

Electronic Supporting Information

for

**Transition State Modeling in the Rational Design of Catalysts for Asymmetric
Diamination Reactions**

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Gaussian 09, Revision **A.02** and **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, J. A. Montgomery, Jr., 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, J. M. 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.

Table S1. Relative Energies (kcal/mol) for the Stereoselectivity Determining Step for Ligand **I**ⁱ

Transition State	L1		L2	
	ΔH	ΔG	ΔH	ΔG
(I - <i>re</i> - a) ₁	3.2	2.0	4.0	4.2
(I - <i>re</i> - a) ₂	1.4	0.0	2.4	1.8
(I - <i>re</i> - a) ₃	4.2	3.9	4.8	4.3
(I - <i>re</i> - a) ₄	0.0	0.1	0.0	0.0
(I - <i>re</i> - b) ₁	4.9	2.8	6.2	4.3
(I - <i>re</i> - b) ₂	5.3	3.7	7.5	5.7
(I - <i>re</i> - b) ₃	6.1	5.1	9.0	8.5
(I - <i>re</i> - b) ₄	4.0	3.1	- ⁱⁱ	- ⁱⁱ
(I - <i>re</i> - c) ₁	10.6	8.7	10.8	9.0
(I - <i>re</i> - c) ₂	8.4	6.6	8.8	7.3
(I - <i>re</i> - c) ₃	12.0	10.5	12.1	11.5
(I - <i>re</i> - c) ₄	7.9	6.5	7.6	6.1
(I - <i>re</i> - d) ₁	9.4	7.7	10.0	8.9
(I - <i>re</i> - d) ₂	10.1	8.6	10.8	8.5
(I - <i>re</i> - d) ₃	10.4	8.9	10.2	8.0
(I - <i>re</i> - d) ₄	9.1	8.1	9.5	8.7
(I - <i>si</i> - a) ₁	8.9	6.5	9.6	8.2

(I-si-a) ₂	7.4	4.8	8.7	8.1
(I-si-a) ₃	6.1	5.2	6.7	5.7
(I-si-a) ₄	9.6	8.1	10.1	8.5
(I-si-b) ₁	10.1	7.6	11.6	9.6
(I-si-b) ₂	9.9	8.4	12.4	11.4
(I-si-b) ₃	10.6	8.6	12.9	11.8
(I-si-b) ₄	11.2	9.9	13.0	11.1
(I-si-c) ₁	6.0	6.7	6.4	5.4
(I-si-c) ₂	4.0	2.6	5.0	3.8
(I-si-c) ₃	4.9	3.6	5.0	3.3
(I-si-c) ₄	6.0	5.0	7.1	6.2
(I-si-d) ₁	4.7	3.4	4.4	4.0
(I-si-d) ₂	5.0	4.2	5.8	5.0
(I-si-d) ₃	5.2	4.5	4.6	3.6
(I-si-d) ₄	4.0	3.1	4.4	4.0

ⁱ *L1*=B3LYP/LANL2DZ(Pd), 6-31G*, *L2*=M06/LANL2DZ(Pd), 6-31G*. **a**, **b**, **c** and **d** represent the different approach of the diene as shown in Figure S1. Subscript **1**, **2**, **3** and **4** refer to the different conformers of the N,N-tetramethylpiperidine group. ⁱⁱ Transition state could not be optimized even after repeated attempts.

Table S2. Relative Energies (kcal/mol) for the Stereoselectivity Determining Step for Ligand **II** ⁱ

Transition State	L1		L2 ⁱⁱ	
	ΔH	ΔG	ΔH	ΔG
(II-re-a) ₁	6.3	6.4	4.4	5.5
(II-re-a) ₂	0.5	1.1	0.0	0.9
(II-re-a) ₃	0.7	0.8	1.2	2.9
(II-re-a) ₄	0.0	0.0	0.7	0.0
(II-re-b) ₁	7.9	8.1	7.4	7.7
(II-re-b) ₂	5.0	4.3	6.7	7.7
(II-re-b) ₃	2.2	1.7	4.2	4.2
(II-re-b) ₄	2.2	1.9	5.1	5.8
(II-re-c) ₁	14.1	13.4	-	-
(II-re-c) ₂	- ⁱⁱⁱ	- ⁱⁱⁱ	-	-
(II-re-c) ₃	7.9	6.7	-	-
(II-re-c) ₄	7.6	6.4	-	-
(II-re-d) ₁	12.6	12.3	-	-
(II-re-d) ₂	12.1	11.2	-	-
(II-re-d) ₃	7.3	6.9	-	-
(II-re-d) ₄	6.0	5.1	-	-

(II- <i>si</i> -a) ₁	12.4	12.0	-	-
(II- <i>si</i> -a) ₂	6.8	6.8	-	-
(II- <i>si</i> -a) ₃	6.8	6.1	-	-
(II- <i>si</i> -a) ₄	6.0	5.6	-	-
(II- <i>si</i> -b) ₁	12.8	12.5	-	-
(II- <i>si</i> -b) ₂	8.8	8.9	-	-
(II- <i>si</i> -b) ₃	6.6	6.1	-	-
(II- <i>si</i> -b) ₄	ⁱⁱⁱ	ⁱⁱⁱ	-	-
(II- <i>si</i> -c) ₁	9.2	9.7	7.6	9.0
(II- <i>si</i> -c) ₂	3.7	4.3	4.7	4.6
(II- <i>si</i> -c) ₃	3.9	2.9	4.5	5.0
(II- <i>si</i> -c) ₄	3.2	3.2	6.0	5.7
(II- <i>si</i> -d) ₁	7.6	7.6	5.9	7.2
(II- <i>si</i> -d) ₂	2.2	2.1	2.1	2.9
(II- <i>si</i> -d) ₃	2.1	2.5	1.6	1.9
(II- <i>si</i> -d) ₄	0.8	0.6	1.9	2.6

ⁱ *L1*=B3LYP/LANL2DZ(Pd), 6-31G*, *L2*=M06/LANL2DZ(Pd), 6-31G*. **a**, **b**, **c** and **d** represent the different approach of the diene as shown in Figure S1. Subscript **1**, **2**, **3** and **4** refer to the different conformers of the isopropyl group. ⁱⁱ Calculations done only for the lowest energy transition states. ⁱⁱⁱ Transition state could not be optimized even after repeated attempts.

Table S3. Relative Energies (kcal/mol) for the Stereoselectivity Determining Step for Ligand **III**ⁱ

Transition State	<i>L1</i>		<i>L2</i>	
	ΔH	ΔG	ΔH	ΔG
III-re-a	0.0	0.0	0.0	0.0
III-re-b	1.1	0.2	2.6	2.9
III-re-c	7.8	6.4	7.2	6.2
III-re-d	5.8	5.2	6.1	6.7
III-si-a	5.6	4.6	6.0	6.0
III-si-b	6.1	5.2	7.0	7.2
III-si-c	3.0	2.8	3.0	4.3
III-si-d	0.5	0.4	1.8	2.8

ⁱ *L1*=B3LYP/LANL2DZ(Pd), 6-31G*, *L2*=M06/LANL2DZ(Pd), 6-31G*. **a**, **b**, **c** and **d** represent the different approach of the diene as shown in Figure S1.

For catalysts V - XXIX only the lowest energy modes are optimized. The lowest energy mode for *re* face is **a** mode as shown in Figure S1 and for the *si* face it is **d** mode. For some catalysts additional optimizations involving the **b** mode for *re* face and **c** mode for *si* face are also carried out. Unless specified, the TSs for *re* and *si* faces belong to **a** and **d** modes respectively.

Table S4. Relative Energies (kcal/mol) for the Stereoselectivity Determining Step for Ligand **IV**ⁱ

Transition State	<i>L1</i>		<i>L2</i>	
	ΔH	ΔG	ΔH	ΔG
(IV- <i>re</i>) ₁	0.0	0.0	0.0	0.0
(IV- <i>re</i>) ₂	4.2	5.0	-0.4	-0.5
(IV- <i>re</i>) ₃	6.2	7.2	0.1	1.6
(IV- <i>re</i>) ₄	2.6	4.0	-2.4	-1.2
(IV- <i>si</i>) ₁	4.5	5.9	-0.3	0.0
(IV- <i>si</i>) ₂	11.1	11.7	4.5	4.6
(IV- <i>si</i>) ₃	6.8	7.9	3.3	4.1
(IV- <i>si</i>) ₄	1.6	2.9	0.8	0.4

ⁱ *L1*=B3LYP/LANL2DZ(Pd), 6-31G*, *L2*=M06/LANL2DZ(Pd), 6-31G*. Only the lowest energy modes, i.e. **a** mode for *re* face and **d** mode for *si* face are optimized. Subscript **1**, **2**, **3** and **4** refer to the different conformers of the amido substituent.

Table S5. Relative Energies (kcal/mol) of TSs for Catalysts **V-XXVII** at the B3LYP/LANL2DZ(Pd), 6-31G* Level of Theory ^a

Catalyst	Transition State	ΔH	ΔG	Calculated % <i>ee</i>
				B3LYP
V	V-<i>re</i>	0.0	0.0	33
	V-<i>re</i>-b	3.5	4.1	
	V-<i>si</i>-c	0.2	0.4	
	V-<i>si</i>	0.1	0.7	
VI	VI-<i>re</i>	0.0	0.0	-17

	VI-<i>si</i>	-0.9	-0.2	
	VI-<i>si-c</i>	0.5	0.5	
VII	VII-<i>re</i>	0.0	0.0	73
	VII-<i>re-b</i>	5.2	4.1	
	VII-<i>si</i>	0.5	1.1	
	VII-<i>si-c</i>	1.4	1.1	
VIII	VIII-<i>re</i>	0.0	0.0	-92
	VIII-<i>re-b</i>	1.7	1.3	
	VIII-<i>si</i>	0.0	0.1	
	VIII-<i>si-c</i>	-0.2	-1.8	
IX	(IX-<i>re</i>)	0.0	0.0	64
	(IX-<i>re</i>)₁	2.9	2.4	
	(IX-<i>re</i>)₂	6.4	6.7	
	(IX-<i>re</i>)₃	1.6	1.0	
	(IX-<i>si</i>)	0.6	1.7	
	(IX-<i>si</i>)₁	2.0	3.1	
	(IX-<i>si</i>)₂	8.0	8.9	
	(IX-<i>si</i>)₃	4.3	5.3	
	(IX-<i>si-c</i>)	0.4	0.9	
X	X-<i>re</i>	0.0	0.0	64
	(X-<i>re</i>)₁	-0.1	0.1	
	(X-<i>re</i>)₂	1.8	2.5	
	(X-<i>re</i>)₃	3.0	3.6	
	X-<i>si</i>	1.3	3.4	
	(X-<i>si</i>)₁	5.3	6.1	
	(X-<i>si</i>)₂	10.8	11.7	
	(X-<i>si</i>)₃	2.7	4.4	
	(X-<i>si-c</i>)	1.3	0.9	
XI	XI-<i>re</i>	0.0	0.0	>99
	XI-<i>si</i>	3.4	5.4	

	XI-<i>si-c</i>	3.5	5.0	
XII	XII-<i>re</i>	0.0	0.0	83
	XII-<i>si</i>	0.8	1.4	
	XII-<i>si-c</i>	1.0	1.8	
XIII	XIII-<i>re</i>	0.0	0.0	83
	XIII-<i>si</i>	0.0	2.4	
XIV	XIII-<i>re</i>	1.6	0.7	92
	(XIV-<i>re</i>)₁	6.1	5.7	
	(XIV-<i>re</i>)₂	0.0	0.0	
	(XIV-<i>re</i>)₃	3.3	2.9	
	XIV-<i>si</i>	3.9	3.1	
	(XIV-<i>si</i>)₁	6.2	6.1	
	(XIV-<i>si</i>)₂	3.4	3.3	
	(XIV-<i>re</i>)₃	3.0	2.7	
	XIV-<i>si-c</i>	2.6	2.9	
	(XIV-<i>si-c</i>)₁	2.7	1.9	
	(XIV-<i>si-c</i>)₂	6.3	5.6	
	(XIV-<i>si-c</i>)₃	4.4	3.8	
XV	XV-<i>re</i>	-0.6	0.9	>99
	(XV-<i>re</i>)₁	0.0	0.0	
	XV-<i>si-c</i>	4.9	6.0	
XVI	XVI-<i>re</i>	0.0	0.0	40
	(XVI-<i>re</i>)₁	2.0	2.2	
	XVI-<i>si</i>	1.2	1.1	
	(XVI-<i>si</i>)₁	2.3	2.0	
	XVI-<i>si-c</i>	-0.2	0.5	
	(XVI-<i>si-c</i>)₁	1.6	1.6	
XVII	XVII-<i>re</i>	-1.6	0.5	98
	(XVII-<i>re</i>)₁	0.0	0.0	
	XVII-<i>si</i>	3.6	4.6	

	(XVII- <i>si</i>) ₁	4.8	4.6	
	XVII- <i>si-c</i>	1.0	2.7	
	(XVII- <i>si-c</i>) ₁	2.5	3.9	
XVIII	XVIII- <i>re</i>	0.0	0.0	25
	XVIII- <i>si</i>	-0.5	0.3	
XIX	XIX- <i>re</i>	0.0	0.0	47
	XIX- <i>re-b</i>	4.3	2.4	
	XIX- <i>si</i>	0.4	0.6	
	XIX- <i>si-d</i>	3.1	3.4	
XX	XX- <i>re</i>	0.0	0.0	80
	(XX- <i>re</i>) ₁	5.1	5.1	
	(XX- <i>re</i>) ₂	1.0	1.2	
	(XX- <i>re</i>) ₃	3.9	3.4	
	XX- <i>si-c</i>	7.2	6.4	
	(XX- <i>si-c</i>) ₁	6.1	5.9	
	(XX- <i>si-c</i>) ₂	5.4	4.6	
	XX- <i>si</i>	1.8	1.5	
	(XX- <i>si</i>) ₁	1.9	1.3	
XXI	XXI- <i>re</i>	0.0	0.0	83
	(XXI- <i>re</i>) ₁	0.5	1.0	
	(XXI- <i>re</i>) ₂	0.6	0.4	
	XXI- <i>si</i>	1.5	1.4	
	(XXI- <i>si</i>) ₁	2.6	3.0	
	(XXI- <i>si</i>) ₂	4.9	4.9	
XXII	XXII- <i>re</i>	0.0	0.0	89
	(XXII- <i>re</i>) ₁	1.6	2.4	
	(XXII- <i>re</i>) ₂	3.5	4.1	
	(XXII- <i>re</i>) ₃	0.8	1.2	
	XXII- <i>si</i>	2.4	1.7	
	(XXII- <i>si</i>) ₁	2.7	2.7	

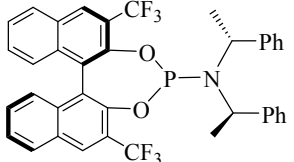
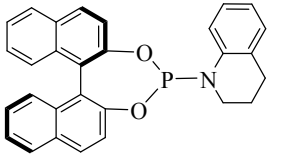
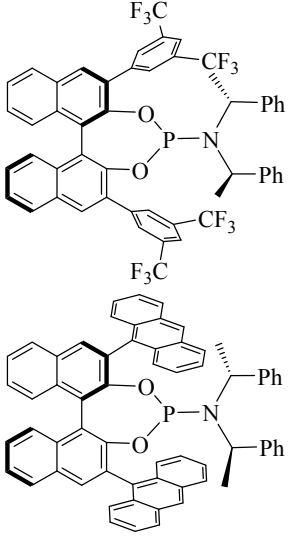
	(XXII- <i>si</i>) ₂	4.7	5.2	
	(XXII- <i>si</i>) ₃	5.2	5.7	
	XXII- <i>re-b</i>	3.0	2.5	
	(XXII- <i>re-b</i>) ₁	4.9	5.3	
	XXII- <i>si-c</i>	5.1	5.1	
XXIII	XXV- <i>re</i>	0.0	0.0	69
	XXIII- <i>re-b</i>	1.0	1.0	
	XXIII- <i>si</i>	0.9	1.0	
	XXIII- <i>si-c</i>	2.0	1.0	
XXIV	XXIV- <i>re</i>	0.0	0.0	83
	XXIV- <i>si</i>	0.7	1.4	
XXV	XXV- <i>re</i>	0.0	0.0	87
	XXV- <i>si</i>	1.3	1.6	
XXVI	XXVI- <i>re</i>	0.0	0.0	95
	(XXVI- <i>re</i>) ₁	4.3	4.0	
	(XXVI- <i>re</i>) ₂	1.0	0.6	
	(XXVI- <i>re</i>) ₃	1.1	1.8	
	(XXVI- <i>re</i>) ₄	1.8	2.3	
	(XXVI- <i>re</i>) ₅	0.7	1.2	
	(XXVI- <i>re</i>) ₆	7.4	7.6	
	(XXVI- <i>re</i>) ₇	2.3	2.2	
	XXVI- <i>si</i>	1.4	2.2	
	(XXVI- <i>si</i>) ₁	3.0	3.3	
	(XXVI- <i>si</i>) ₂	8.2	8.5	
	(XXVI- <i>si</i>) ₃	5.0	5.7	
	(XXVI- <i>si</i>) ₄	4.4	3.5	
	(XXVI- <i>si</i>) ₅	2.7	3.2	
	(XXVI- <i>si</i>) ₆	2.1	2.4	
	(XXVI- <i>si</i>) ₇	8.2	8.1	
XXVII	XXVII- <i>re</i>	0.0	0.0	99

	(XXVII- <i>re</i>) ₁	3.0	2.9	
	(XXVII- <i>re</i>) ₂	2.9	2.4	
	XXVII- <i>si</i>	2.8	2.9	
	(XXVII- <i>si</i>) ₁	5.1	5.1	

^a The *re* and *si* TSs belong to **a** and **d** modes respectively unless specified. For each catalyst the numerical subscripts refer to different conformations of the substituent at the amido part.

Table S6. Calculated %*ee* for Catalysts **V-XXVII** at Different Levels of Theory^a

Catalyst	Calculated % <i>ee</i>		
	M06//B3LYP	SMD _(Benzene) /M06//B3LYP	B3LYP-D//B3LYP
V	8	8	-8
VI	-99	-97	-99
VII	-53	-77	-59
VIII	-64	-64	-69
IX	85	91	40
X	>99	98	93
XI	96	97	98
XII	83	59	97
XIII	99	99	69
XIV	99	98	80
XV	>99	>99	>99
XVI	8	8	-53
XVII	99	98	92
XVIII	-40	-40	-53
XIX	17	25	-33
XX	69	59	73
XXI	89	80	77
XXII	94	91	97
XXIII	83	83	25
XXIV	93	91	83

	2,3-Rearrangement of Amine N-oxides	H. Bao, X. Qi and U. K. Tambar, <i>J. Am. Chem. Soc.</i> , 2011, 133 , 1206.
	Iridium Catalyzed allylic alkylation	W.-B. Liu, C. Zheng, C.-X. Zhuo, L.-X. Dai and S.-L. You, <i>J. Am. Chem. Soc.</i> , 2012, 134 , 4812.
	Synthesis of 3,4-Substitued Pyrrolidines	A. Z. González, D. Benitez, E. Tkatchouk, W. A. Goddard III and F. D. Toste, <i>J. Am. Chem. Soc.</i> , 2011, 133 , 5500.

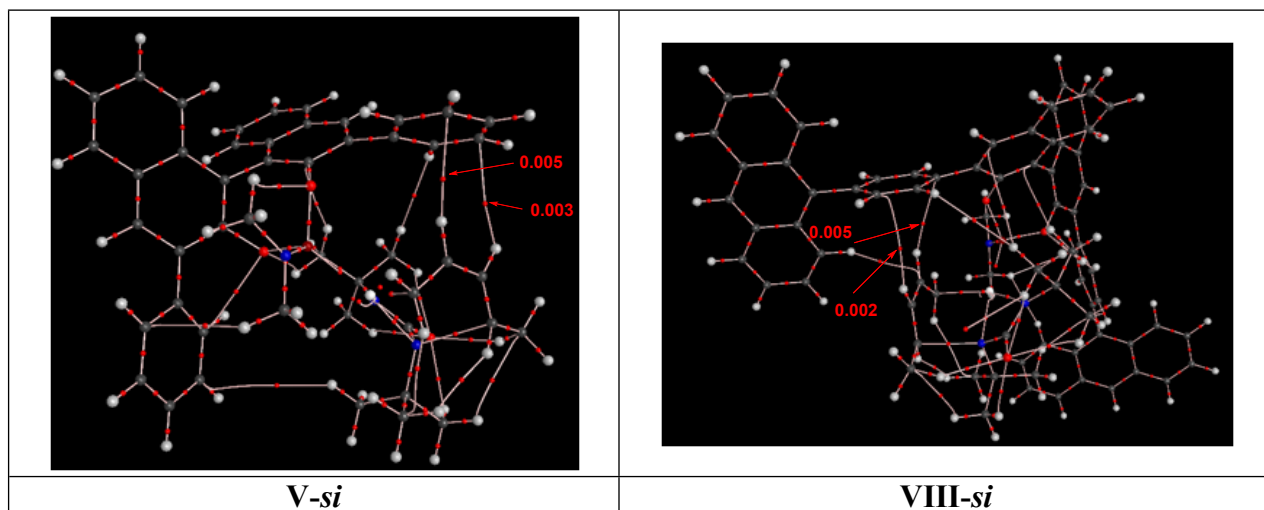


Figure S1. AIM analyses depicting the bond paths as well as bond critical points for TSs **V-*si*** and **VIII-*si***. The ρ_{bcp} values for the C-H $\cdots$ π interactions are provided in atomic units.

Distortion-Interaction Analysis

In the higher energy TS **X-*si***, increased distortion in the reactants is noticed. This results in destabilization with respect to the diastereomeric lower energy TS **X-*re***. The *Distortion-Interaction* model is applied to examine the origin of the energy difference between the stereodetermining TSs, **X-*re*** and **X-*si***. In distortion-interaction model, the activation barrier ($\Delta E^\ddagger$) is considered as arising due to the destabilizing distortion in the reacting partners ($\Delta E^\ddagger_d$) upon going from their respective ground state geometries to that in the transition states and the stabilizing interaction energy between these distorted fragments ($\Delta E^\ddagger_i$) in the TS geometry. It is found that the higher energy TS **X-*si*** exhibits 2.4 kcal/mol higher distortion energy ($\Delta E^\ddagger_d$) and 1.6 kcal/mol lower interaction energy ($\Delta E^\ddagger_i$) than the corresponding values in **X-*re***. Thus both distortion and interaction contribute to the stabilization of the lower energy of TS **X-*re*** (by 4.0 kcal/mol)

Optimized Geometries of Coordinates at the B3LYP Level of Theory for Catalysts IV-XXVII. Electronic energies, enthalpies, Gibbs free energies (in a.u.), and the imaginary frequency (in cm⁻¹) representing the reaction coordinate are provided.

