383200	2.20522100
C	-0.13355600	0.27370800	3.47967500
H	1.54991800	1.01616000	4.61383700
H	-1.63682900	-0.39366100	2.08896000
H	-0.76182900	0.10658600	4.35067300
I	1.69904600	3.41895500	-0.95400600
C	-0.43389700	-0.10743600	-0.31581300
H	-0.38091600	0.77470400	-0.96325400
H	0.11844400	-0.91270500	-0.81417000
H	-1.48267500	-0.40887000	-0.23231600
P	-5.80362000	-1.13364600	0.30704100
C	-7.60589300	-0.89066900	0.55841800
C	-8.65728500	-0.45564000	-0.20512600
O	-8.07562800	-1.28061700	1.79384600
C	-9.83341600	-0.57607400	0.60132000
H	-8.59086500	-0.09083800	-1.21953000
C	-9.41816000	-1.07506700	1.79940200
H	-10.84776500	-0.32404100	0.32425100
H	-9.92710500	-1.33105100	2.71670400
C	-5.21451000	0.56594900	0.67705000
C	-5.79524100	1.80004300	0.79088100
O	-3.86814200	0.67192200	0.95375000
C	-4.75537800	2.71638300	1.14624200
H	-6.84103400	2.02169300	0.63389000
C	-3.61124300	1.98075900	1.22498800
H	-4.84747000	3.78009300	1.31665400
H	-2.58229700	2.21645200	1.45209400
C	-5.72346400	-1.16015000	-1.52059000
C	-5.18799400	-2.11392400	-2.34517900
O	-6.19725500	-0.11765800	-2.28800200
C	-5.34209500	-1.64432600	-3.68785500
H	-4.73433000	-3.04145600	-2.02418300

C	-5.95749900	-0.43296200	-3.58839100	I	0.19909100	-2.51910400	-2.06304700
H	-5.03142000	-2.13722900	-4.59843500	C	-0.47565200	1.69953300	1.02978500
H	-6.27257900	0.30242800	-4.31392300	H	-0.27637800	0.62526700	1.02401600
P	3.76314800	-0.98450500	-0.05452500	H	-0.09888000	2.10738700	1.97724600
C	4.41184400	-1.58516000	-1.64632700	H	-1.56210500	1.83897300	1.01894100
C	4.60421800	-2.82463600	-2.19696900	P	-5.49024800	0.99272600	1.25212000
O	4.73768800	-0.61711600	-2.56486400	C	-6.86398600	-0.05463000	0.63003000
C	5.08410900	-2.60822500	-3.52678300	C	-6.95967600	-1.18467700	-0.13934900
H	4.41916800	-3.77226100	-1.71123100	O	-8.12450800	0.31297900	1.05175400
C	5.14486300	-1.25608400	-3.69188900	C	-8.34621300	-1.52884800	-0.20146200
H	5.34281900	-3.35906600	-4.26010600	H	-6.13070800	-1.70267500	-0.60033000
H	5.43887300	-0.61642000	-4.51026400	C	-9.00026100	-0.58575300	0.53510700
C	5.27570200	-0.85113700	0.95538300	H	-8.79295900	-2.36471500	-0.72201700
C	6.52791300	-1.39725700	0.84509900	H	-10.03919500	-0.42106000	0.77947200
O	5.23866900	-0.00281100	2.03434300	C	-4.96349700	1.74002000	-0.34403900
C	7.30295800	-0.86212300	1.92026700	C	-5.46674200	1.75325900	-1.61570500
H	6.85302600	-2.08938300	0.08137700	O	-3.85835000	2.55781100	-0.28159400
C	6.47017400	-0.02683300	2.60453800	C	-4.61781800	2.61290000	-2.38591800
H	8.33996600	-1.06661400	2.14643700	H	-6.32878400	1.20276900	-1.96244100
H	6.59348400	0.59959000	3.47511600	C	-3.65918800	3.06429800	-1.53223900
C	2.97885800	-2.47720400	0.62830400	H	-4.70648300	2.84955500	-3.43719200
C	3.36922300	-3.39612400	1.56610100	H	-2.79407100	3.69973800	-1.64516300
O	1.71681300	-2.77855800	0.18343400	C	-4.17157100	-0.25245100	1.48315300
C	2.28585500	-4.31913000	1.70461100	C	-3.52980800	-0.64078000	2.63022700
H	4.31244400	-3.40688600	2.09291000	O	-3.65546100	-0.95645100	0.41866200
C	1.31696900	-3.89552200	0.84459600	C	-2.57526900	-1.63823400	2.25556600
H	2.23575600	-5.17657300	2.36075800	H	-3.72166200	-0.25369900	3.62178000
H	0.32987800	-4.25561600	0.59700300	C	-2.69237600	-1.78351800	0.90398800

TS4a-4b

M06/BSII SCF energy in solution: -2468.854693 a.u.