(IV-*re*)₁

E0 = -2797.065371
 E0+ZPE = -2796.112492
 E298 = -2796.057038
 H298 = -2796.056094
 G298 = -2796.202668
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 C 3.132564 -3.168635 0.142434
 C 4.040909 -3.659172 -0.837684
 C 4.384028 -4.992600 -0.889757
 C 3.843565 -5.915277 0.036238
 C 2.743034 -1.782190 0.221761
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 C 1.148006 -2.377550 1.992492
 C 1.576691 -3.681268 1.984678
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 C 2.549483 0.068710 -1.427960
 C 3.078684 0.963356 -2.387857
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 C 7.571932 -0.004008 -0.812302
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 C -0.710939 3.382724 -3.885310
 C -0.975905 4.749537 -4.003627
 C -1.237138 5.493844 -2.854686
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 C -1.299034 -2.599337 -1.792177

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 H 4.128741 -6.962485 -0.011444
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 H 5.298527 -1.799885 0.981224
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 H 2.285962 1.937608 0.635471
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 H 3.026067 4.081173 -0.190474
 H 2.055161 3.276103 -1.430495
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 H -1.441462 5.485023 -0.722428

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 H -1.452354 6.556634 -2.930066
 H -0.985397 5.224859 -4.980753
 H 1.987659 5.346620 1.494524
 H 1.053805 1.407065 2.935340
 H 1.990035 6.194086 3.796202
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 H 1.514995 4.663967 5.702443
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 H -1.481697 3.099306 1.983269
 H -0.811613 4.544700 1.229707
 H -2.467172 4.039773 0.848415

(IV-re)₂

E0 = -2797.058633
 E0+ZPE = -2796.105637
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 H298 = -2796.049338
 G298 = -2796.194658
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 C -2.075677 4.757745 -1.722305
 C -3.216950 5.462176 -1.329593
 C -4.153296 4.857749 -0.490081
 C -3.944142 3.546122 -0.055290
 C -0.627088 2.687042 -1.784654
 C -1.053995 1.714050 -2.903405
 N 0.221523 2.070550 -0.714654
 C 1.227809 2.949592 0.003334
 C 0.767716 3.457276 1.372352
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 C -0.572151 4.908590 2.792479
 C 0.086222 4.434126 3.928793
 C 1.090400 3.475973 3.788144
 C 1.424646 2.994366 2.520936
 P 0.282084 0.387551 -0.562294
 Pd -1.638643 -0.972187 -0.616652
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 H -1.353996 5.657605 2.887912
 H 1.614716 3.100268 4.663084
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 H 0.016710 3.418868 -2.277171
 H -0.194326 1.199782 -3.344262
 H -1.765346 0.960716 -2.552200
 H -1.548009 2.297531 -3.687417

(IV-*re*)₃

E0+ZPE = -2796.102651
 E298 = -2796.047212
 H298 = -2796.046268
 G298 = -2796.191175
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 C -2.333520 6.274525 -0.215778
 C -3.419173 5.758147 0.492132
 C -3.491161 4.384584 0.740559
 C -0.307845 3.116241 -0.980886
 C -0.835951 2.414174 -2.244572
 N 0.269817 2.222221 0.077578
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 C 3.520673 2.379277 1.222405
 C 4.866900 2.661147 0.990032
 C 5.237637 3.821671 0.306373
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 H -1.712194 1.792970 -2.035582
 H -1.139168 3.190815 -2.954549

(IV-*re*)₄

E0 = -2797.0612882
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 E298 = -2796.052942
 H298 = -2796.051998
 G298 = -2796.196311
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 C -1.713468 -1.892149 -2.024553
 C -2.891158 -2.638263 -1.897497
 C -4.169722 -2.153762 -2.180634
 C -5.392890 -2.969560 -1.871078
 C -4.419805 1.451456 -2.604199
 C -6.461713 0.358712 -1.648972
 C -3.545997 -0.512161 2.771624
 C -2.291725 0.116276 3.388888
 C -4.785523 0.178169 3.384691
 C -3.582807 -2.023989 3.086128
 H -5.047467 2.278588 -2.955579
 H -3.414615 1.844039 -2.419362
 H -4.363431 0.720720 -3.418458
 H -7.073220 1.210215 -1.972148
 H -6.456136 -0.374456 -2.462014
 H -6.918727 -0.100957 -0.771854
 H -5.682177 2.821250 -0.681526
 H -5.645991 1.630312 0.631015
 H -4.130573 2.322666 0.025783
 H -3.565514 -2.196566 4.169986
 H -4.490095 -2.471444 2.673105
 H -2.717990 -2.527710 2.639912
 H -4.791961 0.049517 4.474515
 H -4.766640 1.253384 3.170542

H -5.704581 -0.244043 2.973841
 H -2.257833 -0.075712 4.467899
 H -1.380589 -0.283766 2.936655
 H -2.290105 1.201083 3.239462
 H -2.375369 -0.087575 -3.012408
 H -0.797262 -2.382584 -1.696513
 H -4.272656 -1.382345 -2.931946
 H -5.119533 -3.999751 -1.617224
 H -5.915224 -2.544225 -1.006138
 H -2.815935 -3.599721 -1.392985
 H -0.588025 -0.179072 -2.646255
 H -6.087983 -2.987727 -2.718976
 H -0.425465 -2.223562 2.658284
 H -0.343990 -4.673607 2.248760
 H 0.446535 -6.563830 0.905519
 H 3.171593 -5.905339 -2.355521
 H 3.262318 -3.514160 -1.828646
 H 1.793449 -7.458959 -0.971956
 H 5.248417 1.166643 -2.426992
 H 4.324392 -3.201404 0.890672
 H 7.193841 -0.180350 -1.815094
 H 8.204959 -2.057091 -0.550380
 H 6.747804 -3.539565 0.832393
 H 2.814552 1.642965 -2.222179
 H 1.112075 3.633544 1.861060
 H 1.121464 0.988307 3.390902
 H 1.633591 2.570093 4.008372
 H -0.057427 2.293947 3.537593
 H 0.395698 2.675908 -2.172410
 H -0.091715 5.758266 0.783818
 H 1.537745 4.286137 -3.661651
 H 1.071437 7.355842 -0.684789
 H 1.898687 6.635689 -2.918062
 H 3.131359 0.540075 2.490710
 H 2.824641 4.336694 0.500466
 H 5.563083 0.532985 2.104392
 H 5.261019 4.331834 0.109868
 H 6.653117 2.432247 0.926789
 H -1.293202 2.493083 -0.370389
 H -2.127464 2.864123 1.842061
 H -0.985423 4.180731 2.166497
 H -2.229269 4.377089 0.924904

(IV-si)₁

E0+ZPE = -2796.105424
 E298 = -2796.049911
 H298 = -2796.048967
 G298 = -2796.193242
 NImag = 1, (-183.0384
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 C -0.495516 -4.157806 -0.565752
 C -0.913111 -3.658657 -1.810445
 C -1.615857 -4.458706 -2.709560
 C -1.925622 -5.781234 -2.379047
 C -1.517720 -6.291701 -1.147929
 C 0.294774 -3.245527 0.379546

C 1.042693 -3.997872 1.487896
 N -0.546221 -2.121925 0.908760
 C -1.622202 -2.527359 1.880237
 C -3.068426 -2.218086 1.488679
 C -3.744109 -1.075833 1.939632
 C -5.104538 -0.901228 1.680573
 C -5.815069 -1.866362 0.965571
 C -5.152829 -3.003572 0.501180
 C -3.793453 -3.175798 0.763050
 P -0.138478 -0.601122 0.312436
 Pd 2.074632 -0.070746 -0.333739
 N 3.533202 -0.098948 1.261585
 C 4.562182 0.197865 0.461521
 O 5.785434 0.128752 0.651880
 O -1.095204 -0.191891 -1.008293
 C -2.387026 0.300359 -1.009501
 C -2.702866 1.507651 -0.399693
 C -4.083249 1.928901 -0.423500
 C -5.033626 1.195531 -1.208301
 C -4.613637 0.024486 -1.892602
 C -3.328331 -0.433282 -1.768815
 C -4.567009 3.030069 0.337676
 C -5.891727 3.408450 0.289525
 C -6.812766 2.712549 -0.527390
 C -6.386520 1.625321 -1.255435
 C -1.648048 2.316361 0.269925
 C -1.444176 3.713548 -0.033212
 C -0.505396 4.477176 0.738358
 C 0.247213 3.833751 1.755743
 C 0.128535 2.482236 1.961278
 C -0.800317 1.736776 1.202988
 C -2.104818 4.369984 -1.109558
 C -1.886240 5.704094 -1.375741
 C -0.998212 6.464098 -0.579252
 C -0.320280 5.856783 0.452110
 O -0.864198 0.362373 1.457725
 C -1.283436 -2.093507 3.316029
 N 3.998516 0.658418 -0.802042
 C 4.218927 2.144155 -0.987323
 C 3.290769 2.678540 -2.091008
 C 1.682006 -0.356145 -2.507704
 C 2.435014 -1.555809 -2.477570
 C 3.829176 -1.703351 -2.470850
 C 4.740930 -0.654788 -2.559961
 C 6.213810 -0.888866 -2.382449
 C 3.926408 2.934246 0.308859
 C 5.686268 2.410900 -1.399489
 C 3.741193 -0.514392 2.665086
 C 2.374482 -0.644037 3.346750
 C 4.473954 -1.874182 2.701820
 C 4.569850 0.540772 3.432147
 H 4.029920 4.007540 0.109213
 H 2.909866 2.746943 0.665882
 H 4.628760 2.669145 1.103672
 H 5.843523 3.492495 -1.493869
 H 6.374861 2.011968 -0.653436

H 5.918273 1.956405 -2.367880
 H 3.464471 3.752427 -2.225409
 H 2.237447 2.537125 -1.829208
 H 4.691730 0.239678 4.480300
 H 5.557472 0.656580 2.981322
 H 4.060267 1.511368 3.415145
 H 4.616151 -2.211196 3.736733
 H 3.897308 -2.638138 2.168040
 H 5.452217 -1.785241 2.223290
 H 2.489751 -1.034037 4.365066
 H 1.877221 0.329169 3.413726
 H 1.716159 -1.315928 2.790761
 H 2.139179 0.535629 -2.918768
 H 1.865695 -2.477949 -2.356718
 H 4.443712 0.244358 -3.082710
 H 6.441829 -1.960542 -2.388585
 H 6.796495 -0.399572 -3.172156
 H 4.219375 -2.690281 -2.227685
 H 0.614549 -0.430967 -2.686549
 H 6.541748 -0.487111 -1.416098
 H 0.728977 1.963237 2.698502
 H 0.947572 4.418553 2.346102
 H 0.385198 6.420214 1.058050
 H -2.397645 6.174944 -2.210901
 H -2.779769 3.803100 -1.739277
 H -0.841991 7.517551 -0.794188
 H -5.337449 -0.527345 -2.486555
 H -3.881371 3.572631 0.977680
 H -7.086143 1.062595 -1.869253
 H -7.851973 3.027328 -0.565431
 H -6.231395 4.248479 0.889493
 H -3.004039 -1.353604 -2.241669
 H -1.564225 -3.618631 1.863286
 H -1.265804 -1.007926 3.423250
 H -2.028996 -2.499361 4.008857
 H -0.299723 -2.474040 3.604957
 H -0.692980 -2.627753 -2.072643
 H -0.484248 -5.915136 0.692706
 H -1.918834 -4.051757 -3.670878
 H -1.746206 -7.320024 -0.880345
 H -2.473150 -6.407183 -3.078375
 H -3.209283 -0.318596 2.501864
 H -3.291083 -4.073779 0.413616
 H -5.608365 -0.007536 2.037964
 H -5.695127 -3.764893 -0.053938
 H -6.876099 -1.731373 0.772583
 H 3.478957 2.198210 -3.057607
 H 1.070310 -2.759655 -0.223216
 H 0.376393 -4.489565 2.203760
 H 1.679837 -4.769868 1.043329
 H 1.682518 -3.307605 2.039750

(IV-si)₂

E0 = -2797.0473473

E0+ZPE = -2796.095125

E298 = -2796.039410

H298 = -2796.038465
 G298 = -2796.184065
 NImag = 1, (-178.2071)
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 C -1.217735 4.262770 -0.494313
 C -1.117165 5.652717 -0.358731
 C -2.199685 6.412160 0.093169
 C -3.403109 5.785743 0.415509
 C -3.515874 4.398626 0.283694
 C -0.032622 3.466385 -1.039645
 C -0.330351 2.926455 -2.444296
 N 0.502262 2.447030 -0.085219
 C 1.249510 3.087608 1.065600
 C 2.751417 2.799175 1.109133
 C 3.348083 2.032921 2.118053
 C 4.734940 1.884787 2.181790
 C 5.554210 2.501439 1.236062
 C 4.973915 3.266307 0.222649
 C 3.588594 3.413856 0.166215
 P 0.115538 0.796421 -0.255622
 Pd -1.965689 -0.400687 -0.521576
 N -3.295332 -0.479345 1.180960
 C -4.136517 -1.361087 0.634225
 O -5.256353 -1.749428 0.999952
 O 1.031204 0.156709 -1.509878
 C 2.415410 0.090153 -1.515515
 C 3.089431 -0.734093 -0.625158
 C 4.531322 -0.712618 -0.650712
 C 5.209924 0.026144 -1.676684
 C 4.449852 0.758396 -2.625463
 C 3.082964 0.812180 -2.531266
 C 5.329069 -1.367121 0.329318
 C 6.705339 -1.326810 0.275982
 C 7.368536 -0.631937 -0.762341
 C 6.630126 0.033113 -1.713766
 C 2.329541 -1.600133 0.320464
 C 2.564895 -3.021192 0.407509
 C 1.915737 -3.785975 1.433933
 C 1.011975 -3.139609 2.317025
 C 0.706193 -1.811634 2.153715
 C 1.347705 -1.063263 1.142028
 C 3.390974 -3.720713 -0.516999
 C 3.594618 -5.078921 -0.408194
 C 2.989983 -5.819264 0.634566
 C 2.164596 -5.181813 1.531560
 O 1.009005 0.283742 1.048007
 C 0.539939 2.947407 2.416947
 N -3.500178 -1.858727 -0.576756
 C -3.143256 -3.323927 -0.449909
 C -2.123750 -3.704661 -1.536440
 C -1.871297 -0.466506 -2.752244
 C -3.039182 0.330298 -2.819073
 C -4.377042 -0.056477 -2.651172
 C -4.811357 -1.358275 -2.431733
 C -6.244646 -1.654190 -2.095121
 C -2.523598 -3.643529 0.928014

C -4.408277 -4.197015 -0.627773
 C -3.557939 0.128477 2.500599
 C -2.386084 1.054005 2.833729
 C -4.861553 0.956624 2.448137
 C -3.674975 -0.960773 3.588625
 H -2.221370 -4.697241 0.955372
 H -1.638902 -3.029698 1.113714
 H -3.242396 -3.475666 1.734495
 H -4.134459 -5.252141 -0.504567
 H -5.164671 -3.933252 0.112234
 H -4.839442 -4.082084 -1.627118
 H -1.866620 -4.765845 -1.440648
 H -1.201869 -3.122794 -1.438823
 H -3.854762 -0.506206 4.570919
 H -4.500885 -1.639104 3.361177
 H -2.748537 -1.544431 3.648184
 H -5.036452 1.456914 3.409276
 H -4.790273 1.725511 1.670079
 H -5.712781 0.311531 2.221086
 H -2.520306 1.513698 3.820071
 H -1.444396 0.496118 2.837555
 H -2.300145 1.852265 2.091094
 H -1.950480 -1.531619 -2.933715
 H -2.888430 1.403860 -2.926497
 H -4.212642 -2.175789 -2.810373
 H -6.875236 -0.775358 -2.269921
 H -6.633117 -2.490994 -2.687715
 H -5.106228 0.743460 -2.533479
 H -0.937134 -0.028852 -3.088542
 H -6.332769 -1.917508 -1.033911
 H -0.020363 -1.313808 2.785816
 H 0.532868 -3.719681 3.101217
 H 1.672661 -5.740436 2.324265
 H 4.221674 -5.587216 -1.135651
 H 3.853942 -3.173695 -1.329409
 H 3.165905 -6.888437 0.713963
 H 4.968338 1.298067 -3.413974
 H 4.841639 -1.894895 1.140135
 H 7.123895 0.588763 -2.507713
 H 8.454368 -0.615890 -0.798620
 H 7.286843 -1.830795 1.043367
 H 2.489281 1.381697 -3.238048
 H 1.176487 4.151534 0.820835
 H 0.505998 1.917185 2.771826
 H 1.062744 3.553221 3.165663
 H -0.485091 3.316333 2.334232
 H -0.182610 6.149549 -0.612994
 H -2.534657 2.564345 -0.256305
 H -2.098999 7.489609 0.194362
 H -4.448734 3.901587 0.535364
 H -4.247672 6.371047 0.768905
 H 2.729836 1.548618 2.866036
 H 3.151516 4.029111 -0.617428
 H 5.174657 1.285560 2.974678
 H 5.599992 3.756062 -0.518629
 H 6.632956 2.383523 1.284618

H -2.524688 -3.558939 -2.545742
H 0.789566 4.179643 -1.172018
H -1.139969 2.197299 -2.443193
H -0.640899 3.762131 -3.079659
H 0.554414 2.462440 -2.886088

(IV-si)₃

E0 = -2797.0545888
E0+ZPE = -2796.101656
E298 = -2796.046173
H298 = -2796.045229
G298 = -2796.190011
NImag = 1, (-189.1060)
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C -1.937357 3.335345 -0.951270
C -2.184425 4.429521 -0.107089
C -3.473396 4.715575 0.342881
C -4.548000 3.916598 -0.051640
C -4.317395 2.826666 -0.891231
C -0.523546 3.126208 -1.502484
C -0.500138 2.672653 -2.971170
N 0.409877 2.310570 -0.652540
C 1.612555 3.062823 -0.140444
C 1.206049 4.091513 0.919481
C 1.362117 5.471728 0.739126
C 0.988223 6.374248 1.740921
C 0.458464 5.908030 2.942838
C 0.308105 4.531754 3.138819
C 0.678159 3.636385 2.138063
P 0.259522 0.630882 -0.532732
Pd -1.608332 -0.844184 -0.618422
N -2.932450 -0.776964 1.061755
C -3.644140 -1.851878 0.708908
O -4.699841 -2.313332 1.164733
O 1.317615 -0.132193 -1.610238
C 2.693471 -0.021145 -1.601806
C 3.449417 -0.503770 -0.541057
C 4.868798 -0.246295 -0.557282
C 5.472791 0.326738 -1.726430
C 4.654196 0.661369 -2.837717
C 3.291307 0.517825 -2.767052
C 5.707471 -0.502215 0.563732
C 7.059490 -0.239796 0.519430
C 7.656079 0.286349 -0.650208
C 6.873205 0.565282 -1.746734
C 2.797197 -1.270556 0.557269
C 3.256046 -2.584969 0.938911
C 2.677738 -3.231153 2.082598
C 1.630825 -2.585807 2.791475
C 1.128418 -1.385523 2.356187
C 1.699049 -0.753279 1.228882
C 4.240553 -3.301856 0.202074
C 4.654957 -4.556087 0.594208
C 4.114488 -5.168116 1.749039
C 3.142314 -4.516380 2.471772
O 1.164264 0.477075 0.866488

C 2.479477 3.643836 -1.266473
 N -2.931478 -2.478566 -0.399058
 C -2.407828 -3.844673 -0.000838
 C -1.326339 -4.308687 -0.990983
 C -1.344155 -1.372960 -2.783831
 C -2.584968 -0.771208 -3.091792
 C -3.882225 -1.253771 -2.857711
 C -4.193707 -2.505818 -2.337612
 C -5.604412 -2.865507 -1.966446
 C -1.779441 -3.824221 1.409796
 C -3.559185 -4.879133 -0.006026
 C -3.226160 0.002750 2.282379
 C -2.227848 1.162988 2.363616
 C -4.659998 0.574477 2.213397
 C -3.086091 -0.888759 3.534709
 H -1.356834 -4.811079 1.633561
 H -0.974788 -3.087215 1.469739
 H -2.525143 -3.593715 2.174728
 H -3.166513 -5.852045 0.314323
 H -4.355002 -4.571074 0.672736
 H -3.982015 -5.008089 -1.007405
 H -0.964029 -5.299086 -0.692396
 H -0.471672 -3.625050 -0.996931
 H -3.282323 -0.308021 4.444695
 H -3.797116 -1.718427 3.493612
 H -2.072715 -1.301324 3.605576
 H -4.858424 1.198074 3.094762
 H -4.774730 1.196983 1.321321
 H -5.391696 -0.234755 2.175841
 H -2.405977 1.756048 3.268490
 H -1.199282 0.789037 2.394617
 H -2.322312 1.822215 1.496610
 H -1.287642 -2.450477 -2.699207
 H -2.536366 0.246650 -3.478276
 H -3.508862 -3.323404 -2.515835
 H -6.302529 -2.079893 -2.275451
 H -5.910604 -3.810946 -2.431452
 H -4.694690 -0.535102 -2.953910
 H -0.445486 -0.909347 -3.177667
 H -5.693488 -2.978220 -0.879742
 H 0.302989 -0.897679 2.861629
 H 1.206595 -3.071927 3.665995
 H 2.699029 -4.982510 3.348447
 H 5.400726 -5.082681 0.004878
 H 4.658890 -2.857899 -0.693096
 H 4.456016 -6.154082 2.051600
 H 5.119075 1.061819 -3.735083
 H 5.267661 -0.896575 1.472297
 H 7.313023 0.988471 -2.646827
 H 8.724714 0.480471 -0.674536
 H 7.672609 -0.434753 1.395084
 H 2.644114 0.796069 -3.592909
 H 2.219025 2.316517 0.371278
 H 1.963863 4.400848 -1.866629
 H 3.368626 4.116531 -0.835067
 H 2.814106 2.849946 -1.935483

H -1.361539 5.070009 0.195755
 H -2.872229 1.688683 -1.984763
 H -3.637379 5.570057 0.994183
 H -5.142704 2.192482 -1.203422
 H -5.554395 4.140570 0.291590
 H 1.782835 5.860573 -0.182742
 H 0.556012 2.569517 2.294706
 H 1.117539 7.441116 1.577656
 H -0.097953 4.155661 4.074120
 H 0.169989 6.607631 3.722812
 H -1.710128 -4.401972 -2.012883
 H -0.073658 4.120611 -1.481053
 H -0.880143 1.654848 -3.095176
 H -1.115060 3.339168 -3.585642
 H 0.525101 2.692171 -3.353587

(IV-si)₄

E0 = -2797.0632386
 E0+ZPE = -2796.109665
 E298 = -2796.054500
 H298 = -2796.053556
 G298 = -2796.198011
 NImag = 1, (-184.6816)
 C -0.655984 5.129851 -1.646473
 C -0.400204 3.758436 -1.510428
 C -0.010027 3.050619 -2.659458
 C 0.125626 3.687265 -3.893038
 C -0.124846 5.056582 -4.009472
 C -0.516413 5.773083 -2.880284
 C -0.609002 3.014834 -0.178071
 C -1.024956 3.933044 0.979727
 N 0.509693 2.087948 0.182539
 C 1.841096 2.605569 0.657217
 C 1.802238 3.158075 2.093041
 C 2.165158 4.476265 2.400183
 C 2.160952 4.936819 3.719907
 C 1.798906 4.083398 4.760955
 C 1.448415 2.762783 4.470486
 C 1.454143 2.306272 3.152864
 P 0.227436 0.453605 -0.113980
 Pd -1.923126 -0.459056 -0.401867
 N -3.174854 -0.393020 1.350980
 C -4.232120 -0.933885 0.737349
 O -5.428609 -0.971927 1.057665
 O 1.168855 -0.073425 -1.415503
 C 2.551671 -0.167635 -1.407731
 C 3.203490 -1.088492 -0.596826
 C 4.644450 -1.065433 -0.574060
 C 5.354249 -0.215316 -1.486716
 C 4.620503 0.611943 -2.377506
 C 3.249817 0.653191 -2.324965
 C 5.408908 -1.827108 0.353972
 C 6.785797 -1.776876 0.356167
 C 7.481339 -0.966876 -0.571855
 C 6.774899 -0.200789 -1.470134
 C 2.409586 -2.044583 0.222294

C 2.597048 -3.471968 0.145921
 C 1.850227 -4.327566 1.024104
 C 0.906115 -3.757900 1.918688
 C 0.668970 -2.405786 1.919584
 C 1.414194 -1.568530 1.060740
 C 3.464215 -4.086431 -0.800608
 C 3.615825 -5.455113 -0.846544
 C 2.912360 -6.290901 0.052103
 C 2.044976 -5.733909 0.963005
 O 1.150516 -0.200310 1.112791
 C 2.507672 3.559567 -0.342451
 N -3.739394 -1.528822 -0.501598
 C -3.729533 -3.038478 -0.421780
 C -2.866267 -3.617854 -1.555209
 C -1.797722 -0.484492 -2.620497
 C -2.733968 0.579562 -2.661197
 C -4.125602 0.516666 -2.505201
 C -4.857285 -0.655264 -2.329681
 C -6.325135 -0.613108 -2.014379
 C -3.155413 -3.541171 0.922429
 C -5.172849 -3.575350 -0.569919
 C -3.290858 0.288351 2.656549
 C -1.882742 0.644741 3.143896
 C -4.130428 1.573794 2.494685
 C -3.949141 -0.641073 3.701080
 H -3.111790 -4.636937 0.909663
 H -2.144537 -3.157434 1.086879
 H -3.783476 -3.237084 1.764243
 H -5.163876 -4.668399 -0.478230
 H -5.821955 -3.155434 0.199754
 H -5.589976 -3.326066 -1.550601
 H -2.878806 -4.712640 -1.501528
 H -1.825799 -3.287810 -1.472097
 H -3.994165 -0.142028 4.677257
 H -4.960861 -0.911706 3.393511
 H -3.361420 -1.559602 3.816435
 H -4.218160 2.107240 3.449903
 H -3.662075 2.247211 1.767373
 H -5.133192 1.322703 2.139338
 H -1.931000 1.205462 4.084626
 H -1.289201 -0.259773 3.318037
 H -1.353494 1.255019 2.408200
 H -2.135123 -1.489381 -2.845776
 H -2.314008 1.582519 -2.732765
 H -4.467814 -1.574957 -2.744693
 H -6.726415 0.395006 -2.166304
 H -6.890580 -1.315964 -2.637786
 H -4.646950 1.461432 -2.360578
 H -0.782732 -0.274964 -2.942885
 H -6.489058 -0.878212 -0.962867
 H -0.077156 -1.957613 2.565421
 H 0.349150 -4.411648 2.584635
 H 1.479056 -6.364263 1.644767
 H 4.278774 -5.896897 -1.585500
 H 4.003027 -3.464481 -1.505335
 H 3.047231 -7.368102 0.010089

H 5.160616 1.233586 -3.087052
 H 4.894298 -2.445642 1.079928
 H 7.294176 0.441926 -2.177145
 H 8.567413 -0.942102 -0.563599
 H 7.342671 -2.361678 1.083218
 H 2.675556 1.298514 -2.981345
 H 2.471703 1.714555 0.705246
 H 1.970253 4.503811 -0.455785
 H 3.524774 3.782098 -0.002205
 H 2.574260 3.094542 -1.326416
 H 0.204967 1.989407 -2.588959
 H -0.966889 5.716040 -0.788926
 H 0.425923 3.111202 -4.764714
 H -0.718167 6.838654 -2.952799
 H -0.018841 5.555460 -4.968872
 H 2.455624 5.162359 1.611521
 H 1.189241 1.276771 2.939694
 H 2.444004 5.965243 3.929333
 H 1.174091 2.082526 5.272682
 H 1.795651 4.439816 5.787594
 H -3.244176 -3.339350 -2.545193
 H -1.461459 2.339802 -0.340601
 H -0.303062 4.729060 1.175455
 H -1.989981 4.395586 0.746590
 H -1.142351 3.354725 1.896891

V-re

E0 = -2718.4566506
 E0+ZPE = -2717.562078
 E298 = -2717.508294
 H298 = -2717.507350
 G298 = -2717.649309
 NImag = 1, (-189.6513)
 C 6.957800 -0.755913 0.993569
 C 5.648633 -0.930019 0.600219
 C 4.806492 0.186567 0.340016
 C 5.348160 1.499437 0.530568
 C 6.707976 1.644121 0.919405
 C 7.500424 0.542307 1.144614
 C 4.516980 2.630610 0.338639
 C 3.176179 2.520567 0.019663
 C 2.653325 1.201420 -0.155861
 C 3.433875 0.059542 -0.066662
 O 1.309152 1.056927 -0.452114
 P 0.220256 0.472212 0.700074
 O 1.115737 -0.831763 1.259727
 C 1.711235 -1.698765 0.350028
 C 1.177250 -3.019633 0.229077
 C 1.737672 -3.845232 -0.728714
 C 2.785342 -3.420198 -1.581030
 C 3.346485 -2.114803 -1.402800
 C 2.821778 -1.269416 -0.365028
 C 3.295405 -4.268193 -2.601531
 C 4.300433 -3.840989 -3.438079
 C 4.834508 -2.539178 -3.286937
 C 4.373831 -1.700120 -2.295720

Pd -1.875722 0.358012 -0.338624
 N -3.536539 0.016624 0.971183
 C -3.867393 -0.396644 2.351657
 C -2.572236 -0.462961 3.168652
 N -3.802124 0.607453 -1.179510
 C -3.880510 -0.981475 -2.842719
 C -2.796649 -1.769061 -2.459917
 C -1.489838 -1.296747 -2.263830
 C -1.017644 0.035831 -2.362480
 C -4.289920 1.984461 -1.562499
 C -4.370149 2.918518 -0.333214
 C -3.324573 2.617789 -2.579078
 C -5.694268 1.894294 -2.205478
 C -4.470242 0.115641 0.018710
 O -5.683558 -0.139271 0.043001
 C -5.274540 -1.542052 -2.879276
 C -4.829849 0.625328 2.993811
 C -4.518136 -1.798495 2.338313
 N 0.328301 1.404143 2.082698
 C 1.454563 1.412384 3.017569
 C -0.576183 2.546082 2.233177
 H -3.690565 3.612583 -2.858905
 H -2.320813 2.730791 -2.156941
 H -3.251565 2.029495 -3.500572
 H -6.037790 2.902790 -2.467298
 H -5.672433 1.301301 -3.125676
 H -6.404507 1.437968 -1.515336
 H -4.676193 3.921760 -0.652817
 H -5.099767 2.556530 0.395730
 H -3.396723 3.001468 0.161164
 H -4.729721 -2.125751 3.364648
 H -5.450905 -1.782831 1.771347
 H -3.838396 -2.525777 1.881572
 H -5.071955 0.334439 4.023796
 H -4.370700 1.620853 3.020255
 H -5.759155 0.684073 2.421172
 H -2.791460 -0.779322 4.195618
 H -1.871949 -1.181662 2.732345
 H -2.082119 0.513547 3.210685
 H -1.569936 0.744382 -2.968185
 H -0.772150 -2.029135 -1.895236
 H -3.691235 -0.094539 -3.433064
 H -5.259165 -2.631502 -2.764038
 H -5.869294 -1.131975 -2.054544
 H -3.006232 -2.783787 -2.126317
 H 0.055872 0.190598 -2.351679
 H -5.780652 -1.295231 -3.820464
 H 1.373289 -4.864568 -0.823428
 H 2.865293 -5.260442 -2.714442
 H 5.613018 -2.195585 -3.962588
 H 4.787406 -0.702821 -2.201146
 H 4.678075 -4.494116 -4.219822
 H 4.955955 3.618880 0.447335
 H 5.247056 -1.931333 0.496018
 H 7.106928 2.647659 1.047026
 H 8.536465 0.664619 1.447884

H 7.578843 -1.624897 1.193207
 H 1.066075 1.393983 4.043997
 H -0.922672 2.600924 3.272519
 H 2.079570 0.534081 2.866038
 H 2.066463 2.315677 2.893080
 H -0.073506 3.488210 1.977102
 H -1.450573 2.422008 1.588990
 C 2.337441 3.740971 -0.123830
 C 2.475519 4.794788 0.797230
 C 1.431571 3.902049 -1.187146
 C 1.735655 5.970297 0.662326
 H 3.160282 4.684244 1.633835
 C 0.695646 5.078676 -1.323178
 H 1.310769 3.105701 -1.912634
 C 0.841758 6.116826 -0.399515
 H 1.855880 6.768415 1.390186
 H 0.008118 5.185745 -2.158001
 H 0.263659 7.030555 -0.506870
 C 0.112416 -3.550695 1.122017
 C 0.176657 -3.380441 2.515565
 C -0.930348 -4.329147 0.592237
 C -0.764979 -3.981455 3.349823
 H 0.977323 -2.788107 2.945476
 C -1.875377 -4.925359 1.427164
 H -1.004115 -4.461251 -0.483837
 C -1.793759 -4.756786 2.810440
 H -0.692608 -3.845180 4.425487
 H -2.677497 -5.517929 0.995627
 H -2.529210 -5.220336 3.461969

V-re-b

E0 = -2718.451434
 E0+ZPE = -2717.556355
 E298 = -2717.502793
 H298 = -2717.501849
 G298 = -2717.642715
 NImag = 1, (-167.7907)
 C 1.822806 -4.649020 -3.354165
 C 0.696401 -3.902548 -3.708247
 C -0.132870 -3.366042 -2.724036
 C 0.146043 -3.565616 -1.360081
 C 1.280478 -4.321150 -1.019263
 C 2.110973 -4.856475 -2.004359
 C -0.783740 -3.088149 -0.301894
 C -1.433674 -1.816054 -0.353122
 C -2.472189 -1.468590 0.499256
 C -2.750639 -2.313118 1.627192
 C -2.048462 -3.554926 1.749509
 C -1.118798 -3.924859 0.747496
 C -3.668780 -1.954727 2.652362
 C -3.891261 -2.787972 3.726858
 C -3.217533 -4.028443 3.830320
 C -2.315822 -4.400836 2.860228
 O -1.048312 -0.913057 -1.340868
 P -0.234645 0.474528 -0.875563
 N -0.445707 1.318615 -2.312048

C 0.229020 2.615713 -2.430069
 C -3.295672 -0.258666 0.206335
 C -4.708647 -0.372992 -0.039140
 C -5.462861 0.819365 -0.285060
 C -4.795678 2.067270 -0.316331
 C -3.427961 2.185186 -0.153750
 C -2.691383 0.984470 0.097493
 C -6.863236 0.730001 -0.513669
 C -7.499428 -0.489289 -0.534205
 C -6.751241 -1.673334 -0.332670
 C -5.395749 -1.618237 -0.090925
 C -2.793449 3.526746 -0.266060
 C -3.161721 4.379808 -1.322461
 C -2.622768 5.662362 -1.432585
 C -1.703572 6.118376 -0.486141
 C -1.332688 5.283006 0.570304
 C -1.870290 4.000508 0.680423
 O -1.316445 1.064013 0.268086
 Pd 1.996813 0.229154 -0.152590
 C 2.509289 -0.693251 -2.112260
 C 3.059937 0.539239 -2.542138
 C 4.299518 1.106516 -2.214846
 C 5.274895 0.501237 -1.428528
 C 6.499309 1.254033 -0.994444
 N 2.601044 1.353663 1.584736
 C 3.903598 1.174176 1.349316
 O 4.902607 1.798515 1.731103
 N 4.004923 0.014894 0.463009
 C 4.455197 -1.211853 1.221204
 C 5.953337 -1.078561 1.585239
 C 2.080969 2.378621 2.511035
 C 2.152003 3.765038 1.837938
 C 0.628671 2.014780 2.845706
 C 2.883414 2.401837 3.832514
 C 3.651152 -1.420219 2.525766
 C 4.268958 -2.463373 0.349233
 C -1.587319 1.170629 -3.217858
 H 4.623942 -3.345542 0.895330
 H 3.216192 -2.620339 0.100700
 H 4.840645 -2.411256 -0.583853
 H 6.266300 -1.961886 2.155380
 H 6.576986 -1.021881 0.687551
 H 6.131468 -0.183859 2.183600
 H 3.959786 -2.363233 2.993059
 H 3.828144 -0.613753 3.241792
 H 2.576458 -1.466391 2.325195
 H 1.766836 4.546422 2.506805
 H 3.189513 4.007255 1.587107
 H 1.558250 3.779014 0.916559
 H 2.434581 3.126999 4.522925
 H 2.852855 1.417297 4.313751
 H 3.926301 2.668958 3.657949
 H 0.188674 2.768735 3.510728
 H 0.022673 1.942573 1.941776
 H 0.585304 1.044259 3.353399
 H 3.174930 -1.485043 -1.790944

H 2.398873 1.168965 -3.134888
 H 5.323668 -0.578405 -1.405655
 H 6.601314 2.189468 -1.555883
 H 6.414284 1.514511 0.067732
 H 4.442562 2.155066 -2.471943
 H 1.625208 -1.048427 -2.632750
 H 7.409574 0.658307 -1.132031
 H -0.667953 -4.911963 0.800301
 H -1.782177 -5.345359 2.933711
 H -4.587487 -2.487715 4.505097
 H -4.184526 -1.003119 2.590268
 H -3.407359 -4.678082 4.680163
 H -5.385866 2.965624 -0.476425
 H -4.840864 -2.537499 0.052403
 H -7.420094 1.648322 -0.684146
 H -8.569015 -0.547700 -0.715599
 H -7.250019 -2.637870 -0.372705
 H -1.231558 1.257915 -4.252524
 H 0.608189 2.740193 -3.452459
 H -2.048066 0.192575 -3.088621
 H -2.341346 1.950367 -3.045226
 H -0.456284 3.444005 -2.208528
 H 1.074101 2.669346 -1.738372
 H -3.868658 4.027572 -2.069076
 H -1.583119 3.369071 1.512432
 H -2.919002 6.301696 -2.260152
 H -0.622214 5.629122 1.315609
 H -1.280620 7.115809 -0.569456
 H -1.012293 -2.801217 -3.013424
 H 1.520387 -4.477731 0.028363
 H 0.456711 -3.742883 -4.756296
 H 2.986070 -5.431754 -1.714183
 H 2.468142 -5.065239 -4.122880

V-si-c

E0 = -2718.4562262
 E0+ZPE = -2717.561706
 E298 = -2717.507918
 H298 = -2717.506973
 G298 = -2717.648722
 NImag = 1, (-176.0573)
 C -0.728683 6.099716 0.498674
 C -0.510095 5.009188 1.344322
 C -1.249625 3.836823 1.192070
 C -2.231062 3.732575 0.190382
 C -2.441217 4.838477 -0.652793
 C -1.698461 6.010193 -0.501185
 C -3.072493 2.515175 0.037284
 C -4.433259 2.630738 -0.177887
 C -5.270380 1.503687 -0.367766
 C -4.711218 0.187758 -0.274573
 C -3.312187 0.050303 0.026789
 C -2.531132 1.193312 0.103137
 C -6.654392 1.655697 -0.655251
 C -7.455777 0.559355 -0.875513
 C -6.898840 -0.740407 -0.820022

C -5.565111 -0.922184 -0.525066
 O -1.162577 1.052646 0.269456
 P -0.193516 0.509271 -0.989221
 N -0.479078 1.441599 -2.357471
 C 0.315691 2.655374 -2.555714
 C -2.684798 -1.288461 0.240010
 C -1.621670 -1.697238 -0.553410
 C -1.066401 -3.011922 -0.489247
 C -1.565783 -3.866071 0.476116
 C -2.568333 -3.470883 1.393904
 C -3.142363 -2.163473 1.285359
 C -4.113881 -1.777785 2.250627
 C -4.513861 -2.646393 3.242597
 C -3.970447 -3.950466 3.324031
 C -3.015634 -4.349596 2.417979
 O -1.094346 -0.813494 -1.487062
 C -0.031722 -3.502403 -1.438956
 C -0.156685 -3.309937 -2.826113
 C 0.767549 -3.868800 -3.708885
 C 1.837533 -4.626587 -3.225471
 C 1.978242 -4.817371 -1.849404
 C 1.053703 -4.259089 -0.965616
 Pd 2.057059 0.415433 -0.316045
 C 2.785307 0.261246 -2.409104
 C 3.112451 -1.090252 -2.131283
 C 4.236825 -1.588717 -1.457342
 C 5.281056 -0.814010 -0.961723
 C 6.363024 -1.415274 -0.110992
 N 2.420444 -0.099006 1.737681
 C 3.750323 -0.006194 1.646438
 O 4.644874 -0.370070 2.424862
 N 4.044403 0.633503 0.370017
 C 4.620020 2.015497 0.557381
 C 6.081870 1.921132 1.055056
 C 1.758045 -0.642015 2.942663
 C 2.151941 0.181205 4.188522
 C 0.241983 -0.559255 2.749329
 C 2.165084 -2.120204 3.132887
 C 4.610682 2.771603 -0.782577
 C 3.799124 2.835965 1.578834
 C -1.700762 1.409752 -3.164980
 H 4.195674 3.857055 1.633092
 H 2.745621 2.889223 1.284840
 H 3.854453 2.395915 2.578129
 H 6.481414 2.932692 1.199244
 H 6.134864 1.373332 1.996280
 H 6.716735 1.412402 0.322270
 H 5.059685 3.762419 -0.647065
 H 5.193474 2.254335 -1.552559
 H 3.590899 2.912690 -1.154405
 H 1.653023 -0.214352 5.082166
 H 3.232459 0.147648 4.345979
 H 1.846237 1.226825 4.064188
 H 1.647478 -2.551831 3.999174
 H 1.890709 -2.701084 2.244060
 H 3.243508 -2.203659 3.285428

H -0.275196 -0.936676 3.639446
 H -0.074519 0.472866 2.572865
 H -0.075687 -1.159273 1.891569
 H 3.578615 0.999915 -2.441557
 H 2.356348 -1.827450 -2.393719
 H 5.498097 0.132108 -1.439701
 H 6.334248 -2.509576 -0.160232
 H 7.357382 -1.074025 -0.422625
 H 4.203446 -2.636872 -1.167245
 H 1.981423 0.432631 -3.119774
 H 6.214859 -1.128644 0.937416
 H -1.183424 -4.881679 0.531209
 H -2.575986 -5.342243 2.478113
 H -5.250088 -2.323892 3.973759
 H -4.532325 -0.779035 2.211483
 H -4.299325 -4.626725 4.108129
 H -4.883523 3.619585 -0.202272
 H -5.153042 -1.924117 -0.492584
 H -7.065623 2.660977 -0.708736
 H -8.510756 0.687716 -1.101112
 H -7.528567 -1.604179 -1.015006
 H 0.595720 2.741812 -3.613512
 H -2.364906 2.249936 -2.921367
 H -0.247083 3.552192 -2.264482
 H 1.230018 2.607792 -1.959064
 H -2.236345 0.475601 -3.006593
 H -1.426269 1.481866 -4.225430
 H -0.991302 -2.734934 -3.212873
 H 1.178338 -4.398486 0.104505
 H 0.646856 -3.717819 -4.778417
 H 2.809826 -5.399097 -1.460554
 H 2.556157 -5.061084 -3.914938
 H -1.073063 3.000914 1.859345
 H -3.184756 4.772214 -1.442714
 H 0.237094 5.070791 2.130937
 H -1.875815 6.849894 -1.168101
 H -0.148100 7.010349 0.618605

V-si

E0 = -2718.4567456
 E0+ZPE = -2717.561688
 E298 = -2717.508117
 H298 = -2717.507173
 G298 = -2717.648196
 NImag = 1, (-190.8530)
 C 6.821441 -1.443582 0.940945
 C 5.502067 -1.454866 0.543732
 C 4.796430 -0.242101 0.308013
 C 5.488711 0.993291 0.526585
 C 6.854725 0.969853 0.919357
 C 7.512101 -0.221650 1.121193
 C 4.796807 2.217414 0.354622
 C 3.455146 2.270167 0.027313
 C 2.776632 1.026978 -0.167493
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 C -1.543365 5.304601 0.641617
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H -1.819752 -2.975322 -2.538847
H 2.899029 -4.179702 1.516949
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 H 0.339081 -1.261937 2.355466
 H 3.622432 0.802850 -2.442684
 H 2.806189 -2.095404 -1.794615
 H 5.599279 0.462084 -1.217680
 H 6.680841 -1.700989 0.660532
 H 7.556816 -0.274420 0.050042
 H 4.686956 -2.347798 -0.392807
 H 2.147758 -0.121751 -2.994507
 H 6.381632 -0.110009 1.370475
 H -0.952434 -4.962740 1.358258
 H -2.265686 -5.124070 3.412555
 H -4.904112 -1.918666 4.536115
 H -4.263922 -0.657146 2.533992
 H -3.933890 -4.174159 4.979405
 H -5.098523 3.129382 -0.542719
 H -4.900963 -2.391147 0.057086
 H -7.213079 1.936516 -0.741890
 H -8.500696 -0.181167 -0.727244
 H -7.316366 -2.345746 -0.354180
 H 0.666841 1.884603 -3.997985
 H -2.232298 1.226888 -3.526904
 H -0.351458 2.890023 -2.928687
 H 1.164467 2.193489 -2.320536
 H -1.999162 -0.471982 -3.054500
 H -1.095456 0.199371 -4.427592
 H 0.262092 -5.310393 -3.932785
 H 3.322255 -5.054509 -0.946536
 H -0.544656 5.621015 1.529638
 H -1.797450 6.062736 -2.540989
 H -1.897306 -4.614082 -3.538557
 H -2.450975 -4.444064 -1.864310
 H -1.922198 -3.023495 -2.763961
 H 3.578753 -6.591660 -2.923281
 H 2.348979 -6.598597 -4.200019
 H 3.475072 -5.245014 -4.059515
 H 2.980674 -4.084746 1.095913
 H 1.999355 -2.618109 1.003116
 H 1.342469 -4.066134 1.759670
 H -1.451933 3.987087 2.895774
 H -2.752623 2.921482 2.338790
 H -1.068541 2.459605 2.092661
 H -2.800356 4.217604 -3.691048
 H -3.453105 2.805367 -2.837506
 H -4.286818 4.349930 -2.755811
 H 0.785207 7.130662 -0.458604
 H -0.418506 7.762262 -1.592697
 H -0.624361 7.997049 0.150444