Solution-phase enthalpy: -2468.326974 a.u.

Solution-phase Gibbs energy: -2468.456512 a.u

Pd	1.21677000	-0.23382600	-1.10266300	H	-1.89120700	-2.17328000	2.89958100
C	1.01511500	1.76456200	-1.06383700	H	-2.16620300	-2.37555400	0.16822400
C	1.59696200	2.45630900	-2.13239000	P	3.05819700	0.04681800	0.15802900
C	0.16207600	2.39961100	-0.15010200	C	2.76872400	-0.02630100	1.94800400
C	1.29435400	3.80462600	-2.33561600	C	3.37634500	0.57455700	3.02008500
H	2.27603800	1.94731500	-2.81151400	O	1.71668100	-0.79141300	2.38287700
C	-0.11483700	3.76145200	-0.37428000	C	2.66108500	0.14977900	4.18143500
C	0.43734600	4.45885900	-1.44724000	H	4.22480700	1.24222400	2.98130000
H	1.73110300	4.33667300	-3.17698100	C	1.67022500	-0.67380900	3.73274000
H	-0.78181100	4.27372700	0.31727600	H	2.85606600	0.42517800	5.20827900
H	0.20430200	5.51148400	-1.58709200	H	0.88375200	-1.22834800	4.22174700
				C	4.17707100	-1.35193700	-0.14616900
				C	4.74516600	-2.28883200	0.67603000
				O	4.47826800	-1.63689300	-1.45357600
				C	5.44006200	-3.20280900	-0.17440600
				H	4.67033500	-2.32245400	1.75336400

C	5.24235200	-2.75929200	-1.44886500
H	6.00329200	-4.07550500	0.12445700
H	5.55841400	-3.11130600	-2.41908800
C	4.18130700	1.46897200	0.00436800
C	5.42189300	1.59087400	-0.56550100
O	3.74080900	2.69653600	0.42426400
C	5.76726500	2.97589300	-0.48687100
H	6.01037600	0.79179500	-0.99249200
C	4.71456800	3.59368600	0.12053700
H	6.67711000	3.44374400	-0.83539500
H	4.50955500	4.61532100	0.40235100

4b

M06/BSII SCF energy in solution: -2468.856616 a.u.

Solution-phase enthalpy: -2468.327867 a.u.

Solution-phase Gibbs energy: -2468.4602 a.u

Pd	1.17582200	-0.15485800	-0.68602300
C	1.06599800	1.84987800	-0.55063100
C	1.59608300	2.58692700	-1.61562200
C	0.28868200	2.46229100	0.44677100
C	1.31680900	3.95147400	-1.73236900
H	2.22349200	2.10172000	-2.35924000
C	0.03626500	3.83933000	0.31346000
C	0.53697000	4.57870100	-0.75841900
H	1.71698200	4.51731400	-2.56998100
H	-0.56971300	4.33220300	1.07150100
H	0.32749200	5.64331400	-0.82646600
I	0.38344700	-2.62871000	-1.38380000
C	-0.32279100	1.70228700	1.60260100
H	0.23840400	0.79370100	1.83862900
H	-0.36445500	2.32652600	2.50253200
H	-1.35120400	1.40295600	1.36628400
P	-5.38591800	0.89313600	1.03892700
C	-6.61603200	-0.22732300	0.26307800
C	-6.56672600	-1.42993900	-0.39223700
O	-7.93200000	0.16627800	0.38664500
C	-7.91632600	-1.79447600	-0.69358400
H	-5.66708200	-1.98169000	-0.62488300
C	-8.69547100	-0.78978000	-0.20053600
H	-8.25782800	-2.68343900	-1.20580700
H	-9.76074100	-0.61315600	-0.18544500
C	-4.55531700	1.49951900	-0.48583900
C	-4.77326700	1.35685700	-1.82857500
O	-3.50835500	2.36940800	-0.28234600