VII-re

E0 = -3426.078038

E0+ZPE = -3424.673363

E298 = -3424.593601

H298 = -3424.592657
 G298 = -3424.788805
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 C -3.703874 1.666523 -0.135746
 C -3.945370 2.128268 -1.454627
 C -5.057731 1.643233 -2.151136
 C -5.951180 0.726663 -1.596505
 C -5.700679 0.291524 -0.293826
 C -2.588613 2.271207 0.670501
 C -1.203453 2.135628 0.332036
 C -0.212439 2.915008 0.917212
 C -0.539465 3.665617 2.101159
 C -1.907549 3.749075 2.510302
 C -2.897364 3.095983 1.734836
 C 0.440319 4.312299 2.904914
 C 0.081238 5.013316 4.035706
 C -1.276744 5.119723 4.418959
 C -2.248481 4.498055 3.668944
 C 1.145904 3.035599 0.308627
 C 1.659023 4.330155 -0.058815
 C 3.028349 4.438464 -0.458221
 C 3.832531 3.271689 -0.491906
 C 3.328993 2.007361 -0.256567
 C 1.940379 1.917924 0.094917
 C 0.864282 5.510450 -0.075664
 C 1.402397 6.725026 -0.442491
 C 2.766417 6.832941 -0.802113
 C 3.559581 5.708750 -0.810160
 C 4.238245 0.809820 -0.298239
 C 4.539805 0.120829 0.907241
 C 5.372978 -1.000953 0.856084
 C 5.943464 -1.460323 -0.333096
 C 5.689754 -0.730205 -1.494047
 C 4.863147 0.401465 -1.506724
 C 4.084183 0.649710 2.270321
 C 3.981269 -0.424160 3.366734
 C 4.756103 1.186363 -2.818078
 C 4.478704 0.308982 -4.054283
 C 6.826124 -2.701347 -0.343142
 C 6.202003 -3.836245 -1.178104
 O 1.401042 0.666342 0.341141
 P 0.145490 -0.025349 -0.548489
 N 0.582089 -0.110989 -2.159945
 C 1.085711 -1.374109 -2.698035
 O -0.874961 1.295412 -0.720132
 C -3.101868 3.216354 -2.120477
 C -3.853492 4.563777 -2.112606
 C -7.163451 0.245307 -2.383383
 C -8.483951 0.676578 -1.716356
 C -4.457570 0.224691 1.884466
 C -5.563615 0.794422 2.797886
 C -7.135256 -1.276543 -2.618465
 C -2.661156 2.841038 -3.547039
 C -4.451745 -1.312783 1.961822
 Pd -0.268848 -2.134525 0.420914

N -1.646560 -3.378646 -0.641323
 C -1.406273 -4.487890 0.072436
 O -1.968567 -5.591535 0.068322
 N -0.277039 -4.188647 0.943030
 C 0.916290 -5.061926 0.623792
 C 1.152007 -5.176265 -0.899712
 C 0.572870 -1.603257 2.406805
 C -0.724404 -1.746510 2.953145
 C -1.400632 -2.928806 3.293539
 C -0.884465 -4.215672 3.175495
 C -1.752409 -5.421831 3.402862
 C 2.185671 -4.464602 1.255291
 C 0.706271 -6.486492 1.190548
 C 6.043640 2.004589 -3.064498
 C 8.259259 -2.391615 -0.816118
 C 5.028495 1.778820 2.740448
 C 0.783802 1.044709 -3.035123
 C -2.603455 -3.347158 -1.768211
 C -2.690172 -1.907831 -2.292961
 C -2.126695 -4.286964 -2.895920
 C -4.006667 -3.785177 -1.289173
 H 3.044652 -5.103541 1.018464
 H 2.391694 -3.461764 0.868208
 H 2.118470 -4.409530 2.347443
 H 1.574784 -7.106415 0.935702
 H 0.617477 -6.473288 2.281316
 H -0.194173 -6.937396 0.772494
 H 2.043804 -5.785975 -1.087272
 H 0.305400 -5.651616 -1.401151
 H 1.316479 -4.191559 -1.346888
 H -4.718677 -3.730720 -2.122494
 H -3.980872 -4.806676 -0.906251
 H -4.362887 -3.121544 -0.494652
 H -2.818600 -4.253988 -3.746838
 H -1.134167 -3.988918 -3.253739
 H -2.073176 -5.318145 -2.535123
 H -3.399901 -1.852093 -3.127018
 H -3.032903 -1.224489 -1.509547
 H -1.718815 -1.553390 -2.650882
 H 1.295646 -2.395663 2.562691
 H -1.312572 -0.831701 3.032188
 H 0.185280 -4.356466 3.249921
 H -2.723074 -5.130872 3.819162
 H -1.942195 -5.938445 2.454842
 H -2.462240 -2.838264 3.508349
 H 0.995386 -0.605496 2.375059
 H -1.276141 -6.134909 4.086953
 H -3.940980 3.248446 1.994089
 H -3.294853 4.558735 3.958478
 H 0.849665 5.486121 4.641250
 H 1.485976 4.234103 2.629913
 H -1.546468 5.682535 5.308275
 H 4.887625 3.383202 -0.722650
 H -0.184026 5.448337 0.191536
 H 4.605943 5.771346 -1.099549
 H 3.179488 7.798476 -1.080429

H 0.770559 7.608929 -0.458149
 H 0.285762 0.860188 -3.995595
 H 0.725103 -1.496016 -3.726821
 H 0.351665 1.938334 -2.588844
 H 1.848993 1.219623 -3.226001
 H 2.182771 -1.409140 -2.700218
 H 0.708762 -2.209575 -2.104146
 H 6.157425 -1.043495 -2.423337
 H 5.599595 -1.534420 1.774024
 H -5.248827 2.008984 -3.157087
 H -6.386419 -0.415258 0.165822
 H 3.086700 1.082682 2.155649
 H 3.928754 1.896789 -2.725684
 H 6.893050 -3.056155 0.694457
 H -7.120671 0.730995 -3.368126
 H -2.191428 3.359323 -1.534779
 H -3.496559 0.572509 2.276311
 H -7.988163 -1.587925 -3.233657
 H -6.215240 -1.581444 -3.128446
 H -7.187470 -1.827810 -1.672437
 H -9.342671 0.373764 -2.327666
 H -8.600167 0.215295 -0.728304
 H -8.524884 1.763459 -1.584051
 H -1.969391 3.596121 -3.940037
 H -2.155487 1.870500 -3.558644
 H -3.509458 2.787173 -4.239030
 H -3.234715 5.354373 -2.554951
 H -4.784151 4.501872 -2.689236
 H -4.113061 4.865597 -1.091701
 H -4.331574 -1.632207 3.004086
 H -5.392302 -1.743915 1.600619
 H -3.635430 -1.744204 1.374503
 H -5.416576 0.461688 3.832640
 H -5.575253 1.889779 2.792974
 H -6.554833 0.454436 2.475227
 H 5.945746 2.614208 -3.971128
 H 6.273938 2.673014 -2.228865
 H 6.905057 1.339244 -3.197304
 H 4.309414 0.943783 -4.932354
 H 5.325140 -0.345808 -4.289567
 H 3.597306 -0.323970 -3.920455
 H 6.822696 -4.739092 -1.129401
 H 5.200125 -4.089972 -0.814265
 H 6.111786 -3.549981 -2.232905
 H 8.887957 -3.287985 -0.754172
 H 8.271591 -2.050006 -1.858015
 H 8.719048 -1.609080 -0.202487
 H 4.693696 2.183804 3.703464
 H 6.048543 1.397191 2.870361
 H 5.065071 2.602517 2.020829
 H 3.492359 -0.002143 4.252055
 H 3.395881 -1.287462 3.037128
 H 4.967543 -0.782441 3.684704

VII-re-b

E0 = -3426.0692289

E0+ZPE = -3424.665403
 E298 = -3424.585288
 H298 = -3424.584343
 G298 = -3424.782336
 NImag = 1, (-191.3250)
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 C 4.252625 -0.552858 -0.317007
 C 4.892552 0.695259 -0.129521
 C 5.823765 1.133938 -1.080266
 C 6.149563 0.386258 -2.210780
 C 5.520172 -0.850275 -2.368566
 C 3.311602 -1.122372 0.711229
 C 1.933851 -1.386712 0.419002
 C 1.169644 -2.276337 1.163645
 C 1.646608 -2.638754 2.473295
 C 2.968634 -2.248844 2.862283
 C 3.790454 -1.567787 1.926230
 C 0.850292 -3.342236 3.418037
 C 1.336362 -3.645609 4.671680
 C 2.650046 -3.277324 5.044783
 C 3.446932 -2.593929 4.154267
 C -0.051076 -2.927647 0.592890
 C -0.117047 -4.369880 0.520397
 C -1.345159 -4.993755 0.128380
 C -2.470085 -4.182887 -0.168270
 C -2.395335 -2.806935 -0.202946
 C -1.131826 -2.207697 0.103995
 C 0.999601 -5.213537 0.779546
 C 0.897511 -6.584652 0.680370
 C -0.327932 -7.195555 0.327758
 C -1.424452 -6.410340 0.055796
 C -3.641423 -1.993152 -0.420390
 C -4.233484 -1.873058 -1.700652
 C -5.434330 -1.165266 -1.830608
 C -6.077984 -0.576406 -0.739644
 C -5.485964 -0.725002 0.515611
 C -4.284421 -1.418767 0.703950
 C -3.631503 -2.516670 -2.949244
 C -3.451234 -1.509425 -4.100837
 C -3.753995 -1.580869 2.128540
 C -4.639180 -2.555271 2.932504
 C -7.374471 0.206239 -0.901841
 C -7.166192 1.478378 -1.746830
 O -1.065354 -0.824706 0.009062
 P 0.013597 0.090938 -0.856702
 N -0.216552 -0.208291 -2.507016
 C 0.187099 0.851132 -3.441400
 O 1.416240 -0.842968 -0.737467
 C 4.641120 1.589254 1.083385
 C 5.864888 1.616239 2.022381
 C 7.158326 0.885022 -3.237157
 C 8.555077 1.091295 -2.620894
 C 4.051070 -2.764583 -1.642364
 C 4.974414 -3.782936 -0.939512
 C 4.246478 3.019320 0.673626
 C 3.845793 -3.165166 -3.114096

C 6.670705 2.166644 -3.939994
 Pd -0.552533 2.323908 -0.220196
 N -1.011378 4.341899 0.230734
 C -0.618361 4.213963 1.629616
 O -0.828603 5.114974 2.457400
 C -2.247891 2.303430 -1.677139
 C -3.124621 2.143045 -0.573639
 C -3.606574 3.136507 0.287395
 C -3.304691 4.493013 0.174513
 C -3.745061 5.475814 1.221480
 N -0.066352 3.009195 1.773005
 C 0.389404 2.508235 3.085535
 C 1.530095 3.388664 3.636935
 C -3.604014 -0.235908 2.862290
 C -8.508603 -0.662416 -1.477707
 C -4.471690 -3.723630 -3.414225
 C 0.010146 -1.544738 -3.069663
 C -0.789239 2.504524 4.085522
 C 0.883129 1.071442 2.896051
 C -0.266297 5.441633 -0.482907
 C -0.499738 5.324099 -1.999354
 C -0.762599 6.830917 -0.017726
 C 1.250662 5.338539 -0.218377
 H 0.041806 6.124278 -2.517000
 H -0.136289 4.365786 -2.384398
 H -1.558425 5.425113 -2.263165
 H -0.206665 7.609076 -0.555244
 H -1.825791 6.967400 -0.239803
 H -0.614997 6.955813 1.055129
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 H 1.633260 4.362099 -0.531370
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 H -1.611082 1.890039 3.702701
 H 1.877000 3.009178 4.606422
 H 2.379768 3.389721 2.946702
 H 1.184528 4.417515 3.766222
 H 1.257705 0.660599 3.840576
 H 0.072553 0.428161 2.538288
 H 1.692329 1.035370 2.160199
 H -2.172178 3.275801 -2.151815
 H -3.387008 1.118496 -0.317259
 H -3.069080 4.888581 -0.804993
 H -4.490090 5.025692 1.886952
 H -2.889101 5.772584 1.839970
 H -4.115611 2.804800 1.190208
 H -2.179992 1.461640 -2.357889
 H -4.173330 6.378769 0.770595
 H 4.835190 -1.401985 2.175235
 H 4.455666 -2.296459 4.430576
 H 0.701894 -4.168703 5.381987
 H -0.162024 -3.624024 3.150557
 H 3.022946 -3.527348 6.034096
 H -3.422219 -4.665397 -0.373576
 H 1.950946 -4.769200 1.044658

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 H 1.770926 -7.201746 0.872881
 H 1.073712 -1.720215 -3.276764
 H 1.228221 0.716919 -3.769825
 H -0.340551 -2.319008 -2.387765
 H -0.550650 -1.629369 -4.006306
 H -0.462552 0.825785 -4.324738
 H 0.094355 1.830756 -2.967640
 H -5.882386 -1.076669 -2.816786
 H -5.983270 -0.290998 1.379917
 H 5.780928 -1.453369 -3.233732
 H 6.309392 2.093656 -0.925577
 H -2.756410 -2.024943 2.076743
 H -2.639049 -2.895755 -2.687981
 H -7.683868 0.526267 0.102608
 H 7.250805 0.104270 -4.004932
 H 3.071681 -2.833622 -1.163095
 H 3.804300 1.171190 1.649654
 H 7.382604 2.480007 -4.713243
 H 5.696134 2.010478 -4.415643
 H 6.565211 2.994037 -3.228232
 H 9.276784 1.390617 -3.390518
 H 8.541067 1.876474 -1.855700
 H 8.919926 0.172216 -2.149281
 H 3.304460 -4.116852 -3.167103
 H 3.266868 -2.412519 -3.660671
 H 4.795294 -3.306845 -3.643070
 H 4.576968 -4.800508 -1.041663
 H 5.978259 -3.764569 -1.380944
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 H 4.042099 3.627892 1.560906
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 H 5.653743 2.225801 2.909083
 H 6.139114 0.610346 2.359889
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 H -2.942803 -1.986538 -4.947769
 H -4.412482 -1.134098 -4.469720
 H -2.855891 -0.648218 -3.780009
 H -8.092446 2.063439 -1.799465
 H -6.382055 2.113589 -1.320311
 H -6.871761 1.227565 -2.773104
 H -9.443970 -0.092140 -1.525965
 H -8.275279 -1.002312 -2.493876
 H -8.681395 -1.550557 -0.859869
 H -3.147022 -0.391018 3.846550
 H -2.965777 0.451410 2.297895
 H -4.571623 0.253653 3.025578
 H -4.233064 -2.700935 3.940836
 H -5.661291 -2.171428 3.034421
 H -4.697295 -3.534604 2.444159

VII-si

E0 = -3426.0774377
E0+ZPE = -3424.672480
E298 = -3424.592808
H298 = -3424.591864
G298 = -3424.787069
NImag = 1, (-197.6791)
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C 4.835827 -0.405819 -1.028860
C 5.632618 -1.456371 -0.555251
C 5.833233 -1.690876 0.805579
C 5.228879 -0.813530 1.707295
C 3.401882 1.651042 -0.530936
C 4.031799 2.738123 -1.104571
C 3.344761 3.935628 -1.432774
C 1.985497 4.092330 -1.014440
C 1.349496 3.013098 -0.306482
C 2.007018 1.793429 -0.231807
C 3.987708 4.992012 -2.132207
C 3.311191 6.150966 -2.438152
C 1.958514 6.298318 -2.050386
C 1.314682 5.300761 -1.350358
C 0.055309 3.219238 0.408332
C -1.055826 2.415037 0.186330
C -2.338377 2.708092 0.745840
C -2.438962 3.798460 1.584734
C -1.316515 4.573726 1.962758
C -0.040311 4.271603 1.391050
C -1.435146 5.626585 2.909879
C -0.331572 6.341415 3.313627
C 0.940625 6.018023 2.786616
C 1.082859 5.016442 1.850743
C -3.569021 1.904586 0.447057
C -4.231212 2.049377 -0.795675
C -5.431275 1.363753 -1.007159
C -5.998952 0.534292 -0.034327
C -5.326161 0.407996 1.181815
C -4.128244 1.082447 1.452514
C -3.720351 2.995911 -1.881640
C -3.559513 2.304995 -3.247742
C -3.491447 0.920919 2.833153
C -3.104223 -0.538363 3.123087
C -7.334888 -0.164042 -0.256738
C -8.499601 0.845664 -0.209210
O -0.995618 1.358887 -0.708344
P 0.025784 0.039324 -0.655533
N 0.418296 0.031127 -2.281457
C 0.783372 -1.215942 -2.951841
O 1.313252 0.686644 0.234595
C 4.709792 -0.231240 -2.544204
C 5.950644 0.469297 -3.139580
C 6.685813 -2.851668 1.300302
C 6.141079 -4.211717 0.823639
C 3.921235 1.242965 2.352644
C 4.978291 2.340268 2.604032

C 4.492257 -1.565242 -3.288672
 C 3.511071 0.585879 3.682637
 C 8.165978 -2.681101 0.906808
 Pd -0.521465 -2.108967 0.197337
 N -0.907885 -4.137849 0.696455
 C -1.590623 -4.381426 -0.572083
 O -1.847709 -5.524332 -0.976691
 C 1.211052 -2.121402 1.557485
 C 1.968697 -2.752656 0.536393
 C 1.937041 -4.097436 0.144417
 C 1.166928 -5.091199 0.751866
 C 1.068480 -6.464961 0.148210
 N -1.842031 -3.185939 -1.118486
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 C -2.101229 -3.715437 -3.528665
 C -4.400132 1.481420 3.945395
 C -7.374028 -0.986303 -1.556897
 C -4.626544 4.239075 -1.994594
 C 0.528695 1.207042 -3.146669
 C -4.108936 -3.676372 -2.010002
 C -2.933638 -1.539819 -2.554991
 C -1.782373 -4.549051 1.863952
 C -3.243786 -4.083502 1.670697
 C -1.789230 -6.089966 2.015354
 C -1.246503 -3.937273 3.169541
 H -3.819893 -4.308099 2.576382
 H -3.300446 -3.008323 1.484497
 H -3.715218 -4.604211 0.833606
 H -2.465868 -6.365354 2.833701
 H -2.128244 -6.565400 1.094507
 H -0.795860 -6.475777 2.265229
 H -1.886311 -4.246392 4.004197
 H -0.231531 -4.278506 3.400933
 H -1.246883 -2.844759 3.131903
 H -4.773818 -3.539916 -2.872177
 H -4.005874 -4.746652 -1.816069
 H -4.577331 -3.204043 -1.139183
 H -2.746647 -3.584880 -4.406859
 H -1.123581 -3.278895 -3.757754
 H -1.967422 -4.783711 -3.343518
 H -3.601543 -1.392200 -3.412060
 H -3.379600 -1.048235 -1.684198
 H -1.984455 -1.041816 -2.772034
 H 0.846451 -2.719491 2.383193
 H 2.581436 -2.091524 -0.074635
 H 0.960932 -5.003542 1.809563
 H 1.779369 -6.578687 -0.677797
 H 1.268097 -7.245221 0.892810
 H 2.420585 -4.345638 -0.799278
 H 1.491025 -1.106746 1.816116
 H 0.063237 -6.630336 -0.255750
 H -3.411517 4.052179 1.998615
 H -2.418015 5.845071 3.320480
 H 1.817907 6.561904 3.126286
 H 2.069627 4.782192 1.470540
 H -0.430304 7.139982 4.043623

H 5.097584 2.684599 -1.304054
 H 0.277162 5.427446 -1.062022
 H 5.024819 4.861457 -2.431983
 H 3.809020 6.949118 -2.981691
 H 1.421043 7.206701 -2.308476
 H 0.170934 -1.338110 -3.853659
 H 1.576766 1.417560 -3.398685
 H 1.836742 -1.204471 -3.249631
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 H 0.099903 2.082872 -2.665244
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 H -5.946069 1.493224 -1.955639
 H -5.758159 -0.227904 1.951732
 H 5.394887 -0.970734 2.769226
 H 6.106696 -2.115984 -1.276123
 H -2.729535 3.351367 -1.584032
 H -7.473732 -0.864047 0.578751
 H -2.565946 1.502429 2.851312
 H 3.028723 1.738838 1.964192
 H 3.840502 0.407295 -2.738458
 H 6.633829 -2.842480 2.397615
 H 8.771286 -3.499650 1.314503
 H 8.289374 -2.686231 -0.182936
 H 8.571276 -1.735711 1.284252
 H 6.714299 -5.033299 1.269827
 H 5.087683 -4.337710 1.096486
 H 6.217010 -4.310293 -0.266104
 H 4.608920 3.071717 3.333355
 H 5.903671 1.904526 2.999962
 H 5.226859 2.875171 1.681228
 H 3.020902 1.327746 4.323374
 H 2.812635 -0.242627 3.526225
 H 4.373143 0.200480 4.239319
 H 5.839740 0.591917 -4.224010
 H 6.117720 1.458668 -2.704780
 H 6.852219 -0.128080 -2.958930
 H 4.197230 -1.374586 -4.327293
 H 5.409435 -2.164017 -3.323162
 H 3.717642 -2.178237 -2.818010
 H -4.234455 4.936553 -2.745133
 H -5.645018 3.962979 -2.292719
 H -4.691779 4.769638 -1.038020
 H -3.131991 3.003781 -3.977460
 H -2.897955 1.436578 -3.172493
 H -4.520900 1.962422 -3.647853
 H -9.463574 0.332049 -0.309564
 H -8.504618 1.401244 0.735138
 H -8.421451 1.574845 -1.024830
 H -8.325273 -1.525599 -1.638936
 H -7.282854 -0.345656 -2.442148
 H -6.561797 -1.719448 -1.589406
 H -3.903538 1.405923 4.920371
 H -4.644213 2.535435 3.769892
 H -5.345116 0.929103 4.009064
 H -2.597165 -0.613613 4.093204
 H -3.980420 -1.196150 3.154363

H -2.425243 -0.919754 2.352233

VII-si-c

E0 = -3426.0753065
E0+ZPE = -3424.671271
E298 = -3424.591335
H298 = -3424.590390
G298 = -3424.787131
NImag = 1, (-188.6695)
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C -4.388739 0.815183 1.156546
C -5.560856 0.174001 0.730340
C -6.088851 0.342199 -0.549331
C -5.411647 1.202860 -1.418813
C -2.508436 2.448112 0.705923
C -1.199588 2.263063 0.155693
C -0.121479 3.068463 0.498091
C -0.271275 3.991101 1.595600
C -1.568426 4.178434 2.169197
C -2.658251 3.425885 1.668254
C 0.815449 4.715273 2.161942
C 0.620503 5.589709 3.209099
C -0.671313 5.799945 3.745787
C -1.741484 5.103485 3.234073
C 1.185429 2.999246 -0.224272
C 1.766267 4.177720 -0.811780
C 3.122305 4.125412 -1.266626
C 3.866219 2.931807 -1.076521
C 3.297009 1.765725 -0.603923
C 1.899814 1.810466 -0.287069
C 1.041360 5.386697 -1.001683
C 1.630068 6.481163 -1.597719
C 2.978685 6.433708 -2.022694
C 3.706958 5.277491 -1.857362
C 4.173746 0.587163 -0.266279
C 4.752088 -0.230975 -1.267138
C 5.618551 -1.263390 -0.885631
C 5.938065 -1.517195 0.448410
C 5.378099 -0.682455 1.416656
C 4.513261 0.369223 1.095909
C 4.508772 -0.008168 -2.760461
C 4.313569 -1.323069 -3.541573
C 4.047414 1.308519 2.212519
C 3.879283 0.625984 3.581276
C 6.862468 -2.660141 0.846803
C 8.258519 -2.528461 0.209493
O 1.258647 0.625787 0.046477
P -0.006351 0.035356 -0.897434
Pd -0.654458 -2.165341 -0.365277
C -3.153655 -2.203682 -0.996574
C -3.598606 -3.292616 -0.229080
C -3.153034 -4.604972 -0.356674
C -3.568575 -5.668531 0.620630
O -1.069712 1.326598 -0.854282
C -3.919304 0.568629 2.592073