C	-3.79995900	2.17203300	-2.49232200
H	-5.52730200	0.73361300	-2.28616600
C	-3.05799600	2.75420000	-1.51063500
H	-3.66786900	2.29649600	-3.55824800
H	-2.21062100	3.42292800	-1.50763100
C	-4.14412200	-0.30949600	1.63543100
C	-3.72246100	-0.56773600	2.91360500
O	-3.45318400	-1.11923200	0.76202100
C	-2.72834300	-1.59284700	2.82516000
H	-4.08345700	-0.07824800	3.80791400
C	-2.60423400	-1.88387400	1.49812500
H	-2.17736000	-2.04709000	3.63693600
H	-1.96769200	-2.54944600	0.93242200
P	3.19690900	-0.05698600	0.28123600
C	3.17783400	-0.45503500	2.05084700
C	4.01624600	-0.12841500	3.08578300
O	2.13854900	-1.21495600	2.52127100
C	3.46474500	-0.72855800	4.25839300
H	4.91286400	0.47059500	3.01493300
C	2.33087800	-1.37123900	3.85370100
H	3.85651100	-0.68257000	5.26472400
H	1.58298100	-1.95717100	4.36611800
C	4.28268600	-1.32506200	-0.43316800
C	4.97768500	-2.37145100	0.11180200
O	4.40272000	-1.34668400	-1.79890400
C	5.56182500	-3.08001400	-0.98292000
H	5.05350600	-2.60962100	1.16278800
C	5.17903000	-2.41672600	-2.11098200
H	6.17573700	-3.96816500	-0.93412400
H	5.36150800	-2.56806300	-3.16400600
C	4.26673700	1.41247800	0.23063400
C	5.43281600	1.67048800	-0.44243800
O	3.85620200	2.53755000	0.89533600
C	5.76060900	3.03543800	-0.17215500
H	5.98335000	0.97343000	-1.05729200
C	4.77229800	3.50673800	0.64051100
H	6.61626700	3.58706500	-0.53510300
H	4.58252000	4.46072300	1.10861800

4c

M06/BSII SCF energy in solution: -2468.904135 a.u.

Solution-phase enthalpy: -2468.375226 a.u.

Solution-phase Gibbs energy: -2468.500201 a.u

Pd	-0.02264900	-0.03191300	0.03120500
----	-------------	-------------	------------

C	-0.01341500	2.01603600	0.11523500
C	-0.14822500	2.63021400	1.36442500
C	0.12304700	2.80282400	-1.04392400
C	-0.14524400	4.02434700	1.48330800
H	-0.25538800	2.02395800	2.26093700
C	0.12785400	4.19973900	-0.90548600
C	-0.00422700	4.81262800	0.34179700
H	-0.25110600	4.48497600	2.46307800
H	0.23285500	4.81507700	-1.79760100
H	0.00126300	5.89754400	0.41806100
I	-0.04615900	-2.81863800	-0.03402500
C	0.25081800	2.18386300	-2.41817100
H	-0.60897000	1.54411800	-2.65055000
H	0.31846100	2.95466400	-3.19415500
H	1.14246500	1.55028500	-2.49668200
P	2.35395800	-0.03644200	0.06233800
C	3.11482700	-1.02475100	-1.26600600
C	4.19189800	-1.86639100	-1.31899300
O	2.51082300	-0.96654900	-2.49629800
C	4.25213300	-2.36347300	-2.65844800
H	4.85458000	-2.10237300	-0.49929400
C	3.21149900	-1.78568500	-3.32261300
H	4.96823300	-3.06343700	-3.06567200
H	2.84512200	-1.84973800	-4.33587900
C	3.29961700	1.51740600	-0.11268900
C	4.14659300	1.98102500	-1.08401400
O	3.13421700	2.47505700	0.85121900
C	4.52384200	3.30479400	-0.69372400
H	4.46585700	1.44187400	-1.96397800
C	3.88122500	3.54766500	0.48308400
H	5.18439200	3.97961200	-1.21993600
H	3.84642700	4.39105000	1.15561500
C	3.04736300	-0.73205700	1.58889800
C	2.46750200	-1.40240300	2.63141800
O	4.39721000	-0.58379500	1.82564300
C	3.51272100	-1.68737300	3.56391800
H	1.42538500	-1.67949400	2.69669700
C	4.65263600	-1.17034400	3.02416500
H	3.42402500	-2.20850600	4.50679500
H	5.68082100	-1.13123500	3.35224300
P	-2.39476400	-0.01105600	0.03823800
C	-3.15953600	-0.44412800	-1.55709100
C	-4.42967500	-0.28293400	-2.04996400
O	-2.36571100	-1.01440500	-2.51609800

C	-4.41808400	-0.79725800	-3.38216300
H	-5.26391300	0.15717100	-1.52181000
C	-3.14114800	-1.22456600	-3.60593700
H	-5.24442200	-0.83879100	-4.07790800
H	-2.64450200	-1.67992200	-4.44932800
C	-3.15965500	-1.18247300	1.20734300
C	-4.15361400	-2.11560300	1.10043800
O	-2.65180600	-1.18840100	2.48172000
C	-4.26264300	-2.73961800	2.38278900
H	-4.72254500	-2.34045700	0.21040400
C	-3.33047800	-2.14052800	3.17549300
H	-4.93699200	-3.53482000	2.66810700
H	-3.03411500	-2.26689800	4.20570900
C	-3.32753400	1.50088300	0.46915400
C	-4.18337400	1.79924100	1.49702000
O	-3.13659100	2.61198900	-0.30819100
C	-4.53775800	3.17668600	1.34242600
H	-4.51495700	1.12026100	2.26906400
C	-3.87342400	3.61401900	0.23561100
H	-5.19547800	3.75855300	1.97281200
H	-3.81552500	4.56294300	-0.27523800

5b

M06/BSII SCF energy in solution: -1785.211121 a.u.

Solution-phase enthalpy: -1784.74645 a.u.

Solution-phase Gibbs energy: -1784.854203 a.u

C	1.10108300	2.37753600	-1.14748700
C	0.56713300	1.54866200	-2.10378600
Pd	0.98988900	0.21175600	-0.26345100
C	3.03255200	0.35955700	-0.31204000
C	3.77050300	-0.35176600	-1.27157600
C	3.66679900	1.22893600	0.57882400
C	5.15724100	-0.12821000	-1.32860500
C	5.04854800	1.42997800	0.50597300
C	5.79597900	0.75090700	-0.45576200
H	5.74166500	-0.66866400	-2.07104100
H	5.53041100	2.11331800	1.20077200
H	6.87045700	0.89958700	-0.52417200
P	-1.50605600	-0.46558400	-0.24229500
C	-2.81154000	0.44941400	-1.16590500
C	-3.15461200	0.47912600	-2.49199400
O	-3.58178000	1.34406700	-0.47303300
C	-4.20454500	1.44447400	-2.62166600
H	-2.73114300	-0.13321400	-3.27603700