C -3.747552 -0.927977 2.911364
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 C -7.103609 -1.358582 -2.135300
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 C -4.546228 4.131090 -2.144372
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 N 0.384041 0.190966 -2.523177
 C 0.464607 1.444065 -3.275375
 C 0.716271 -0.981856 -3.327329
 C 5.016078 2.504519 2.346345
 C 6.236550 -4.032026 0.528526
 C 5.660776 0.792536 -3.405066
 N -0.191157 -2.926141 1.579854
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 C -0.173721 -5.034116 -2.356761
 C 1.497415 -4.960042 -0.500202
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 H 0.470565 -5.743167 -2.889294
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 H 1.770515 -4.194404 3.007545
 H 2.461522 -2.762659 2.203360
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 H -3.958696 -6.554329 0.103829
 H -4.213138 -3.054273 0.636286
 H -2.108053 -1.296590 -2.625194
 H -2.713183 -5.981656 1.230102
 H -3.647387 3.612401 2.076695
 H -2.738361 5.237414 3.647258
 H 1.470660 6.119716 3.629900

H 1.815267 4.564432 1.773114
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 H 4.930130 2.947340 -1.294724
 H 0.005795 5.436979 -0.684857
 H 4.742226 5.224191 -2.185879
 H 3.432821 7.306705 -2.483124
 H 1.051601 7.389275 -1.744153
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 H 1.503983 1.679727 -3.540705
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 H 0.052831 2.268931 -2.698833
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 H -5.814995 1.370669 -2.414028
 H -6.082422 -0.480371 1.424801
 H 5.634423 -0.856376 2.457384
 H 6.056182 -1.889672 -1.657237
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 H -2.938350 1.035723 2.717143
 H 3.066986 1.709249 1.938214
 H 3.593232 0.585032 -2.866057
 H 6.991986 -2.603556 1.936251
 H 8.920096 -3.328749 0.562145
 H 8.207281 -2.599675 -0.883587
 H 8.720979 -1.567455 0.460569
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 H 6.092244 -4.161131 -0.550981
 H 4.673962 3.189313 3.132292
 H 6.020811 2.156687 2.615907
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 H -6.322919 -2.082981 -1.878772
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 H -4.699795 -1.469426 2.858857
 H -3.043477 -1.408822 2.225401

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H -4.985667 2.297782 3.437718
H -5.877588 0.776446 3.554026

VIII-*re*

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E0+ZPE = -3793.853322
E298 = -3793.779218
H298 = -3793.778274
G298 = -3793.966085
NImag = 1, (-194.3303)
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C -6.920320 -1.841254 -2.268639
C -5.642476 -2.356715 -2.660795
C -5.534125 -3.422247 -3.517132
C -6.695759 -4.058160 -4.040734
C -9.363154 -2.056529 -2.405804
C -9.527088 -0.971011 -1.540992
C -8.361018 -0.287111 -1.026793
C -7.065744 -0.739458 -1.389035
C -10.829651 -0.515669 -1.163894
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C -9.848601 1.261667 0.146604
C -8.582818 0.852476 -0.185512
C -5.861819 -0.038270 -0.845234
C -5.002574 0.691107 -1.683674
C -3.925947 1.408732 -1.167052
C -3.675610 1.440380 0.215402
C -4.505515 0.675112 1.050172
C -5.573396 -0.054507 0.529220
C -2.682195 2.390076 0.786116
C -1.369928 2.568961 0.248257
C -0.559163 3.642443 0.592955
C -0.951965 4.479118 1.693645
C -2.221407 4.252492 2.316642
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O -0.914792 1.648460 -0.689740
P 0.311521 0.589983 -0.244502
N 0.776331 0.161318 -1.790795
C 1.619494 -1.021311 -1.968045
C 0.697034 3.902190 -0.171808
C 0.907263 5.136174 -0.878208
C 2.158984 5.340564 -1.545582
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C 2.927666 3.104306 -0.889972
C 1.667618 2.916340 -0.241088
C 2.389554 6.559756 -2.239498
C 1.418850 7.532608 -2.302395
C 0.169189 7.319330 -1.673701
C -0.080118 6.155112 -0.979789
C 3.980904 2.054519 -0.915720

C 4.693227 1.804172 -2.101450
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 C 8.528863 -0.446122 -1.057398
 C 9.590353 -1.426567 -1.111172
 C 9.268781 -2.786880 -1.138757
 C 7.942387 -3.227833 -1.117958
 C 6.871621 -2.257226 -1.070852
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 C 11.258473 0.351494 -1.090697
 C 10.217081 1.321266 -1.023444
 C 8.901281 0.936899 -1.005818
 C 7.619539 -4.621068 -1.149353
 C 6.318246 -5.046261 -1.142233
 C 5.258889 -4.094407 -1.107122
 C 5.526203 -2.750040 -1.073968
 Pd 0.148025 -1.122594 1.347990
 C 0.660351 0.217149 3.049193
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 C -0.713218 -3.555009 1.854549
 O -1.205406 -4.617373 2.262049
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 H 2.978531 -4.669865 1.540051
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 H -2.493104 -2.683606 -2.285046
 H -2.212872 -1.364258 -1.128243

H -0.840093 -2.189115 -1.889745
 H 1.405597 -0.360553 3.582841
 H -1.356339 0.912279 3.096476
 H 0.374519 -2.011272 4.850671
 H -2.495504 -2.935826 5.358847
 H -1.448333 -4.074483 4.505017
 H -2.408541 -0.920932 4.167651
 H 1.008369 1.177304 2.684225
 H -1.016620 -3.544694 6.144308
 H -4.070719 3.143729 2.220079
 H -3.589575 4.890217 3.865943
 H 0.141376 7.024226 3.698559
 H 0.863437 5.661529 1.789380
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 H 4.099927 4.510077 -1.988163
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 H 3.349289 6.703643 -2.730135
 H 1.603905 8.458063 -2.840483
 H -0.603872 8.079833 -1.741814
 H 0.328625 0.471050 -3.814780
 H 1.281421 -1.583358 -2.847384
 H 0.074186 1.887254 -2.774687
 H 1.729378 1.401441 -3.225805
 H 2.671748 -0.740850 -2.114353
 H 1.540493 -1.673698 -1.093963
 H 4.429359 2.344448 -3.006791
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 H -5.200246 0.718926 -2.751688
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 H -9.984118 2.131274 0.784270
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 H -10.244372 -2.563969 -2.793263
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 H 8.119947 1.686677 -0.947239
 H 10.472249 2.376838 -0.981597
 H 11.735472 -1.732105 -1.175054
 H 10.071101 -3.521021 -1.177377
 H 12.295470 0.675728 -1.105129
 H 4.709236 -2.037346 -1.048936
 H 4.229070 -4.440858 -1.107892
 H 8.436987 -5.337627 -1.180795
 H -4.747098 -1.895855 -2.261846
 H -4.550859 -3.792381 -3.795269
 H -8.834447 -4.093425 -4.063415
 H -6.589749 -4.901288 -4.717905
 H 6.086722 -6.107549 -1.166715

VIII-re-b

E0+ZPE = -3793.850628

E298 = -3793.776455

H298 = -3793.775511

G298 = -3793.964017
 NImag = 1, (-159.5849)
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 C 7.038755 -2.184538 -1.415242
 C 8.147640 -3.077586 -1.668825
 C 7.943977 -4.489894 -1.568933
 C 6.719014 -5.007050 -1.243466
 C 5.619475 -4.133503 -1.005584
 C 7.232380 -0.784294 -1.509420
 C 8.506551 -0.262381 -1.844622
 C 9.603185 -1.167546 -2.107153
 C 9.394138 -2.546319 -2.012062
 C 10.884150 -0.631910 -2.451344
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 C 10.020165 1.616683 -2.243447
 C 8.775971 1.143692 -1.914936
 C 6.091049 0.149456 -1.259674
 C 5.524415 0.889507 -2.309094
 C 4.477577 1.779905 -2.074164
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 C 4.504594 1.204860 0.262787
 C 5.559276 0.324022 0.028001
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 C 0.959334 5.050262 -0.159714
 C 0.739656 3.733281 0.379268
 C 1.674792 2.738494 0.137897
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 H 6.578385 -6.081790 -1.167978

VIII-si

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 C 7.848094 -3.302377 -0.869412
 C 7.468517 -4.681441 -0.842522

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 C 9.567761 -1.569751 -0.924741
 C 8.546356 -0.546361 -0.920508
 C 7.182416 -0.921113 -0.895378
 C 10.943675 -1.179863 -0.950999
 C 11.304484 0.140819 -0.965727
 C 10.302032 1.153065 -0.951141
 C 8.971964 0.821868 -0.928192
 C 6.117149 0.130355 -0.885941
 C 5.728750 0.782024 -2.065156
 C 4.717229 1.743587 -2.052833
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 C 4.451900 1.438418 0.320251
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 C 0.979636 5.160099 -0.854445
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VIII-si-c

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 H 7.782851 1.243651 0.203530
 H 9.909490 1.686261 1.337484
 H 11.346757 -2.234419 0.299047
 H 9.939379 -3.742127 -1.008004
 H 11.702211 -0.050283 1.403743
 H 4.852035 -1.959509 -2.387134
 H 8.562752 -5.279503 -2.313399
 H 6.435900 -5.809923 -3.458133
 H 4.581103 -4.138700 -3.477855
 H 1.164134 -1.537012 -3.207352
 H 2.545625 -0.622774 -2.543202
 H 0.170712 0.523799 -4.133322
 H -0.162675 1.894404 -3.054785

(IX-re)

E0 = -2875.6993067
 E0+ZPE = -2874.690810
 E298 = -2874.631817
 H298 = -2874.630873
 G298 = -2874.782742
 NImag = 1, (-200.2966)
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 C 2.699507 3.491736 -0.626506
 C 1.743642 3.619834 -1.650279
 C 1.175683 4.858951 -1.944638
 C 1.543938 5.996566 -1.222194
 C 2.493078 5.885219 -0.205184
 C 3.375309 2.195196 -0.349150
 C 4.742310 2.162078 -0.145280
 C 5.449576 0.956560 0.084286
 C 4.748210 -0.290197 0.014205
 C 3.340177 -0.276479 -0.277159
 C 2.680471 0.942199 -0.341202
 C 6.842702 0.960694 0.366092
 C 7.520466 -0.213733 0.599523
 C 6.824613 -1.445231 0.560798
 C 5.477539 -1.483996 0.272123
 C 2.591036 -1.545005 -0.515237
 C 1.506267 -1.883683 0.280234
 C 0.885897 -3.171028 0.228846
 C 1.303130 -4.039340 -0.762794
 C 2.300124 -3.691700 -1.706887
 C 2.970037 -2.432028 -1.583340

C 2.662387 -4.577490 -2.757847
 C 3.627743 -4.229352 -3.674119
 C 4.269234 -2.972103 -3.574780
 C 3.953234 -2.099193 -2.556324
 C -0.092822 -3.641059 1.245421
 C -1.240861 -4.349177 0.855137
 C -2.094427 -4.908737 1.806689
 C -1.814167 -4.771365 3.167061
 C -0.679390 -4.062735 3.568439
 C 0.171282 -3.498931 2.618581
 O 1.033104 -0.959609 1.203650
 P 0.187665 0.387786 0.655835
 Pd -1.878620 0.323222 -0.502085
 C -1.407182 -1.176489 -2.543502
 C -2.704212 -1.605494 -2.860826
 C -3.752023 -0.764614 -3.233829
 C -5.148334 -1.293763 -3.406728
 O 1.307747 0.953995 -0.485710
 N 0.293570 1.310757 2.053292
 C 1.484548 1.205036 2.955698
 C 1.186048 0.392456 4.228169
 C -0.786764 2.330548 2.240468
 C -0.454588 3.702595 1.630508
 C -1.276986 2.469999 3.688584
 N -3.748409 0.661403 -1.441718
 C -4.198033 2.076038 -1.726209
 C -3.150631 2.791173 -2.597192
 N -3.633558 -0.190358 0.631459
 C -4.057847 -0.713151 1.945743
 C -4.926910 0.331569 2.677004
 C -0.918089 0.152807 -2.500526
 C -4.505711 0.067466 -0.348062
 O -5.729475 -0.123343 -0.416865
 C -4.855530 -2.025327 1.766426
 C -2.798980 -1.016337 2.764402
 C 2.158996 2.544532 3.281973
 C -5.546906 2.073261 -2.483955
 C -4.367893 2.884621 -0.419419
 H -3.485033 3.815048 -2.801523
 H -2.180824 2.843804 -2.092141
 H -3.013959 2.296674 -3.565261
 H -5.859462 3.108755 -2.667761
 H -5.456511 1.577432 -3.456159
 H -6.313609 1.561445 -1.902029
 H -4.634365 3.920463 -0.660662
 H -5.160186 2.466101 0.206371
 H -3.438089 2.898494 0.158679
 H -5.112041 -2.443970 2.748213
 H -5.771508 -1.845406 1.201690
 H -4.249747 -2.763651 1.229948
 H -5.228178 -0.035730 3.666205
 H -4.370061 1.265968 2.815760
 H -5.829596 0.546395 2.097943
 H -3.068054 -1.397587 3.756642
 H -2.184565 -1.768492 2.262772
 H -2.190995 -0.117745 2.895214

H -1.425836 0.916219 -3.078051
 H -0.722432 -1.950515 -2.196969
 H -3.515803 0.165248 -3.734123
 H -5.156233 -2.388994 -3.378948
 H -5.792074 -0.939064 -2.593395
 H -2.947809 -2.643518 -2.641007
 H 0.153112 0.289481 -2.409817
 H -5.585931 -0.963056 -4.356513
 H 0.869040 -5.034565 -0.807938
 H 2.151579 -5.534815 -2.828480
 H 5.016342 -2.689684 -4.311433
 H 4.448210 -1.136812 -2.501015
 H 3.891765 -4.910637 -4.478133
 H 5.303982 3.091836 -0.176693
 H 4.958768 -2.435605 0.254119
 H 7.361397 1.915742 0.403684
 H 8.583868 -0.198736 0.821502
 H 7.357014 -2.370376 0.764228
 H 2.215828 0.624291 2.391852
 H 2.787330 6.761540 0.366375
 H 0.445520 4.935502 -2.746026
 H -0.452029 -3.952127 4.625431
 H -2.980624 -5.447858 1.483389
 H 2.129053 0.156151 4.736490
 H 0.557133 0.938893 4.936031
 H 0.688307 -0.547339 3.974494
 H 3.096067 2.341701 3.813773
 H 2.398139 3.103302 2.374538
 H 1.548260 3.178828 3.930807
 H -1.633468 1.932642 1.667785
 H -1.352918 4.332036 1.645649
 H 0.328774 4.229086 2.182092
 H -0.129744 3.602708 0.591340
 H -2.170676 3.104334 3.690058
 H -1.551794 1.506370 4.123355
 H -0.539635 2.949343 4.339464
 H 1.058965 -2.963258 2.939161
 H -1.468904 -4.453374 -0.202118
 H -2.477401 -5.207988 3.908634
 H 1.452488 2.747522 -2.224167
 H 3.796137 4.570268 0.887227
 H 1.095994 6.959696 -1.450934

(IX-re)₁

E0 = -2875.6946036
 E0+ZPE = -2874.686248
 E298 = -2874.627144
 H298 = -2874.626200
 G298 = -2874.778987
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 C -1.176834 -4.541178 0.701041
 C -1.912387 -5.221473 1.671676
 C -1.553950 -5.128585 3.017202
 C -0.459613 -4.342259 3.384930

C 0.809239 -3.166783 0.009767
 C 1.415328 -1.874844 0.128267
 C 2.488786 -1.488737 -0.661717
 C 2.818880 -2.279460 -1.817928
 C 2.128605 -3.515241 -2.030512
 C 1.181023 -3.945793 -1.070459
 C 3.772533 -1.868846 -2.790268
 C 4.035302 -2.644737 -3.898597
 C 3.369825 -3.878483 -4.091276
 C 2.436323 -4.301929 -3.173437
 C 3.298181 -0.283159 -0.319735
 C 4.707771 -0.393526 -0.058512
 C 5.472362 0.805125 0.114287
 C 4.823829 2.059772 0.005259
 C 3.458309 2.176959 -0.176644
 C 2.699453 0.965104 -0.263677
 C 5.379302 -1.640923 0.068857
 C 6.730879 -1.696089 0.332386
 C 7.488493 -0.509451 0.475072
 C 6.867873 0.713974 0.368449
 C 2.849978 3.524576 -0.344748
 C 3.236383 4.588090 0.489073
 C 2.728841 5.873588 0.295969
 C 1.827818 6.123043 -0.740262
 C 1.440572 5.076654 -1.581130
 C 1.942914 3.791150 -1.385164
 O 1.327441 1.048136 -0.383260
 P 0.204567 0.431703 0.728747
 N 0.434720 1.201998 2.203807
 C -0.402285 2.383653 2.600190
 C -0.487470 3.456838 1.506900
 O 0.961016 -1.019845 1.125380
 Pd -1.894607 0.527251 -0.400098
 C -0.957197 0.817919 -2.390954
 C -1.325448 -0.517855 -2.693909
 C -2.581806 -0.983495 -3.102344
 C -3.692326 -0.168509 -3.322204
 C -5.042822 -0.758767 -3.613975
 N -3.786762 0.886645 -1.291432
 C -4.495328 0.026075 -0.353376
 O -5.692767 -0.264069 -0.508412
 N -3.625804 -0.332915 0.593917
 C -4.037686 -1.196773 1.723209
 C -2.805231 -1.504709 2.580101
 C 1.533884 0.822881 3.148386
 C 2.514747 1.969140 3.441836
 C 0.970147 0.218189 4.442344
 C -1.792365 2.014920 3.132173
 C -4.363493 2.284068 -1.311951
 C -4.610857 2.811121 0.119718
 C -3.388419 3.243070 -2.016552
 C -5.706377 2.305897 -2.080851
 C -5.104712 -0.484933 2.582842
 C -4.606653 -2.528596 1.182062
 H -3.809827 4.255081 -2.017813
 H -2.420771 3.278913 -1.506243

H -3.219665 2.962777 -3.062273
 H -6.106091 3.327676 -2.075955
 H -5.571464 2.007944 -3.125642
 H -6.427493 1.632797 -1.617054
 H -4.989060 3.839309 0.071203
 H -5.350495 2.201317 0.645028
 H -3.686214 2.816375 0.704287
 H -4.860441 -3.196514 2.015195
 H -5.501026 -2.349450 0.582954
 H -3.858497 -3.031025 0.559520
 H -5.398709 -1.114902 3.432142
 H -4.713468 0.458644 2.980930
 H -5.994452 -0.270099 1.985173
 H -3.069986 -2.191812 3.391705
 H -2.023590 -1.974689 1.978573
 H -2.393937 -0.596902 3.026059
 H -1.537842 1.626837 -2.817674
 H -0.573284 -1.282181 -2.499388
 H -3.525367 0.853574 -3.635989
 H -4.965205 -1.836120 -3.797576
 H -5.709817 -0.618388 -2.755093
 H -2.740367 -2.060243 -3.089778
 H 0.098440 1.027455 -2.271829
 H -5.505790 -0.284889 -4.488085
 H 0.758798 -4.941856 -1.170463
 H 1.910258 -5.243362 -3.312468
 H 4.758545 -2.303278 -4.634068
 H 4.284665 -0.922103 -2.663393
 H 3.591659 -4.483020 -4.966291
 H 5.429678 2.961068 0.047640
 H 4.812514 -2.559476 -0.030593
 H 7.435222 1.634324 0.485082
 H 8.554678 -0.568055 0.675440
 H 7.219191 -2.661397 0.434558
 H 2.101142 0.042303 2.644130
 H 3.036272 6.678298 0.958602
 H 0.746975 5.261839 -2.397049
 H -0.170588 -4.265472 4.429850
 H -2.770542 -5.818028 1.374977
 H 1.791614 -0.129262 5.080645
 H 0.395343 0.952484 5.018294
 H 0.319700 -0.633110 4.220338
 H 3.377431 1.566625 3.985310
 H 2.878659 2.424599 2.518099
 H 2.078608 2.754520 4.069081
 H 0.147395 2.830104 3.432353
 H -2.287901 2.918408 3.508818
 H -2.422980 1.583436 2.350429
 H -1.726943 1.298613 3.955796
 H -1.023997 4.330430 1.895235
 H 0.504083 3.777946 1.181139
 H -1.038496 3.094028 0.631656
 H 1.134011 -3.067062 2.710932
 H -1.468701 -4.611274 -0.343117
 H -2.125111 -5.659976 3.773524
 H 1.641225 2.990057 -2.050776

H 3.931099 4.401822 1.303613
H 1.431289 7.123133 -0.892538

(IX-re)₂

E0 = -2875.6888963
E0+ZPE = -2874.680572
E298 = -2874.621612
H298 = -2874.620668
G298 = -2874.772034
NImag = 1, (-205.2753)
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C -1.409482 -4.201061 0.766450
C -2.227689 -4.816348 1.714660
C -1.852270 -4.837403 3.058870
C -0.652276 -4.238768 3.448465
C 0.746199 -3.085352 0.117482
C 1.412324 -1.823272 0.215910
C 2.490334 -1.491313 -0.593767
C 2.797367 -2.330218 -1.721461
C 2.069053 -3.549971 -1.896638
C 1.093108 -3.910564 -0.936367
C 3.766776 -1.982600 -2.703421
C 4.011407 -2.805113 -3.781441
C 3.309514 -4.024403 -3.934745
C 2.357674 -4.385643 -3.009594
C 3.317805 -0.283947 -0.304383
C 4.724838 -0.399563 -0.030983
C 5.497001 0.795776 0.133165
C 4.857769 2.054178 0.006953
C 3.497010 2.174396 -0.198093
C 2.729503 0.970654 -0.286119
C 5.386279 -1.649447 0.125252
C 6.734681 -1.710271 0.403295
C 7.499708 -0.527320 0.535211
C 6.888814 0.698567 0.403696
C 2.893933 3.522953 -0.375509
C 3.165194 4.550834 0.541740
C 2.665646 5.839090 0.341548
C 1.891669 6.123643 -0.784459
C 1.618565 5.110337 -1.707149
C 2.110657 3.821681 -1.503658
O 1.359786 1.067417 -0.417164
P 0.233500 0.489163 0.719966
N 0.420734 1.354930 2.153322
C -0.170192 2.733032 2.287953
C -0.649594 3.380745 0.985693
O 1.002874 -0.923675 1.199260
Pd -1.856509 0.464383 -0.450133
C -0.888865 0.389970 -2.443965
C -1.306150 -0.962459 -2.533240
C -2.576608 -1.448144 -2.869658
C -3.665433 -0.648657 -3.217286
C -5.031951 -1.245210 -3.411104
N -3.738990 0.728340 -1.400258
C -4.476911 0.082846 -0.322748