C	-4.42221500	1.93356900	-1.37008900	C	0.77777400	0.91952800	-1.49058500
H	-4.73002400	1.72331500	-3.52437200	Pd	-1.34314500	1.01935700	-1.28985500
H	-5.11251700	2.65434400	-0.95861400	C	-1.22437900	3.18166400	-1.29107100
C	-1.68504900	-2.09285100	-1.03591000	C	-1.36950300	3.89596200	-0.08424700
C	-0.75518400	-2.95486000	-1.55223800	C	-1.62882500	3.74377800	-2.50883000
O	-2.94569200	-2.62859700	-1.20041700	C	-1.92949800	5.17865900	-0.14967500
C	-1.47302700	-4.08181800	-2.06035300	C	-2.20678300	5.01224400	-2.54397000
H	0.31436700	-2.80839500	-1.53929700	C	-2.34574200	5.73591500	-1.35929200
C	-2.78969800	-3.82916300	-1.81692200	H	-2.05528400	5.74211500	0.77241100
H	-1.06069000	-4.96030000	-2.53623100	H	-2.53869700	5.43159900	-3.49006700
H	-3.70100600	-4.37406000	-2.01423800	H	-2.77569600	6.73383900	-1.37435300
C	-2.28095400	-0.69487000	1.39159800	P	-1.53397700	-1.34274200	-1.42377000
C	-3.19878600	-1.57617400	1.89619100	C	0.00631400	-2.29056600	-1.74254300
O	-1.86027600	0.15289500	2.38520000	C	0.77095900	-3.15506000	-1.00712000
C	-3.35026000	-1.25651000	3.28069000	O	0.60546900	-2.07063300	-2.95962000
H	-3.69693000	-2.35792600	1.34208600	C	1.90075900	-3.49615800	-1.81958200
C	-2.51727700	-0.20364700	3.51825400	H	0.54700000	-3.52115000	-0.01626700
H	-3.98682300	-1.75040400	4.00141000	C	1.74585400	-2.81602400	-2.98812400
H	-2.28111000	0.37779500	4.39644900	H	2.71152400	-4.16413100	-1.56426900
H	3.08977100	1.75949400	1.33089800	H	2.32107800	-2.75347900	-3.89940800
C	3.14779000	-1.37820300	-2.19197700	C	-2.13480200	-2.19444900	0.06061100
H	2.24304000	-1.00492100	-2.68603200	C	-2.58752100	-1.71118100	1.25776100
H	3.85266200	-1.68781700	-2.97122100	O	-2.19425700	-3.57378700	0.06762600
H	2.85720600	-2.27185700	-1.62456200	C	-2.94497700	-2.84621500	2.04987000
H	1.21379100	1.10961100	-2.85755900	H	-2.68805700	-0.66757600	1.51653100
H	-0.50297000	1.50412000	-2.27596000	C	-2.68985300	-3.94065600	1.27971600
C	0.34035800	3.31900000	-0.27372100	H	-3.34585500	-2.84230600	3.05358500
O	0.90020300	4.16604100	0.39460000	H	-2.79747800	-5.00375800	1.43626800
O	-0.99463400	3.16187700	-0.34502200	C	-2.63493900	-1.90536200	-2.76304800
C	-1.79339000	4.11519000	0.40474100	C	-3.40082100	-3.02302500	-2.96187700
H	-2.76081200	4.09517400	-0.09999800	O	-2.76260400	-1.06005000	-3.83470400
H	-1.34245700	5.10440900	0.29164900	C	-4.04419100	-2.85251100	-4.22609800
C	-1.91780400	3.72668300	1.86911800	H	-3.49416000	-3.85785600	-2.28297300
H	-0.94497900	3.77528800	2.36546500	C	-3.61945700	-1.64861700	-4.70585300
H	-2.59768200	4.42337200	2.37416900	H	-4.73518900	-3.53092900	-4.70659600
H	-2.31727600	2.71392600	1.96689200	H	-3.82600800	-1.09007300	-5.60609200
I	1.45583300	-1.75145000	1.49069100	H	-1.50253900	3.18316300	-3.42900500
H	2.16543000	2.57360300	-1.12664200	C	-1.04306000	3.29644600	1.26191200
				H	-0.12544400	2.69606400	1.24964600
				H	-0.92933800	4.07330600	2.02511100
				H	-1.85500500	2.62772200	1.57438300
				H	1.09063800	0.37592700	-0.60092100
				H	0.99464800	0.43912700	-2.43927700
				C	1.23415000	3.15155200	-2.59738100

TS6b

M06/BSII SCF energy in solution: -1785.19418 a.u.

Solution-phase enthalpy: -1784.730753 a.u.

Solution-phase Gibbs energy: -1784.838159 a.u

O	1.84218500	4.19001100	-2.44748500	H	-5.66779100	0.89928100	-2.89736500
O	1.00814700	2.55886400	-3.78641300	C	-2.78204100	0.42082800	1.45547400
C	1.56113800	3.22075700	-4.95316600	C	-4.12785600	0.35386900	1.70083900
H	1.71217800	2.41097300	-5.67088500	O	-2.08666200	0.18101000	2.61065800
H	2.52734700	3.65181800	-4.68048600	C	-4.26913400	0.04810000	3.08921900
C	0.62013400	4.28315200	-5.49971000	H	-4.91508100	0.50024000	0.97579800
H	0.46014900	5.07456900	-4.76254100	C	-3.00230000	-0.04439700	3.58572200
H	1.05831600	4.73193600	-6.39883000	H	-5.18940300	-0.09207700	3.63872400
H	-0.34764600	3.84906700	-5.77150500	H	-2.59857500	-0.25785500	4.56370700
I	-4.04689200	1.21507200	-0.81055700	H	2.39516700	0.12198300	1.69480800
H	1.00393200	2.81259300	-0.49770000	C	3.29564300	-1.53974000	-2.63008300

7b

M06/BSII SCF energy in solution: -1785.236681 a.u.

Solution-phase enthalpy: -1784.770084 a.u.

Solution-phase Gibbs energy: -1784.876754 a.u.

C	2.54059100	0.84324100	-0.92988900
C	1.25317800	1.44227600	-0.36146400
Pd	0.20820500	-0.31788400	-0.02040900
C	2.72646600	-0.56655500	-0.32979500
C	3.10282300	-1.67365500	-1.13643000
C	2.59634800	-0.73989700	1.06690700
C	3.31489800	-2.90382500	-0.51359400
C	2.81551700	-1.98772300	1.66266400
C	3.16948700	-3.06940700	0.86823400
H	3.59725800	-3.75745300	-1.12449700
H	2.70068000	-2.10047100	2.73628000
H	3.33269000	-4.04666500	1.31302100
P	-1.79959900	0.74235000	-0.04306700
C	-1.79353800	2.56757700	-0.15428100
C	-2.12573500	3.46911400	-1.12947900
O	-1.28747300	3.23189000	0.93478300
C	-1.81749300	4.76597800	-0.60656600
H	-2.55395300	3.23918200	-2.09373700
C	-1.31716200	4.56076300	0.64314500
H	-1.95664200	5.71878300	-1.09784700
H	-0.95656300	5.21684600	1.42081600
C	-2.89775500	0.30817300	-1.41661400
C	-2.80390800	-0.66484000	-2.37383800
O	-4.07906400	1.00471600	-1.57600400
C	-3.98576500	-0.56693100	-3.17184500
H	-2.00131600	-1.38276000	-2.46130300
C	-4.71722400	0.45398300	-2.64345300
H	-4.25331400	-1.18087800	-4.02014200

H	4.01517000	-0.75046300	-2.87555300
H	3.66235000	-2.47878800	-3.05459900
H	2.35380000	-1.29622600	-3.13814200
H	0.74148900	2.09734300	-1.06871000
H	1.38488300	1.95279100	0.59440600
C	3.81601200	1.66848500	-0.73865500
O	4.65434200	1.82640100	-1.60239500
O	3.91345500	2.17220900	0.50974600
C	5.12046400	2.91036800	0.82233600
H	4.82467700	3.57578300	1.63712000
H	5.40230500	3.50501600	-0.04998600
C	6.24630600	1.97710200	1.24188900
H	6.53856900	1.32983600	0.41033700
H	7.12127100	2.56356300	1.54549700
H	5.94040700	1.35184000	2.08710700
I	-0.83025700	-2.85871000	0.18571500
H	2.43835500	0.74309300	-2.01076200

TS22b

M06/BSII SCF energy in solution: -1824.995307 a.u.

Solution-phase enthalpy: -1824.485543 a.u.

Solution-phase Gibbs energy: -1824.620116 a.u.

Pd	-1.37163000	-0.86244400	1.11782700
C	0.16411900	-2.28253900	-0.18769800
C	0.76109300	-3.31128800	0.60041000
C	-0.85847500	-2.66992600	-1.12944800
C	0.37222100	-4.64052500	0.41800400
C	-1.20579700	-4.02795800	-1.27590000
H	-1.25628000	5.63214900	0.07931900
C	-0.58846800	-5.01238000	-0.52160400
H	0.86089800	-5.40766700	1.01387300
H	-1.95430700	-4.30501500	-2.01015100
H	-0.84715800	-6.05782000	-0.66213000

C	0.04855200	4.27272300	-0.19145500
O	0.21043500	3.10886500	-0.64508900
O	0.86264300	5.04759500	0.34252200
O	-1.27721100	4.74897200	-0.32482000
Cs	-2.49882300	2.01828900	-1.33465700
C	0.71489300	-0.84438700	-0.19849400
C	0.43677300	0.07004900	0.93306400
H	0.32788700	1.10595700	0.59193200
H	0.39726400	-0.36006100	-1.11720800
Cs	3.17675200	3.00239600	0.18453300
I	-3.20890400	0.56236500	2.35965500
C	1.84304600	-3.02415200	1.61357400
H	1.42303500	-2.60468400	2.53125700
H	2.36354400	-3.94909200	1.88209000
H	2.58657300	-2.32584200	1.22025000
C	6.15389800	-0.45559500	-2.64845400
C	5.21542700	-1.27579400	-2.00950000
C	5.43368700	-2.65873300	-1.96041600
C	6.57654900	-3.21133100	-2.53887600
C	7.50922800	-2.38728600	-3.17418600
C	7.29491100	-1.00723000	-3.22950800
H	5.96525600	0.61254000	-2.68378800
H	4.69837600	-3.28564000	-1.46797000
H	6.73976600	-4.28535900	-2.49663200
H	8.39881900	-2.81887500	-3.62635400
H	8.01692500	-0.36405600	-3.72679900
C	3.98739200	-0.65020500	-1.38634100
O	3.16754500	-1.49721100	-0.84857500
O	3.84174700	0.58242600	-1.41636200
C	-1.60413600	-1.70857900	-2.00309100
O	-1.10808500	-0.68940200	-2.49432400
C	-3.05338300	-1.99000700	-2.32145000
C	-3.94380800	-2.55937300	-1.39686000
C	-3.54542900	-1.56271200	-3.56701300
C	-5.29706000	-2.69362600	-1.71154500
H	-3.58286100	-2.87855200	-0.42458100
C	-4.89209100	-1.71927000	-3.88871700
H	-2.85274600	-1.12142200	-4.27736100
C	-5.77234700	-2.28115400	-2.95796200
H	-5.97876200	-3.11886400	-0.98045400
H	-5.25645400	-1.40677100	-4.86383700
H	-6.82427400	-2.39720200	-3.20488000
H	2.00079700	-1.02721700	-0.44742600
C	1.21368900	0.14901300	2.23234300