O -5.689113 -0.168856 -0.414820
 N -3.610881 -0.135480 0.670686
 C -4.046612 -0.669654 1.977312
 C -2.795054 -0.908531 2.827308
 C 1.230662 0.971131 3.363534
 C 0.611722 -0.181624 4.163959
 C 2.727993 0.756627 3.109915
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 C -4.276601 2.114949 -1.681408
 C -4.580942 2.882807 -0.373921
 C -3.244556 2.919994 -2.489374
 C -5.585062 2.031729 -2.504081
 C -4.975937 0.341212 2.682573
 C -4.789101 -2.012504 1.792721
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 H -2.297291 3.014111 -1.949290
 H -3.042746 2.464989 -3.465538
 H -5.968394 3.045904 -2.672085
 H -5.414238 1.576373 -3.484794
 H -6.334711 1.446735 -1.970798
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 H -3.698108 2.943932 0.268627
 H -5.035831 -2.441374 2.772748
 H -5.706880 -1.868756 1.220738
 H -4.150877 -2.725227 1.261012
 H -5.280733 -0.032779 3.668233
 H -4.465695 1.300968 2.825646
 H -5.875273 0.511282 2.083990
 H -3.068382 -1.283927 3.820863
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 H -2.230890 0.019092 2.952187
 H -1.433194 1.142301 -3.002526
 H -0.581961 -1.710974 -2.214038
 H -3.473152 0.302478 -3.695890
 H -4.979341 -2.339551 -3.425753
 H -5.692373 -0.957400 -2.584782
 H -2.766823 -2.504312 -2.686041
 H 0.173619 0.578736 -2.345714
 H -5.489132 -0.902998 -4.347389
 H 0.617069 -4.884041 -1.017816
 H 1.801898 -5.313695 -3.119495
 H 4.748583 -2.512198 -4.523964
 H 4.306792 -1.048008 -2.606768
 H 3.517673 -4.665998 -4.786384
 H 5.464985 2.954335 0.059002
 H 4.814469 -2.565781 0.035400
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 H 8.563220 -0.590403 0.747995
 H 7.214452 -2.677473 0.526074
 H 1.161655 1.861765 3.996523
 H 2.882171 6.619142 1.066751
 H 1.022573 5.323994 -2.590446
 H -0.347275 -4.256091 4.491404
 H -3.162906 -5.272463 1.402367
 H 3.243626 0.691425 4.075768

H 2.925171 -0.164327 2.559623
 H 3.161624 1.592123 2.553082
 H 1.186672 -0.336304 5.085476
 H -0.422416 0.039546 4.440987
 H 0.615070 -1.112220 3.595829
 H 0.662275 3.353925 2.647149
 H -1.587295 3.819163 3.514545
 H -2.173802 2.234902 2.974093
 H -0.993581 2.347250 4.293018
 H -0.939175 4.413924 1.208390
 H 0.129111 3.410959 0.222640
 H -1.526805 2.871292 0.574446
 H 1.115600 -3.195411 2.805152
 H -1.713499 -4.176628 -0.276256
 H -2.490579 -5.314835 3.797118
 H 1.896151 3.041186 -2.226830
 H 3.765326 4.333669 1.421577
 H 1.504663 7.126474 -0.943289

(IX-re)₃

E0 = -2875.6964034
 E0+ZPE = -2874.688531
 E298 = -2874.629342
 H298 = -2874.628398
 G298 = -2874.781178
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 C -1.320808 -4.338727 0.848693
 C -2.111872 -4.962952 1.813565
 C -1.740271 -4.923789 3.158353
 C -0.572686 -4.254081 3.530972
 C 0.771836 -3.131007 0.165887
 C 1.423140 -1.860101 0.259436
 C 2.476755 -1.505031 -0.571126
 C 2.765807 -2.327980 -1.716695
 C 2.051755 -3.557027 -1.884435
 C 1.107026 -3.941778 -0.902798
 C 3.700092 -1.954950 -2.722954
 C 3.925965 -2.762347 -3.816546
 C 3.240552 -3.991788 -3.961829
 C 2.322153 -4.377617 -3.013141
 C 3.301012 -0.293566 -0.292755
 C 4.719630 -0.406047 -0.081006
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 C 4.851972 2.045977 -0.079898
 C 3.481344 2.167390 -0.206587
 C 2.710736 0.960055 -0.241857
 C 5.388681 -1.653717 0.057929
 C 6.748978 -1.711041 0.272405
 C 7.518971 -0.526731 0.352014
 C 6.901420 0.697241 0.234405
 C 2.873934 3.517714 -0.349162
 C 3.312720 4.577621 0.462743
 C 2.807932 5.867418 0.295528
 C 1.855009 6.124641 -0.691394

C 1.412185 5.081207 -1.508209
 C 1.912882 3.790819 -1.338793
 O 1.339236 1.064437 -0.307847
 P 0.188607 0.409385 0.760331
 N 0.187044 1.256159 2.209819
 C -0.750042 2.426889 2.254810
 C -1.625430 2.455762 3.515435
 O 1.014820 -0.967966 1.251828
 Pd -1.840654 0.441867 -0.486244
 C -0.815419 0.508001 -2.455441
 C -1.258505 -0.822468 -2.660713
 C -2.530680 -1.251051 -3.065792
 C -3.590692 -0.404019 -3.385486
 C -4.963794 -0.949749 -3.661825
 N -3.687973 0.825561 -1.454356
 C -4.462980 0.099318 -0.458386
 O -5.676938 -0.118849 -0.595249
 N -3.621188 -0.234182 0.524871
 C -4.089453 -0.892169 1.761494
 C -2.863739 -1.224765 2.617810
 C 1.078813 1.090810 3.401522
 C 0.649587 -0.096520 4.274948
 C 2.580851 1.061150 3.098856
 C -0.015105 3.760055 2.063967
 C -4.177243 2.246758 -1.612550
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 C -3.122459 3.080924 -2.359507
 C -5.493271 2.279469 -2.425745
 C -5.037176 0.046112 2.538480
 C -4.825466 -2.208085 1.418568
 H -3.483577 4.109986 -2.471083
 H -2.174844 3.109187 -1.811982
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 H -5.345351 1.887554 -3.437321
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 H -5.233560 2.402483 0.303199
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 H -5.105714 -2.732087 2.341479
 H -5.723753 -2.005889 0.833066
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 H -5.374601 -0.426615 3.469566
 H -4.527195 0.981665 2.796451
 H -5.916027 0.283914 1.932679
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 H -2.202892 -1.921811 2.096839
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 H -3.365571 0.579393 -3.777071
 H -4.938096 -2.041569 -3.749239
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 H -2.747946 -2.313136 -2.966598
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H 0.647459 -4.923298 -0.980685
 H 1.778349 -5.313517 -3.116281
 H 4.635754 -2.449367 -4.577329
 H 4.227940 -1.012911 -2.633019
 H 3.434346 -4.621567 -4.825597
 H 5.463258 2.944600 -0.076990
 H 4.813973 -2.571294 0.007427
 H 7.477369 1.616954 0.304901
 H 8.591530 -0.587085 0.514171
 H 7.234393 -2.676678 0.384993
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 H 3.156745 6.669684 0.940426
 H 0.676630 5.272325 -2.285146
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 H -3.023450 -5.472126 1.513587
 H 3.131178 1.082772 4.047039
 H 2.877315 0.158527 2.561070
 H 2.885294 1.932191 2.512881
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 H -0.400426 -0.013164 4.569360
 H 0.776774 -1.040306 3.741562
 H -1.425377 2.290809 1.400580
 H -0.735986 4.586104 2.070555
 H 0.702232 3.945008 2.872787
 H 0.525309 3.784144 1.115959
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 H -2.165455 1.518092 3.657678
 H -1.045860 2.665807 4.421530
 H 1.140942 -3.140379 2.860974
 H -1.623183 -4.361032 -0.194539
 H -2.356634 -5.408640 3.910363
 H 1.566403 2.991482 -1.984428
 H 4.044725 4.382872 1.241897
 H 1.460253 7.128357 -0.823404

(IX-si)

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 H298 = -2874.629903
 G298 = -2874.780027
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 C 2.475163 -2.762323 -1.536406
 C 1.615274 -3.906322 -1.579857
 C 0.632359 -4.070322 -0.573401
 C 3.453143 -2.618737 -2.559270

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 C 2.747427 -4.704616 -3.580574
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 C 3.799967 4.235463 0.001943
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 C 2.045779 4.751434 -2.096515
 C 2.385699 3.436190 -1.780495
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 C -4.190041 -2.161004 -1.299959
 O 0.898846 -0.895837 1.237063
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 C -2.775444 2.945520 -2.260119
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 H -1.958381 0.329705 2.812383
 H -1.420565 0.644557 -3.184259
 H -0.788784 3.184122 -1.563421
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 H 2.863592 -5.443189 -4.368877
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 H 4.476789 -3.062449 0.217850
 H 7.595638 0.810078 0.271236
 H 8.443547 -1.480458 0.691191
 H 6.859099 -3.407628 0.681975
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 H -3.604371 -4.870341 2.016528
 H 1.370373 4.945129 -2.925668
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 H -1.720598 3.714019 3.468701
 H -1.366368 2.062738 3.988811
 H -0.143267 3.339758 4.159666
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 H 2.805908 2.975873 2.268391
 H 1.954416 3.243577 3.801984
 H 2.081200 0.220936 4.757744
 H 0.627650 1.219425 4.878172
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 H -0.706909 4.683824 1.358749
 H 0.909793 4.393668 2.011137
 H 0.474881 3.744179 0.426998
 H 4.482405 4.040329 0.824634
 H 1.980169 2.621474 -2.369864
 H 2.305762 6.838380 -1.606405
 H -2.942252 -4.508126 4.388659
 H 0.749115 -2.741196 3.072561
 H -2.096923 -4.173111 0.187405

(IX-sf)₁

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 C -2.269084 -4.127146 3.822889
 C -0.996852 -3.593320 4.039093
 C 0.214302 -3.026435 0.487353
 C 1.068593 -1.880002 0.422888
 C 2.105353 -1.775190 -0.492868
 C 2.163105 -2.715605 -1.581054
 C 1.241194 -3.810014 -1.599256
 C 0.328528 -3.958584 -0.527278
 C 3.070041 -2.585342 -2.669140
 C 3.073884 -3.496492 -3.703090
 C 2.180160 -4.593499 -3.702623
 C 1.283249 -4.743653 -2.670174
 C 3.158959 -0.729890 -0.342765
 C 4.540320 -1.110633 -0.195108
 C 5.543898 -0.089530 -0.184735
 C 5.150751 1.264388 -0.319294
 C 3.825884 1.646906 -0.383971
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 C 4.961571 -2.458619 -0.021022
 C 6.294898 -2.774810 0.127333
 C 7.285190 -1.764900 0.103284
 C 6.911706 -0.449325 -0.047725
 C 3.488509 3.088299 -0.537692
 C 4.099654 4.047513 0.286949
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 C 2.988603 5.839521 -0.899286
 C 2.379026 4.896618 -1.731254
 C 2.623905 3.535526 -1.551460
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 P 0.269213 0.590029 0.748738
 Pd -1.729468 0.567368 -0.556010
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 C -3.789985 -0.819113 -2.518235
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 O 0.881815 -0.849192 1.347851
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 C 1.307925 1.393338 3.294940
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 H 5.923079 2.026870 -0.379370
 H 4.218588 -3.246824 0.008771
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 H 8.333128 -2.029300 0.213806
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(IX-si)₂

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 H -3.083141 -4.394777 4.461576
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(IX-si)₃

E0 = -2875.6926543
 E0+ZPE = -2874.683830
 E298 = -2874.625023
 H298 = -2874.624079
 G298 = -2874.774329
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 C 3.182377 5.784298 -0.968009
 C 2.517279 4.848767 -1.764339
 C 3.820427 1.571402 -0.349896
 C 5.129223 1.139101 -0.243775
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 C 7.147160 -1.974659 0.135695
 C 6.125597 -2.951569 0.070061
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 C 1.128929 -3.737583 -1.888617

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 H 4.886533 3.639543 1.048183
 H 2.198715 2.764966 -2.188378
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(IX-si-c)

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 C -1.914689 -4.552043 3.532040

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 C 0.863456 -3.165687 0.549338
 C 1.463275 -1.867908 0.499453
 C 2.510712 -1.561231 -0.356453
 C 2.889268 -2.517628 -1.362971
 C 2.262851 -3.804528 -1.362263
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 C 3.829930 -2.234143 -2.392267
 C 4.150463 -3.179468 -3.342184
 C 3.556183 -4.463326 -3.314694
 C 2.629788 -4.764867 -2.343819
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 C 6.774282 -1.221636 0.519026
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(X-re)₁

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 C 5.409140 -0.702143 -0.382889
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 C -3.517576 0.791760 -3.632480
 C -4.977089 0.785521 -3.989557
 N -3.272485 1.909481 -1.626381
 C -3.223079 3.416695 -1.727702
 C -4.404207 3.942255 -2.577403
 C -4.302113 1.467306 -0.698066
 O -5.505820 1.699049 -0.886253
 C -3.430901 -0.479813 2.345032
 C -4.929365 1.547571 2.305094
 C 2.144374 1.312094 3.927619
 C -3.287277 4.076947 -0.331285
 C -1.908188 3.848530 -2.399328
 H -1.878929 4.941806 -2.474715
 H -1.038486 3.524919 -1.818614

H -1.815408 3.451972 -3.416447
 H -4.346347 5.036245 -2.636552
 H -4.363182 3.552252 -3.599571
 H -5.357035 3.653651 -2.133281
 H -3.192852 5.164453 -0.434582
 H -4.236659 3.863556 0.166465
 H -2.471197 3.723794 0.307345
 H -6.061887 -0.977778 1.986083
 H -6.325907 -0.004065 0.513549
 H -5.229067 -1.398009 0.474538
 H -5.450762 1.208450 3.209045
 H -4.103323 2.199086 2.613523
 H -5.629291 2.133846 1.702647
 H -3.917395 -0.804380 3.272954
 H -3.098372 -1.371125 1.806856
 H -2.544152 0.099972 2.607972
 H -0.801333 1.568788 -3.033317
 H -1.175232 -1.450293 -2.569417
 H -2.936448 1.646832 -3.952125
 H -5.340512 -0.238950 -4.126397
 H -5.567165 1.239235 -3.184536
 H -3.432724 -1.302992 -3.276731
 H 0.391989 0.357237 -2.372074
 H -5.165713 1.351618 -4.909908
 H -0.618291 -4.990454 -1.399465
 H 0.258481 -5.390834 -3.653008
 H 3.469507 -2.959436 -5.162639
 H 3.485840 -1.650147 -3.087771
 H 1.876204 -4.857382 -5.452268
 H 5.974260 1.365951 -0.163174
 H 3.811146 -3.718936 -0.682503
 H 7.557520 -0.478072 -0.290169
 H 8.023408 -2.905909 -0.488565
 H 6.122982 -4.516402 -0.648555
 H 1.922018 -0.348172 2.633418
 H 4.433846 5.114249 2.335453
 H 2.368323 5.413415 -1.401430
 H -0.969939 -5.013925 4.082497
 H -4.344104 -4.334340 1.534906
 H 1.364680 -1.198555 4.829416
 H -0.035594 -0.128205 4.970867
 H -0.028293 -1.416719 3.750052
 H 2.951177 0.790142 4.455390
 H 2.596192 1.990425 3.202976
 H 1.604618 1.905421 4.670881
 H -1.353280 2.035525 1.830254
 H -0.460115 4.224691 2.237082
 H 1.021020 3.600022 2.971296
 H 0.716339 3.340535 1.247767
 H -1.847015 2.991281 3.971776
 H -1.731422 1.238971 4.167803
 H -0.420960 2.292386 4.734282
 H 2.390847 3.650237 -2.914885
 H 3.201610 2.113896 -2.567761
 H 1.540987 2.369902 -2.035848
 H 3.845616 7.316059 1.468695

H 3.219767 7.483743 -0.181544
 H 2.120046 7.111522 1.146882
 H 4.959918 3.011613 3.267814
 H 4.773817 1.483567 2.388125
 H 6.112498 2.561682 2.014680
 H 1.188073 -4.759337 3.346572
 H 1.512025 -4.733886 1.605974
 H 1.394725 -3.219600 2.501544
 H -3.198730 -5.932264 4.688444
 H -4.022966 -4.370325 4.678508
 H -4.594645 -5.668212 3.627289
 H -4.161893 -3.389595 -0.529088
 H -2.788392 -2.327632 -0.852415
 H -2.779544 -3.988067 -1.449403

(X-re)₂

E0 = -3111.5800684
 E0+ZPE = -3110.404791
 E298 = -3110.335625
 H298 = -3110.334680
 G298 = -3110.507079
 NImag = 1, (-212.5731)
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 C 0.784816 -3.933515 0.167048
 C 0.647823 -4.589056 -1.076847
 C 1.729892 -5.312411 -1.589259
 C 2.941719 -5.417755 -0.903617
 C 3.054427 -4.766057 0.327252
 C -0.421467 -3.317559 0.808029
 C -1.098419 -2.156115 0.316800
 C -2.367110 -1.802890 0.760020
 C -2.899697 -2.454430 1.930981
 C -2.190669 -3.563008 2.490997
 C -0.993792 -3.990277 1.869360
 C -4.087879 -2.026945 2.588813
 C -4.551521 -2.673724 3.713736
 C -3.863445 -3.791301 4.242150
 C -2.704370 -4.222707 3.640170
 C -3.193165 -0.757886 0.086423
 C -4.520020 -1.052392 -0.382107
 C -5.383034 0.033313 -0.737811
 C -4.918081 1.363166 -0.570594
 C -3.615903 1.655159 -0.212076
 C -2.731961 0.546107 0.002446
 C -5.009936 -2.378832 -0.533288
 C -6.282704 -2.614666 -1.006212
 C -7.140347 -1.539001 -1.338412
 C -6.696412 -0.243095 -1.204401
 C -3.222494 3.068950 0.091738
 C -2.905391 3.413686 1.429975
 C -2.573374 4.735806 1.735027
 C -2.559931 5.742738 0.764383
 C -2.925334 5.394362 -0.535568
 C -3.267046 4.082295 -0.890317
 C -2.994654 2.406026 2.556449
 C -3.696683 3.821137 -2.318983

C -2.160170 7.156906 1.115201
 O -1.393050 0.791930 0.247181
 P -0.127406 0.178286 -0.708569
 N -0.446697 0.480696 -2.334181
 C 0.122240 1.695900 -3.008402
 C -0.009173 2.974621 -2.170553
 O -0.502902 -1.456673 -0.723393
 C -0.651468 -4.562587 -1.850323
 C 4.104249 -6.189061 -1.483344
 C 2.210559 -3.318587 2.198785
 Pd 1.898859 1.017268 0.230437
 N 3.718619 1.913818 0.872295
 C 4.540755 0.906491 0.213157
 O 5.767960 0.844006 0.385325
 N 3.725030 0.158470 -0.537275
 C 4.251142 -0.895136 -1.433281
 C 5.120138 -0.266907 -2.544573
 C 0.893183 1.898194 1.988636
 C 1.400068 0.800091 2.729500
 C 2.696322 0.639279 3.237538
 C 3.716556 1.586277 3.123744
 C 5.120578 1.261454 3.553544
 C 5.099233 -1.904833 -0.627362
 C 3.062991 -1.634721 -2.059755
 C -1.307353 -0.401735 -3.186691
 C -2.587772 0.284152 -3.684503
 C -0.519960 -1.019835 -4.352381
 C 1.565098 1.517844 -3.500674
 C 4.116951 3.310732 0.444823
 C 3.019416 4.318731 0.825730
 C 5.430422 3.737478 1.144432
 C 4.331603 3.394714 -1.083704
 H 3.319084 5.320922 0.497860
 H 2.067454 4.076320 0.344142
 H 2.859236 4.369682 1.908294
 H 5.700190 4.748484 0.814633
 H 5.312564 3.764966 2.232337
 H 6.238875 3.049112 0.898147
 H 4.577680 4.426517 -1.361755
 H 5.154526 2.751721 -1.405277
 H 3.428411 3.103087 -1.626954
 H 5.427269 -2.723919 -1.280623
 H 5.974676 -1.415620 -0.197950
 H 4.502838 -2.334890 0.182733
 H 5.496027 -1.042316 -3.224088
 H 4.538368 0.448822 -3.136359
 H 5.977147 0.254352 -2.108901
 H 3.418040 -2.443619 -2.708980
 H 2.425640 -2.072355 -1.287368
 H 2.452661 -0.957616 -2.663094
 H 1.376753 2.860737 2.094579
 H 0.735940 -0.058543 2.832382
 H 3.445892 2.633376 3.090897
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 H 5.781872 1.200022 2.681698
 H 2.969136 -0.353494 3.590147

H -0.174198 1.946595 1.818327
 H 5.518482 2.029068 4.228762
 H -0.509287 -4.890802 2.237729
 H -2.153877 -5.070978 4.040036
 H -5.454106 -2.317454 4.202797
 H -4.625778 -1.166970 2.209096
 H -4.245356 -4.296415 5.124960
 H -5.620689 2.179460 -0.716562
 H -4.361032 -3.212044 -0.286812
 H -7.343279 0.592563 -1.460955
 H -8.144019 -1.739550 -1.702830
 H -6.630948 -3.636857 -1.126882
 H -1.617821 -1.220257 -2.540788
 H -2.948969 6.164482 -1.304302
 H -2.334919 4.989542 2.766128
 H 1.613980 -5.821353 -2.544315
 H 3.989993 -4.832848 0.878396
 H -1.150666 -1.753856 -4.867604
 H -0.222929 -0.269553 -5.093542
 H 0.378150 -1.530943 -3.993418
 H -3.191726 -0.443877 -4.238605
 H -3.189664 0.652737 -2.851148
 H -2.384981 1.118341 -4.366073
 H -0.511580 1.832824 -3.889245
 H 1.870170 2.408817 -4.063586
 H 2.254054 1.393643 -2.661123
 H 1.669362 0.652524 -4.159263
 H 0.273097 3.839408 -2.782370
 H -1.028074 3.124967 -1.811066
 H 0.655992 2.955359 -1.299936
 H -2.832455 2.895690 3.521507
 H -3.982120 1.929441 2.584121
 H -2.255305 1.604782 2.463540
 H -1.068256 7.274507 1.109023
 H -2.569725 7.878710 0.400682
 H -2.508266 7.435236 2.116234
 H -3.298410 4.592401 -2.986324
 H -3.363317 2.848412 -2.685596
 H -4.789780 3.842379 -2.420474
 H -0.605314 -5.241399 -2.707508
 H -1.501065 -4.864493 -1.226476
 H -0.871183 -3.558665 -2.230887
 H 4.807544 -5.518843 -1.995515
 H 4.668777 -6.711751 -0.703130
 H 3.768450 -6.931736 -2.214957
 H 3.252992 -3.405985 2.520155
 H 1.974743 -2.251201 2.123098
 H 1.581012 -3.732429 2.994806

(X-re)₃

E0 = -3111.5777276
 E0+ZPE = -3110.402895
 E298 = -3110.333577
 H298 = -3110.332633
 G298 = -3110.505311
 NImag = 1, (-195.9681)