O	0.65394900	-0.45666800	3.28327900
O	2.23903500	0.80990500	2.29914000
C	1.22843000	-0.19062100	4.59279000
H	0.38648100	-0.32874100	5.27370400
H	1.54921400	0.85351800	4.61840000
C	2.37910200	-1.12883800	4.92196900
H	3.20684000	-0.99189400	4.22083700
H	2.74378200	-0.91256600	5.93305400
H	2.05815800	-2.17492200	4.89413700

TS22c

M06/BSII SCF energy in solution: -2109.147492a.u.

Solution-phase enthalpy: -2108.61479 a.u.

Solution-phase Gibbs energy: -2108.764058 a.u

Pd	-1.32581100	0.72928600	-0.88049500
C	-3.36393600	0.98689000	2.29045200
C	-4.58411200	1.72320700	2.37530800
C	-3.41771600	-0.39791700	2.63815700
C	-5.76844500	1.08706700	2.74518500
C	-4.64590700	-1.01041800	2.96367200
H	5.45004900	-0.68108900	2.99501000
C	-5.81926700	-0.27815100	3.03218600
H	-6.68102900	1.67869400	2.79345500
H	-4.65707900	-2.06993600	3.20274300
H	-6.75713600	-0.75616900	3.30355000
C	4.04754000	-0.45751700	4.26012800
O	2.96459900	-0.94667600	4.65478300
O	4.64195700	0.58875200	4.59597100
O	4.65993800	-1.20266500	3.21228300
Cs	1.64113100	-1.73123200	1.99503700
C	-2.14981100	1.73229800	1.88255600
C	-1.02669300	1.10623100	1.15145200
H	-0.79319000	0.09976100	1.47607700
H	-1.65075100	2.18840700	2.99379200
Cs	1.74285100	1.92820800	4.90730100
I	-3.88868500	0.14798200	-1.47316000
C	-4.62270600	3.20596200	2.07725700
H	-4.40768800	3.40131900	1.01779600
H	-5.62135300	3.60627800	2.29090200
H	-3.88314700	3.75514700	2.67545600
C	-2.23550100	-1.27963900	2.84062900
O	-1.21251800	-0.92981300	3.43633000
C	-2.29671700	-2.69998800	2.33115200
C	-2.90809600	-3.01330600	1.10765700