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 C 0.405858 -4.491287 -1.563460
 C 1.331522 -5.113554 -2.406929
 C 2.699942 -5.122465 -2.125581
 C 3.127730 -4.498653 -0.951949
 C -0.148258 -3.256671 0.545417
 C -0.948170 -2.111912 0.236785
 C -2.099995 -1.795819 0.947946
 C -2.329673 -2.455316 2.206708
 C -1.471613 -3.533822 2.593268
 C -0.440860 -3.939979 1.709750
 C -3.357675 -2.062264 3.108872
 C -3.530700 -2.708056 4.313622
 C -2.696844 -3.791396 4.679309
 C -1.688904 -4.193113 3.833449
 C -3.111999 -0.837875 0.408632
 C -4.469921 -1.263569 0.191835
 C -5.451603 -0.285432 -0.168367
 C -5.060447 1.071055 -0.294783
 C -3.747328 1.479854 -0.174942
 C -2.768583 0.474090 0.115765
 C -4.885847 -2.621410 0.285480
 C -6.196684 -2.981578 0.059441
 C -7.169275 -2.006545 -0.264734
 C -6.798863 -0.686289 -0.377189
 C -3.419029 2.941464 -0.246630
 C -3.026517 3.621933 0.930854
 C -2.764274 4.993906 0.874441
 C -2.887961 5.725793 -0.309928
 C -3.313334 5.045327 -1.451910
 C -3.589647 3.672296 -1.443450
 C -2.924799 2.910480 2.261062
 C -4.081858 3.031580 -2.723883
 C -2.564673 7.201184 -0.351516
 O -1.444095 0.850688 0.211672
 P -0.170775 0.239256 -0.731330
 N -0.441150 0.693546 -2.332358
 C -0.172449 2.107254 -2.768827
 C 0.063960 3.110344 -1.634321
 O -0.619097 -1.364619 -0.890039
 C -1.068564 -4.593042 -1.889204
 C 3.686617 -5.776086 -3.064562
 C 2.790191 -3.176760 1.152528
 Pd 1.807956 0.925080 0.438840
 N 3.514761 1.824939 1.320985
 C 4.451540 1.131918 0.446436
 O 5.678742 1.186418 0.621810
 N 3.727543 0.504432 -0.485953
 C 4.360243 -0.159287 -1.645125
 C 5.092287 0.879754 -2.521704
 C 0.758928 1.073101 2.389345
 C 1.473236 -0.064618 2.837838
 C 2.790546 -0.123954 3.311528
 C 3.634606 0.975329 3.452523
 C 5.083780 0.796438 3.809522

C 5.367360 -1.233387 -1.174431
 C 3.255343 -0.836528 -2.462014
 C -1.041933 -0.144895 -3.429695
 C -0.099216 -1.245308 -3.935797
 C -2.451860 -0.689983 -3.156719
 C 0.976258 2.193193 -3.785215
 C 3.705131 3.325457 1.244016
 C 2.462805 4.036711 1.807168
 C 4.937348 3.756814 2.075254
 C 3.922697 3.802069 -0.211102
 H 2.603343 5.122061 1.743352
 H 1.560767 3.776176 1.244502
 H 2.294157 3.795096 2.862478
 H 5.069738 4.842016 1.984194
 H 4.806164 3.528021 3.137399
 H 5.835487 3.253588 1.715984
 H 3.974107 4.897134 -0.233601
 H 4.857504 3.409958 -0.618997
 H 3.103225 3.486086 -0.862452
 H 5.780727 -1.764468 -2.041647
 H 6.182536 -0.776408 -0.611146
 H 4.868296 -1.966447 -0.533088
 H 5.545839 0.397710 -3.396936
 H 4.394220 1.645683 -2.879434
 H 5.884286 1.370665 -1.949190
 H 3.675598 -1.317947 -3.353526
 H 2.742077 -1.601206 -1.871372
 H 2.511730 -0.103614 -2.783725
 H 1.059435 2.054605 2.737050
 H 0.970661 -1.023400 2.714131
 H 3.194096 1.943470 3.650467
 H 5.283557 -0.235919 4.117520
 H 5.717057 1.009474 2.940126
 H 3.231652 -1.112670 3.421485
 H -0.305786 0.954209 2.233178
 H 5.383475 1.469781 4.621599
 H 0.135861 -4.828518 1.954383
 H -1.033288 -5.016999 4.105039
 H -4.313572 -2.379409 4.991659
 H -4.000599 -1.229402 2.848302
 H -2.849258 -4.295967 5.629317
 H -5.828660 1.815657 -0.487631
 H -4.154910 -3.384637 0.525403
 H -7.531501 0.073895 -0.637883
 H -8.200649 -2.303929 -0.432616
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 H -1.155701 0.573655 -4.248430
 H -3.439481 5.597259 -2.381456
 H -2.468207 5.506570 1.787706
 H 0.968449 -5.622135 -3.298028
 H 4.186193 -4.510511 -0.701154
 H -2.882126 -1.039425 -4.103141
 H -2.444989 -1.528698 -2.460243
 H -3.112770 0.079699 -2.750947
 H -0.558320 -1.752182 -4.793659
 H 0.857405 -0.828393 -4.261005

H 0.101668 -1.992628 -3.165984
 H -1.097055 2.422269 -3.271995
 H 1.035795 3.211493 -4.187669
 H 1.931912 1.960273 -3.306336
 H 0.840026 1.511145 -4.629904
 H 0.110937 4.113878 -2.071490
 H -0.739100 3.105057 -0.895970
 H 1.013664 2.926048 -1.122328
 H -2.796089 3.630536 3.075072
 H -3.823988 2.319807 2.470876
 H -2.073254 2.223432 2.286129
 H -2.860396 7.702781 0.576683
 H -1.486819 7.368910 -0.479346
 H -3.073130 7.700001 -1.183366
 H -3.919185 3.700372 -3.575179
 H -3.575876 2.085876 -2.934413
 H -5.155784 2.811041 -2.685428
 H -1.227360 -5.234175 -2.761767
 H -1.635627 -5.017845 -1.052285
 H -1.510815 -3.616174 -2.112021
 H 3.219416 -6.581553 -3.641458
 H 4.088414 -5.049939 -3.783992
 H 4.539541 -6.196953 -2.521015
 H 2.220720 -3.427992 2.052722
 H 3.831340 -3.469587 1.319877
 H 2.769628 -2.086028 1.046454

X-si

E0 = -3111.5811802
 E0+ZPE = -3110.404986
 E298 = -3110.336340
 H298 = -3110.335396
 G298 = -3110.505706
 NImag = 1, (-188.0010)
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 C 3.146973 3.035623 -0.376981
 C 3.212815 4.143134 0.498165
 C 2.815022 5.406111 0.037343
 C 2.385553 5.620633 -1.271236
 C 2.390148 4.526148 -2.142123
 C 3.584465 1.666318 0.045231
 C 4.888694 1.446065 0.446072
 C 5.388632 0.150721 0.734518
 C 4.568024 -0.987521 0.450426
 C 3.244970 -0.777366 -0.073238
 C 2.739099 0.515142 -0.089887
 C 6.696119 -0.043816 1.255864
 C 7.172798 -1.308811 1.514465
 C 6.355616 -2.434973 1.256043
 C 5.091146 -2.280215 0.730142
 C 2.471639 -1.894935 -0.691339
 C 1.182001 -2.222652 -0.291970
 C 0.501223 -3.379665 -0.781634
 C 1.133633 -4.138835 -1.744351
 C 2.387239 -3.781308 -2.294040
 C 3.066648 -2.631709 -1.780540

C 2.969415 -4.535316 -3.348777
 C 4.166022 -4.156468 -3.910724
 C 4.821758 -2.995372 -3.438505
 C 4.291438 -2.256784 -2.403203
 C -0.831037 -3.839386 -0.275919
 C -0.924176 -4.505133 0.963991
 C -2.158561 -5.027448 1.364358
 C -3.302808 -4.914567 0.570185
 C -3.183498 -4.265597 -0.662760
 C -1.968439 -3.729898 -1.103616
 C 0.293087 -4.704814 1.838621
 C -1.892572 -3.065155 -2.461245
 C -4.633070 -5.459381 1.035412
 O 0.553835 -1.494553 0.708021
 P 0.143625 0.124523 0.644142
 N 0.446102 0.485427 2.264043
 C -0.309315 1.653095 2.815266
 C 0.464849 2.979098 2.736658
 O 1.392940 0.707960 -0.350674
 C 3.744101 4.052236 1.913229
 C 1.931267 6.983843 -1.737327
 C 2.821649 2.140414 -2.761258
 Pd -1.926956 0.847417 -0.312493
 C -0.959368 2.374545 -1.590310
 C -1.325592 3.362417 -0.641839
 C -2.575019 3.971000 -0.467599
 C -3.691494 3.729501 -1.265528
 C -5.035298 4.298528 -0.906781
 N -3.807603 1.437767 -1.098190
 C -4.515218 1.035530 0.113439
 O -5.679419 1.393520 0.347086
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 C -4.465589 0.543201 3.138190
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 H -5.589372 -0.786488 -1.315741
 H -6.149149 0.954188 -3.590297
 H -6.408578 1.524798 -1.921841
 H -5.490667 2.513574 -3.078664
 H -3.827786 0.300735 -4.352710
 H -3.159119 1.827815 -3.777180
 H -2.466026 0.290209 -3.215533
 H -5.633777 -1.905258 2.616409
 H -6.183238 -0.738874 1.390736
 H -5.097079 -2.071536 0.930923

H -4.740498 0.017329 4.061867
 H -3.613741 1.195942 3.356536
 H -5.305586 1.168061 2.824656
 H -3.224060 -1.915359 3.378385
 H -2.712880 -2.097496 1.687173
 H -2.054415 -0.783409 2.668734
 H -1.531452 2.293919 -2.506573
 H -0.566820 3.616944 0.096063
 H -3.533722 3.445136 -2.297187
 H -4.936598 5.069295 -0.134018
 H -5.534817 4.736206 -1.778993
 H -2.723045 4.546795 0.444727
 H 0.097715 2.164974 -1.693050
 H -5.680112 3.507881 -0.504567
 H 0.642002 -5.037695 -2.108011
 H 2.439010 -5.412580 -3.711495
 H 5.752571 -2.677789 -3.900601
 H 4.808178 -1.366217 -2.068308
 H 4.600500 -4.734159 -4.721813
 H 5.563869 2.292833 0.534622
 H 4.473840 -3.151113 0.539240
 H 7.311048 0.830507 1.455966
 H 8.170803 -1.445879 1.921370
 H 6.728382 -3.431676 1.475890
 H 2.001586 -0.871428 2.345443
 H -2.224019 -5.544653 2.319639
 H -4.057800 -4.178690 -1.304769
 H 2.103820 4.674823 -3.181405
 H 2.854225 6.246890 0.727588
 H -1.179378 1.750413 2.154493
 H -1.524047 2.283893 4.470512
 H -1.447733 0.526202 4.314158
 H -0.074163 1.427289 4.990066
 H 3.225898 -0.079498 4.262028
 H 3.005718 1.239306 3.106792
 H 2.044694 1.185988 4.601404
 H 1.562114 -2.000893 4.383394
 H 0.344284 -0.836650 4.908623
 H 0.023238 -1.881323 3.511016
 H -0.220510 3.813956 2.928299
 H 1.265228 3.033782 3.479704
 H 0.910125 3.124056 1.749104
 H 4.824597 4.248399 1.942303
 H 3.267192 4.801679 2.553377
 H 3.585950 3.070791 2.361173
 H 2.043704 1.385322 -2.607249
 H 2.690048 2.552025 -3.766613
 H 3.785251 1.618466 -2.736147
 H 2.304754 7.777206 -1.081460
 H 2.276753 7.194639 -2.755793
 H 0.835468 7.054356 -1.747625
 H 1.076091 -5.265274 1.312736
 H 0.733359 -3.749657 2.143722
 H 0.034662 -5.260325 2.745592
 H -1.215899 -3.596110 -3.140195
 H -2.878816 -3.031948 -2.931683

H -1.521283 -2.035911 -2.385057
H -5.238236 -4.672857 1.505202
H -5.217244 -5.860489 0.199596
H -4.503455 -6.258393 1.773181

(X-si)₁

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H298 = -3110.329008
G298 = -3110.501341
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C 1.231720 -4.357754 -1.317463
C 2.312684 -4.905865 -2.011401
C 3.604881 -4.928635 -1.477580
C 3.786758 -4.403161 -0.199065
C 0.270614 -3.303807 0.757615
C -0.599535 -2.234729 0.355579
C -1.849283 -2.056569 0.936986
C -2.137967 -2.730858 2.178689
C -1.223509 -3.717022 2.661987
C -0.076614 -4.015072 1.889289
C -3.282018 -2.440092 2.974130
C -3.507813 -3.097725 4.164072
C -2.613897 -4.094150 4.621569
C -1.493944 -4.394605 3.881222
C -2.921279 -1.219240 0.321533
C -4.208655 -1.795294 0.034814
C -5.303727 -0.923329 -0.262699
C -5.091899 0.477592 -0.231592
C -3.840178 1.039778 -0.064184
C -2.737023 0.137341 0.106093
C -4.442624 -3.198024 0.008439
C -5.689397 -3.704219 -0.289187
C -6.775427 -2.838011 -0.559138
C -6.582616 -1.475618 -0.543873
C -3.709656 2.526193 0.067002
C -3.231975 3.076383 1.285103
C -3.156667 4.464384 1.426344
C -3.544114 5.340338 0.407713
C -4.055973 4.782949 -0.763246
C -4.163903 3.398215 -0.948974
C -2.851459 2.209370 2.465998
C -4.807505 2.916536 -2.233743
C -3.407903 6.835643 0.573478
O -1.454898 0.652181 0.175519
P -0.166253 0.208085 -0.831036
Pd 1.690265 1.351939 0.165979
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C 4.352282 -0.132795 -1.444081
C 5.484778 -0.974166 -0.815194
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C -0.149528 -4.459892 -1.924121
C 4.763873 -5.492954 -2.264958

C 3.030717 -3.346116 1.934046
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 C -0.502794 -1.384587 -4.290313
 C -0.334909 1.534061 -3.263187
 C -1.161353 2.739648 -2.801557
 C 1.155667 1.860607 -3.411568
 C 0.515045 3.157379 0.772091
 C 1.212899 3.945842 -0.172662
 C 2.496254 4.503126 -0.075413
 C 3.318978 4.415753 1.040350
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 C 4.306092 1.510220 0.388663
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 C 4.944666 0.817382 -2.508758
 C 2.261399 1.989148 3.548844
 C 3.683174 0.093868 2.771360
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 H 2.845458 -0.411281 2.283814
 H 4.606124 -0.217669 2.274265
 H 4.876159 1.916021 4.362052
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 H 2.086073 3.070274 3.577338
 H 1.360461 1.499659 3.165394
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 H 5.076722 -1.662693 -0.067749
 H 5.436878 0.243463 -3.304511
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 H -0.789034 -5.148770 4.222958
 H -4.381099 -2.844379 4.759065
 H -3.976189 -1.674413 2.648857
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 H -3.620186 -3.875151 0.209603
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 H 2.135649 -5.345923 -2.991058
 H 4.778052 -4.427812 0.249357
 H -2.793480 4.872608 2.367538
 H -4.391695 5.442418 -1.561544
 H -0.688892 1.279617 -4.265494
 H -0.947528 3.610977 -3.432317
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 H -0.948118 3.010071 -1.765216
 H -3.244066 -1.171209 -4.165033
 H -3.369594 0.030568 -2.872515
 H -2.669489 0.473563 -4.446120
 H -1.024823 -2.237551 -4.739541
 H -0.296055 -0.669466 -5.095107
 H 0.452089 -1.736371 -3.888685
 H 1.271948 2.722532 -4.079840
 H 1.628828 2.105643 -2.456699
 H 1.696264 1.017690 -3.849821
 H -5.898663 2.846974 -2.128714
 H -4.612847 3.621602 -3.048949
 H -4.456166 1.930257 -2.542126
 H -1.900362 1.691680 2.303382
 H -2.751172 2.819037 3.369309
 H -3.608503 1.441612 2.661886
 H -4.051384 7.377532 -0.127485
 H -3.670507 7.152091 1.589352
 H -2.375364 7.162468 0.391580
 H -0.862970 -4.909531 -1.223208
 H -0.545404 -3.479351 -2.202535
 H -0.129220 -5.079908 -2.825825
 H 2.987494 -4.167635 2.662398
 H 4.038541 -2.922693 1.988664
 H 2.324317 -2.584316 2.266619
 H 5.230880 -4.719807 -2.889808
 H 5.542832 -5.889788 -1.605154
 H 4.441176 -6.298919 -2.933388

(X-si)₂

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 E0+ZPE = -3110.390242
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 H298 = -3110.320199
 G298 = -3110.492338
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 C -2.064175 5.079677 -2.330143
 C -3.444095 4.967508 -2.144773
 C -3.893411 4.251764 -1.033727
 C -0.635588 3.161074 0.613942
 C 0.350024 2.165762 0.302605
 C 1.486781 2.000893 1.087116
 C 1.492415 2.556267 2.416450

C 0.438095 3.439580 2.804877
 C -0.552491 3.772430 1.850001
 C 2.492573 2.244585 3.379329
 C 2.450085 2.783701 4.646898
 C 1.417284 3.676979 5.018243
 C 0.433016 3.997275 4.111685
 C 2.727804 1.353309 0.569709
 C 3.963889 2.095567 0.551483
 C 5.179134 1.408477 0.235288
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 C 4.037928 3.495463 0.796965
 C 5.242014 4.164654 0.750403
 C 6.443712 3.473944 0.468083
 C 6.407473 2.122054 0.215097
 C 3.986331 -2.170826 -0.282237
 C 3.627583 -3.002944 0.806063
 C 3.721661 -4.390105 0.664572
 C 4.172866 -4.987723 -0.516820
 C 4.558445 -4.149234 -1.563426
 C 4.483609 -2.753527 -1.467018
 C 3.201325 -2.424325 2.137957
 C 4.960819 -1.922057 -2.639896
 C 4.232051 -6.491491 -0.652433
 O 1.533349 -0.624614 -0.022580
 P 0.190138 -0.216817 -0.969289
 Pd -1.533201 -1.445965 0.204095
 N -3.623206 -0.948931 -0.213236
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 C 1.180029 0.693213 -3.505832
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 C 0.252384 -1.631048 -3.342454
 C 1.236562 -2.741970 -2.960424
 C -1.208855 -2.089619 -3.306219
 C -0.186361 -3.137108 0.744938
 C -0.914678 -4.027098 -0.083350
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 C -4.888226 -1.628371 -2.226699
 C -1.714574 -1.985939 3.650641
 C -3.316449 -0.210884 2.951913
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 H -2.535406 0.330724 2.410698
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 H 0.830033 -2.908175 0.448347
 H -4.964401 -4.322359 1.460137
 H -1.267328 4.553434 2.094843
 H -0.372352 4.675212 4.384103
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 H 3.286457 1.555935 3.113801
 H 1.400627 4.100163 6.018780
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 H -1.685992 5.671269 -3.161802
 H -4.962957 4.171960 -0.850802
 H 3.445745 -5.020944 1.507425
 H 4.931930 -4.589828 -2.485935
 H 0.446518 -1.386333 -4.390510
 H 1.046319 -3.640886 -3.559173
 H 2.266501 -2.426081 -3.141575
 H 1.160159 -3.013410 -1.904555
 H 0.557713 2.316655 -4.811709
 H -0.672474 1.058816 -4.591523
 H -0.362923 2.221953 -3.293436
 H 2.847125 2.012069 -3.768565
 H 2.131352 2.153562 -2.159400
 H 3.143755 0.761626 -2.553930
 H -1.308338 -2.996622 -3.914947
 H -1.567630 -2.317956 -2.299540
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 H 5.965259 -1.514653 -2.468672
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 H 3.066341 -3.219989 2.877084
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 H 3.237414 -6.912746 -0.850585
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 H 0.885166 3.842723 -1.915838
 H 0.481412 5.468034 -2.472736
 H -4.671822 2.988828 1.075485
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(X-si)₃

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 G298 = -3110.504005
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 C 2.796469 -5.318192 -1.753728
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 C -0.156197 -3.322850 0.697931
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 C -2.100632 -1.833162 0.980695
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 C -5.439066 -0.373285 -0.219873
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 C -2.759227 0.405758 0.059131
 C -4.853811 -2.698889 0.257644
 C -6.157311 -3.075434 0.014993
 C -7.135721 -2.113740 -0.329903
 C -6.778537 -0.789796 -0.444796
 C -3.444420 2.873276 -0.199635
 C -3.071663 3.487300 1.021193
 C -2.827984 4.862821 1.047854
 C -2.957743 5.662395 -0.092368
 C -3.374269 5.047109 -1.273376
 C -3.631210 3.671449 -1.348064
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C -4.131524 3.102627 -2.658885
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 H 2.446540 -0.649232 -2.438916
 H 1.067568 2.756718 2.310028
 H 0.565756 3.791045 -0.539763
 H 3.089070 3.898562 2.319582
 H 4.875382 5.223535 0.228062
 H 5.152889 5.155976 1.987347

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 H -0.398480 2.520516 1.248587
 H 5.514130 3.748315 0.965663
 H 0.056422 -4.851956 2.164147
 H -1.179287 -4.953027 4.281841
 H -4.455646 -2.251428 4.966710
 H -4.057398 -1.179925 2.798335
 H -3.037218 -4.161186 5.719059
 H -5.836804 1.729568 -0.506295
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 H -8.161248 -2.423676 -0.510503
 H -6.435120 -4.123533 0.086414
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 H 1.145890 -5.725341 -3.071027
 H 4.186599 -4.789366 -0.203501
 H -2.542376 5.325111 1.990687
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 H 1.152579 1.987835 -2.047261
 H 1.888356 2.454227 -4.296630
 H 2.055614 0.721220 -3.998936
 H 0.729677 1.334160 -5.010668
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 H 0.799517 -1.171881 -4.392287
 H 0.032435 -2.201635 -3.179981
 H -2.901223 -1.039207 -4.023244
 H -2.443339 -1.503847 -2.380871
 H -2.981234 0.147295 -2.713489
 H 0.017457 3.791411 -3.324631
 H -1.227995 2.662016 -3.867278
 H -1.097817 3.067334 -2.148007
 H -5.220152 2.962924 -2.648835
 H -3.900470 3.781123 -3.486303
 H -3.690330 2.128961 -2.884709
 H -2.245556 1.915500 2.289648
 H -2.772707 3.364339 3.153790
 H -3.965116 2.214443 2.526765
 H -3.142309 7.679863 -0.860961
 H -2.978104 7.587460 0.901937
 H -1.572031 7.326270 -0.131086
 H -1.583132 -5.083149 -1.036778
 H -1.365886 -3.633879 -2.013434
 H -1.064912 -5.222967 -2.724316
 H 2.500058 -4.153574 2.408170
 H 3.757875 -3.256810 1.554626
 H 2.162535 -2.532478 1.808239
 H 4.267261 -5.309453 -3.341801
 H 4.644241 -6.417848 -2.020414
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 E298 = -3110.336369
 H298 = -3110.335425
 G298 = -3110.509668

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 C 2.521030 -5.063741 -2.611047
 C 1.157590 -4.974529 -2.906167
 C -0.292433 -3.413651 0.232206
 C -1.024559 -2.204036 0.026347
 C -2.100037 -1.831932 0.819051
 C -2.331411 -2.562089 2.040072
 C -1.567937 -3.745393 2.297507
 C -0.600951 -4.162039 1.349750
 C -3.262477 -2.142999 3.031450
 C -3.443146 -2.866486 4.190024
 C -2.713587 -4.056491 4.421092
 C -1.794026 -4.482745 3.491217
 C -3.021909 -0.724255 0.426755
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 C -3.442024 1.696366 0.119284
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 C -7.237685 -1.383454 0.147279
 C -6.732846 -0.103875 0.138138
 C -2.980024 3.120936 0.055203
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 C -3.024987 5.314709 -0.995913
 C -2.194673 5.852696 -0.013402
 C -1.793265 5.009137 1.025611
 C -2.169963 3.664254 1.084607
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 Pd 2.079422 0.653099 -0.068000
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 C 2.608342 -3.563650 0.899251
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 C -1.433142 -0.068830 -3.359101
 C -0.801685 -1.100182 -4.311739
 C 0.345862 1.819495 -2.967352
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 C -0.420501 3.142022 -2.804150
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 H 2.878871 3.185735 -1.419408
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 H -6.749772 -3.496240 0.210410
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 H 3.043295 -6.429632 -4.210224
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 H 2.189243 -4.124644 1.741698
 H -1.524571 3.510799 3.133000
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 H -2.437538 7.911476 -0.644385
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 H -0.828961 3.235873 -1.795611
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 H -2.855361 1.588571 -3.437033
 H -1.885687 1.430199 -4.912591
 H -3.171058 0.272408 -4.575166
 H 0.188553 1.727325 -5.163322
 H 1.622905 2.541098 -4.543426
 H 1.526300 0.774975 -4.495122
 H -1.592601 -1.702393 -4.775994
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XI-re