C	-1.62539200	-3.70648400	3.04578000	Pd	-0.84929300	0.28416900	-0.99036000
C	-2.83912500	-4.31641400	0.60836300	P	1.10516800	-1.10314400	-1.09148900
H	-3.39988400	-2.23230700	0.53274200	C	0.88269700	-2.69720500	-0.23934000
C	-1.58114100	-5.01098400	2.55660200	C	-0.23398500	-3.33773200	0.22959900
H	-1.15408300	-3.44957000	3.99092500	O	1.99134400	-3.48523600	-0.01866500
C	-2.18493200	-5.31612000	1.33091000	C	0.20642300	-4.58458600	0.77104000
H	-3.29405000	-4.54363100	-0.35202200	H	-1.24781100	-2.97362400	0.15349100
H	-1.07857200	-5.78924600	3.12683500	C	1.55740400	-4.61728500	0.59007200
H	-2.14199100	-6.33097800	0.94191600	H	-0.40404300	-5.35239400	1.22508300
H	-2.39671000	2.69684400	1.44095700	H	2.32321100	-5.34017500	0.82977200
C	0.25182700	1.89401100	1.22404600	C	1.77050400	-1.48380900	-2.74024700
O	0.14267200	3.15057900	0.75010900	C	1.29014300	-1.23962000	-3.99936700
O	1.29241400	1.44923400	1.70094200	O	2.97831300	-2.13794800	-2.82364400
C	1.33804900	3.93961200	0.64542600	C	2.25397600	-1.76988900	-4.91152100
H	1.50518800	4.10254900	-0.42418800	H	0.34572400	-0.77045600	-4.23328900
H	2.17805000	3.37119100	1.04867300	C	3.24820400	-2.29964400	-4.14333000
C	1.14444800	5.25271100	1.39252000	H	2.20597700	-1.76200600	-5.99132000
H	0.96305100	5.05940100	2.45777900	H	4.17516300	-2.80486500	-4.37101700
H	2.04158200	5.87735900	1.27991700	C	2.62421700	-0.51951300	-0.24204800
H	0.28779100	5.79806000	0.97507000	C	3.08356800	-0.64846000	1.04091700
C	-1.01168000	4.01465900	4.12443300	O	3.46713600	0.29593600	-0.95177100
O	-0.98262700	2.69678800	4.04853800	C	4.28451500	0.12678000	1.12505000
O	0.04563200	4.60424600	4.60888700	H	2.63421300	-1.24246500	1.82369300
O	-2.03257900	4.66877900	3.72194900	C	4.46877200	0.67303800	-0.10891300
Cs	-0.89168400	7.27424000	3.97626900	H	4.92698000	0.24670000	1.98628600
C	2.95894100	1.88563500	-2.80994000	H	5.22837900	1.30658900	-0.54123700
C	4.11416800	2.26701700	-3.49399200	I	-2.25660500	-1.54202500	-2.51157100
C	5.21694900	1.40962000	-3.54275200	C	-3.41896400	1.95425000	-1.70738700
C	5.15539000	0.16642700	-2.90704000	C	-4.80604200	2.11897000	-1.67457300
C	3.99785000	-0.21357500	-2.22721200	C	-5.53521200	1.64147600	-0.58865300
C	2.89100600	0.64226300	-2.16800600	C	-4.86719800	1.00159300	0.45690500
H	2.09151500	2.53549600	-2.76351200	C	-3.47851500	0.82601400	0.44501700
H	4.15507900	3.23373200	-3.99177300	C	-2.74780000	1.30185400	-0.66777900
H	6.11797800	1.70735000	-4.07501400	H	-2.87610400	2.32039300	-2.56982400
H	6.00975900	-0.50644700	-2.94348600	H	-5.30737200	2.61426000	-2.50221700
H	3.92355800	-1.17728800	-1.73352300	H	-6.61407100	1.76581500	-0.54973800
C	1.64086600	0.20596200	-1.41509700	H	-5.43409300	0.62497300	1.30600200
O	1.62430500	-0.93147600	-0.90766500	C	-2.81804500	0.10971100	1.60125900
O	0.71456400	1.09323600	-1.37813000	H	-1.92593000	0.63728200	1.96237900
TS6' M06/BSII SCF energy in solution: -1712.10747a.u. Solution-phase enthalpy: -1711.617257 a.u. Solution-phase Gibbs energy: -1711.715619 a.u.				H	-3.50881500	0.00549700	2.44478000
				H	-2.49323200	-0.89590600	1.30793200
				C	0.21095300	1.78708300	0.13754700
				C	1.25950600	2.70278800	-0.53041300
				C	-0.75628000	3.68990500	-0.87451500

C	-1.03922300	2.46412400	0.00301200
H	0.47381100	1.28473600	1.06649700
H	-1.69411100	2.58984000	0.85430800
C	0.60531600	4.08559100	-0.22637800
H	1.09561600	4.92880600	-0.72996200
H	0.53025100	4.30530500	0.84427400
C	1.13513300	2.67975000	-2.07095600
H	1.91994200	3.30166600	-2.51709800
H	1.23474700	1.67556100	-2.48808600
C	-0.27921400	3.29550900	-2.30358300
H	-0.23144100	4.19140400	-2.93221600
H	-0.95029600	2.58756500	-2.79093700
H	2.27335300	2.54828800	-0.15875800
H	-1.55373900	4.43535800	-0.85976700