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 E0+ZPE = -3581.793257
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 C -1.654652 4.993370 3.431720
 C 1.222364 2.972485 -0.095327
 C 1.793122 4.166782 -0.655290
 C 3.178471 4.162966 -1.010371
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 C 2.997935 6.456686 -1.800596
 C 3.757942 5.331526 -1.573155
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 C 4.274148 0.333514 1.550320
 C 5.095033 -0.711563 1.985586
 C 5.959114 -1.398631 1.130811
 C 6.016465 -0.978439 -0.196760
 C 5.213964 0.055623 -0.697597
 C 3.505238 1.147790 2.599798
 C 4.293127 2.431186 2.947088
 C 5.457339 0.486887 -2.146707
 C 5.575770 -0.691594 -3.134530
 C 6.827744 -2.536493 1.650202
 C 6.527873 -3.864633 0.929623
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 N 0.375098 -0.045735 -2.371665
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XI-si

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 C 5.555762 -2.101421 -2.158018
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 C 3.534151 -2.886498 -1.018225
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 C -0.567402 6.725697 1.253293
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 C 5.514114 1.412130 0.433894
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 C -0.991374 -2.310059 -2.563035
 C -0.547511 1.774075 -4.212053
 C 1.441722 3.421152 3.689713
 C 3.420463 3.545937 2.189403
 C 2.627345 3.594952 -2.020545
 C 4.012280 4.277231 -1.932864
 C 2.815084 2.175346 -2.571647
 C 1.722885 4.424819 -2.958070
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 H 3.295354 2.513015 1.853235
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 H 2.978295 5.680196 3.775195
 H 2.694637 6.238439 2.104823
 H 1.348366 6.127756 3.253490
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 H 0.481233 3.840929 4.007735
 H 1.301672 2.361769 3.452992
 H 4.478392 4.302498 -2.926135
 H 3.917261 5.298127 -1.559333
 H 4.678770 3.722864 -1.264358
 H 2.150093 4.479773 -3.967743
 H 0.726068 3.978710 -3.030248
 H 1.617022 5.440265 -2.567471
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 H -0.672797 7.348026 2.149959
 H -2.081958 4.974593 -0.126120
 H -1.523619 1.252940 1.907772
 H 0.446485 6.859550 0.857943
 H 4.053989 -2.141029 2.588356
 H 3.536242 -2.169794 4.995359
 H -0.569203 -2.369216 6.266337
 H -1.323473 -2.198171 3.931679
 H 1.864286 -2.372377 6.812327
 H -4.799080 -3.409923 0.669560
 H 0.408568 -4.469710 2.261513
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H -3.599157 -1.396842 -3.812952
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H 3.920173 -5.522957 -0.186721
H 3.209521 -4.582051 1.134847
H 1.279070 -5.396599 -1.995425
H 1.845214 -4.024402 -2.963252
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H 8.056462 -3.585119 -4.087847
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H 4.679671 1.853415 -0.114640
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H 6.088108 -1.497083 2.276071
H 7.223501 -0.600597 1.266342
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H -0.927852 2.766356 -4.476979
H 0.540569 1.804336 -4.283904
H -0.930178 1.073652 -4.962290
H 0.954344 -2.073335 -4.471223
H 1.352305 -0.359933 -4.263431
H 1.701373 -1.506390 -2.961353
H -1.118615 -3.042388 -3.368606
H -0.336148 -2.747499 -1.809756
H -1.968137 -2.134014 -2.111193
H -2.957071 2.395185 -3.039915
H -2.978916 0.676288 -3.442085
H -2.938403 1.174845 -1.747605

XI-si-c

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C 5.914307 -1.770056 0.946876
C 5.122849 -1.047303 1.840425
C 3.435420 1.572896 -0.340104
C 4.039103 2.743684 -0.761908
C 3.328498 3.950126 -0.984909
C 1.957896 4.021370 -0.586600
C 1.333009 2.842837 -0.051244
C 2.010662 1.630646 -0.128107
C 3.960430 5.100438 -1.528424
C 3.262132 6.274675 -1.697815
C 1.899563 6.343252 -1.321810
C 1.265620 5.249770 -0.772008
C 0.031902 2.952787 0.677546
C -1.099349 2.236926 0.308607
C -2.385678 2.477684 0.894032
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C -0.037122 3.827291 1.821653
C -1.406094 4.939845 3.546879
C -0.286754 5.543332 4.070265
C 0.979376 5.285702 3.493870
C 1.101940 4.457101 2.399640
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C -5.496832 1.601428 -1.128148
C -6.181845 0.725653 -0.277900
C -5.600296 0.438704 0.954232
C -4.360438 0.965377 1.348100
C -3.652275 3.232858 -1.699510
C -4.068031 3.111264 -3.175837
C -3.853438 0.614362 2.749093
C -4.706359 1.308510 3.832895
C -7.516127 0.108187 -0.675276
C -8.594354 1.175736 -0.940232
O -1.021471 1.343520 -0.748304
P -0.035490 -0.008953 -0.839262
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C 0.687366 -1.172029 -3.150735
C 2.189412 -1.471916 -3.183912
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C 5.404302 0.177565 -2.287749
C 6.690961 1.029006 -2.400052
C 6.734375 -2.962803 1.419574
C 6.274764 -4.269966 0.745612
C 3.654477 0.880609 2.534263

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 C 3.471144 0.158568 3.879756
 C 8.246326 -2.740733 1.224281
 Pd -0.911669 -2.165716 -0.318231
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 H 0.220255 5.314554 -0.491050
 H 5.007022 5.032701 -1.815787
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 H -2.563821 3.123237 -1.661515
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 H -2.829232 0.984809 2.848060
 H 2.655009 1.161424 2.190217
 H 4.559357 0.797500 -2.602882
 H 6.554850 -3.068994 2.498144
 H 8.815724 -3.587117 1.626811
 H 8.502443 -2.644267 0.162321
 H 8.582514 -1.830419 1.732960
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 H 1.850856 1.028570 -4.817422
 H -0.822268 2.751515 -4.366845
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 H -1.721014 1.450992 -3.569211
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 H 2.631746 -1.341295 -2.191927

XVIII-re

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 E298 = -2929.631465
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 G298 = -2929.767366
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 C -6.468580 -2.289391 0.798435
 C -7.309599 -1.319202 1.292975
 C -4.271321 -2.968123 -0.103816
 C -2.969559 -2.671114 -0.429287
 C -2.508756 -1.327800 -0.319424
 C -3.364788 -0.288659 0.010511
 O -1.186957 -1.071266 -0.598861
 P -0.093445 -0.635736 0.632857
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 C -1.270836 2.858017 0.529667
 C -1.967678 3.792805 -0.197816
 C -3.099157 3.428565 -0.967273
 C -3.554347 2.070540 -0.944964
 C -2.875889 1.114838 -0.106686
 C -3.768406 4.385377 -1.776566
 C -4.832979 4.018539 -2.566416
 C -5.261048 2.670443 -2.580373
 C -4.643125 1.723431 -1.792606
 Pd 2.028920 -0.358397 -0.276331
 N 3.537521 0.135369 1.162500
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 C 2.393487 0.376236 3.320214
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 C 2.833880 1.873598 -2.335108
 C 1.584340 1.245287 -2.234488
 C 1.285771 -0.135096 -2.360471
 C 4.706539 -1.672028 -1.311892
 C 4.810510 -2.595667 -0.076600

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 C 6.133292 -1.401872 -1.845863
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 C 0.787678 -2.756802 2.063514
 H 4.411130 -3.356488 -2.640711
 H 2.894445 -2.650981 -2.052762
 H 3.835016 -1.836478 -3.323707
 H 6.622514 -2.357922 -2.069867
 H 6.107251 -0.816937 -2.771108
 H 6.724591 -0.857918 -1.108466
 H 5.254141 -3.554056 -0.371398
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 H 3.821669 -2.794559 0.349281
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 H 2.507571 0.695940 4.362905
 H 1.581464 0.957670 2.876146
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XVIII-si

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 C 2.026371 -2.429270 -1.734047
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 C 4.166037 2.544297 -0.880242
 C 5.773603 1.222432 -2.281261
 C 4.534668 0.001629 0.287914
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 H 5.910787 0.407246 -2.998878
 H 3.660836 2.405523 -3.528886
 H 3.470282 0.663627 -3.718082
 H 2.338615 1.574010 -2.690999
 H 4.850968 1.621657 3.948898
 H 5.655523 1.357005 2.384291
 H 4.223007 2.407742 2.486790
 H 4.593300 -0.904132 4.256400
 H 3.776993 -1.871560 3.010546
 H 5.382002 -1.184845 2.683806
 H 2.588278 0.636022 4.395996
 H 1.954776 1.440035 2.947163
 H 1.734638 -0.301990 3.157263
 H 1.946751 -0.637912 -2.938061
 H 1.357080 -3.148280 -1.261282
 H 4.178008 -1.249726 -3.008371
 H 5.957240 -3.268313 -1.572512
 H 6.433239 -2.159539 -2.883074
 H 3.689847 -3.599605 -1.103054
 H 0.338499 -1.256598 -2.333969
 H 6.290846 -1.569372 -1.214309
 H -1.557525 4.862187 -0.298886
 H -3.285814 5.439744 -1.921728
 H -5.986578 2.417815 -3.357626
 H -4.939560 0.751260 -1.903912
 H -5.194348 4.782638 -3.362095
 H -4.699912 -3.901528 -0.112893
 H -5.256363 1.528662 0.964506
 H -6.865807 -3.173216 0.760084
 H -8.367034 -1.374139 1.568287
 H -7.532613 0.972555 1.687645
 H 1.148045 -2.631712 3.185813
 H -1.904793 -2.716755 2.626171
 H 0.419504 -3.646319 1.911556
 H 1.674002 -2.446905 1.502177
 H -2.064444 -0.941353 2.703104
 H -1.032238 -1.786161 3.871148
 C -0.037907 3.316323 1.291038
 C -2.103054 -3.717445 -0.847050
 F 1.079698 2.661571 0.898230
 F 0.216526 4.637566 1.167580
 F -0.205315 3.064647 2.605635
 F -1.023441 -3.891361 -0.040426
 F -2.741003 -4.906103 -0.899712
 F -1.626006 -3.462533 -2.082548

XII-re

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 E0+ZPE = -4065.681932
 E298 = -4065.613168
 H298 = -4065.612224

G298 = -4065.791823
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 C 4.390517 1.513837 2.102800
 C 3.301283 2.103153 1.464243
 C 3.202990 2.089456 0.063828
 C 4.221743 1.467956 -0.668861
 C 5.305542 0.869659 -0.023275
 C 2.091138 2.772975 -0.648157
 C 0.721607 2.623209 -0.267367
 C -0.298586 3.353648 -0.862480
 C 0.006317 4.171887 -2.005487
 C 1.370744 4.304460 -2.419710
 C 2.379618 3.617424 -1.703503
 C -0.991668 4.830856 -2.776515
 C -0.652993 5.598666 -3.869367
 C 0.700155 5.756866 -4.251971
 C 1.689157 5.118365 -3.540720
 O 0.425998 1.752526 0.772000
 P -0.380077 0.300066 0.493000
 N -1.070485 0.158787 2.007055
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 C -1.693162 3.248166 -0.341552
 C -2.428451 4.395495 0.116393
 C -3.793966 4.226064 0.519366
 C -4.379795 2.936482 0.469154
 C -3.660309 1.819089 0.093243
 C -2.293277 2.001159 -0.278624
 C -4.535516 5.352073 0.969620
 C -3.952158 6.595319 1.051212
 C -2.594516 6.759442 0.687554
 C -1.853316 5.691399 0.230626
 C -4.296673 0.476016 0.081348
 C -5.069091 0.053741 1.169783
 C -5.679963 -1.203812 1.169236
 C -5.546220 -2.054288 0.075674
 C -4.788533 -1.632861 -1.021050
 C -4.163550 -0.388438 -1.018736
 O -1.545431 0.882244 -0.594917
 C -6.399912 -1.662094 2.409448
 F -7.114840 -0.661220 2.969171
 C -4.696757 -2.527417 -2.230788
 F -5.815074 -2.452327 -2.986486
 C 4.503939 1.568105 3.604545
 F 5.048479 0.436220 4.102698
 C 6.317939 0.119645 -0.847317
 F 7.475473 -0.070481 -0.184653
 Pd 0.544341 -1.642143 -0.417046
 C 0.185183 -1.024871 -2.528253
 C 1.587908 -0.850773 -2.626852
 C 2.576901 -1.830777 -2.801492
 C 2.327807 -3.190903 -2.973950
 C 3.451061 -4.187465 -3.011972
 N 1.787349 -2.777311 0.909128
 C 1.986016 -3.793794 0.061963
 O 2.756501 -4.761865 0.124642

N 1.089342 -3.583978 -1.065478
 C 0.043786 -4.670220 -1.158469
 C 0.671077 -5.965645 -1.725710
 C 2.516365 -2.674520 2.191695
 C 4.039661 -2.666985 1.926692
 C 2.123160 -1.360444 2.876004
 C 2.151798 -3.860321 3.109925
 C -0.569982 -4.982914 0.225547
 C -1.087552 -4.217993 -2.094297
 C -1.440512 1.263444 2.893893
 F -5.521341 -2.086962 3.349159
 F -7.245238 -2.682103 2.161577
 F -4.549163 -3.823386 -1.876799
 F -3.655640 -2.199107 -3.025809
 F 3.301571 1.735845 4.195571
 F 5.290985 2.592622 4.005757
 F 6.603491 0.769824 -1.997883
 F 5.850466 -1.103848 -1.197915
 H -1.863630 -4.989826 -2.141164
 H -1.553152 -3.295873 -1.736308
 H -0.733007 -4.052158 -3.117970
 H -0.101482 -6.741724 -1.791045
 H 1.067148 -5.804672 -2.733649
 H 1.482029 -6.315266 -1.086014
 H -1.351620 -5.743796 0.116805
 H 0.182748 -5.365097 0.920014
 H -1.025881 -4.089321 0.664833
 H 4.585784 -2.485705 2.861105
 H 4.358316 -3.621357 1.503884
 H 4.299670 -1.874949 1.216566
 H 2.675680 -3.780407 4.070729
 H 1.073789 -3.873619 3.309832
 H 2.431562 -4.806005 2.638361
 H 2.706009 -1.218104 3.792827
 H 2.311347 -0.509138 2.215383
 H 1.062804 -1.355691 3.143131
 H -0.269034 -1.909538 -2.958060
 H 1.953663 0.159708 -2.444156
 H 1.386395 -3.493868 -3.413932
 H 4.421836 -3.680768 -3.025096
 H 3.426064 -4.824524 -2.120374
 H 3.606577 -1.528284 -2.622000
 H -0.434866 -0.135682 -2.567609
 H 3.377509 -4.834281 -3.895139
 H 3.416176 3.770015 -1.992257
 H 2.732037 5.215839 -3.832125
 H -1.434857 6.084220 -4.446708
 H -2.034391 4.714329 -2.506012
 H 0.952020 6.371111 -5.111707
 H -5.428718 2.831175 0.734779
 H -0.812682 5.834296 -0.036480
 H -5.573339 5.207817 1.259904
 H -4.525682 7.448044 1.403075
 H -2.129902 7.737821 0.773114
 H -1.034399 1.070876 3.895139
 H -1.207440 -1.325514 3.489872

H -1.031587 2.203044 2.527424
 H -2.531737 1.354768 2.974194
 H -2.644961 -1.200449 2.446280
 H -1.142427 -1.942379 1.829385
 H -5.180806 0.700843 2.033921
 H -3.568936 -0.086492 -1.871546
 H -6.015928 -3.031021 0.078207
 H 2.523122 2.570271 2.054880
 H 4.163123 1.436211 -1.751849
 H 6.235592 0.416510 1.866645

XII-si

E0 = -4066.5938263
 E0+ZPE = -4065.680462
 E298 = -4065.611876
 H298 = -4065.610931
 G298 = -4065.789513
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 C -4.803540 -1.439277 -0.730232
 C -4.086468 -0.251764 -0.859385
 C -4.187441 0.753695 0.117133
 C -5.024038 0.530898 1.217577
 C -5.728805 -0.668852 1.349820
 C -3.443151 2.034654 -0.005050
 C -4.078503 3.243082 0.201669
 C -3.385151 4.477092 0.131302
 C -1.994521 4.486292 -0.217985
 C -1.342448 3.237028 -0.506666
 C -2.052408 2.060461 -0.328599
 C -4.044625 5.704514 0.412403
 C -3.359650 6.897118 0.384411
 C -1.978632 6.906453 0.076241
 C -1.314592 5.735808 -0.219780
 O -1.399239 0.851406 -0.481405
 P -0.313576 0.305380 0.685865
 N -1.041409 0.383899 2.195636
 C -1.692316 -0.806879 2.745596
 C 0.077200 3.172755 -0.965763
 C 1.010205 2.440185 -0.244706
 C 2.404821 2.451743 -0.556760
 C 2.807520 3.154904 -1.676119
 C 1.888297 3.824511 -2.518245
 C 0.498768 3.834276 -2.171273
 C -0.407299 4.471270 -3.063886
 C 0.041856 5.088366 -4.211081
 C 1.420414 5.109590 -4.529642
 C 2.322139 4.486467 -3.698858
 O 0.601266 1.707968 0.859880
 C 3.422946 1.791417 0.301582
 C 3.391897 1.908994 1.700556
 C 4.401882 1.352535 2.484602
 C 5.472165 0.675139 1.897232
 C 5.509659 0.554058 0.509300
 C 4.494036 1.098290 -0.280327
 Pd 0.535019 -1.803408 0.110743

C 1.398752 -2.137204 2.143453
 C 2.678674 -2.008290 1.552304
 C 3.415558 -2.963620 0.833866
 C 3.015281 -4.274095 0.607778
 C 3.783903 -5.181580 -0.307381
 N 0.716312 -2.240210 -1.977054
 C 1.129265 -3.500727 -1.801719
 O 1.610746 -4.314414 -2.602517
 N 0.932935 -3.817569 -0.395144
 C -0.138318 -4.861458 -0.198695
 C 0.387935 -6.251000 -0.630725
 C 0.674074 -1.612290 -3.315757
 C -0.240001 -2.423416 -4.259925
 C 0.114454 -0.193970 -3.177150
 C 2.104190 -1.538029 -3.896389
 C -0.528332 -4.932281 1.287796
 C -1.406157 -4.529847 -1.016093
 C -1.336267 1.605972 2.947140
 H -2.196683 -5.254308 -0.788439
 H -1.778533 -3.529960 -0.775563
 H -1.209278 -4.568561 -2.090645
 H -0.404074 -6.996275 -0.487080
 H 0.690721 -6.241724 -1.678003
 H 1.247616 -6.554827 -0.024353
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 H 0.139220 -3.441130 -4.380185
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 H 2.754584 -0.957068 -3.231372
 H 2.524231 -2.539996 -4.005590
 H 0.064956 0.290208 -4.159593
 H -0.890297 -0.211607 -2.746115
 H 0.750113 0.417242 -2.527987
 H 1.030826 -3.123540 2.403039
 H 3.111298 -1.010960 1.583682
 H 2.328612 -4.738026 1.302992
 H 4.761373 -4.752217 -0.552767
 H 3.933402 -6.171339 0.140491
 H 4.290260 -2.603654 0.297361
 H 1.102010 -1.350597 2.831853
 H 3.236032 -5.312545 -1.248686
 H 3.865376 3.208964 -1.918766
 H 3.382429 4.478208 -3.938981
 H -0.671851 5.558995 -4.881528
 H -1.468042 4.455268 -2.843477
 H 1.760052 5.605754 -5.434244
 H -5.142186 3.256262 0.425718
 H -0.255304 5.761505 -0.447099
 H -5.102415 5.679843 0.662764
 H -3.871341 7.828851 0.607897
 H -1.434535 7.846868 0.076083
 H -1.355036 -0.972746 3.776874
 H -2.414244 1.816042 2.952850

H -2.784711 -0.694620 2.750618
 H -1.434446 -1.686698 2.151592
 H -0.811618 2.456842 2.517091
 H -1.005264 1.477828 3.985923
 H 2.581953 2.446542 2.177840
 H 4.530851 0.974813 -1.358043
 H 6.258513 0.251450 2.509211
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 H -5.110014 1.288452 1.990005
 H -6.165734 -2.594033 0.485089
 C -4.733297 -2.483988 -1.815884
 C -6.512980 -0.913737 2.610899
 C 6.630069 -0.189061 -0.171002
 C 4.285041 1.438375 3.983911
 F 7.188430 0.554604 -1.151261
 F 6.183644 -1.326548 -0.757530
 F 7.608917 -0.536673 0.687176
 F 5.459374 1.199017 4.601684
 F 3.851950 2.654786 4.381953
 F 3.393017 0.533954 4.454978
 F -3.587270 -2.397459 -2.522840
 F -4.807749 -3.732977 -1.305667
 F -5.754246 -2.354360 -2.692408
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 F -5.692777 -1.285188 3.624706
 F -7.158863 0.199672 3.022098

XII-si-c

E0 = -4066.593673
 E0+ZPE = -4065.680096
 E298 = -4065.611621
 H298 = -4065.610676
 G298 = -4065.788960
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 C 3.924011 2.112739 2.494402
 C 5.117292 1.524661 2.078372
 C 5.280265 1.208674 0.728709
 C 2.039266 2.469678 -0.780818
 C 0.639550 2.316729 -0.540698
 C -0.325630 2.893552 -1.352719
 C 0.081559 3.471397 -2.603973
 C 1.479296 3.554260 -2.905894
 C 2.421360 3.089570 -1.955701
 C -0.845052 3.928623 -3.580971
 C -0.410564 4.454543 -4.778265
 C 0.971821 4.562106 -5.061132
 C 1.894934 4.120008 -4.141760
 C -1.747377 2.917887 -0.900296
 C -2.445643 4.161594 -0.711550
 C -3.821190 4.127712 -0.312329
 C -4.446271 2.878380 -0.083158
 C -3.765370 1.681372 -0.195781
 C -2.392769 1.729900 -0.592297

C -1.827941 5.434260 -0.864022
 C -2.539575 6.597800 -0.667533
 C -3.908447 6.558866 -0.311378
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 C -4.411082 -0.697596 -0.768977
 C -5.140318 -1.853227 -0.494114
 C -5.935648 -1.943690 0.651573
 C -5.992687 -0.857922 1.520521
 C -5.268978 0.305770 1.246939
 C -5.052047 -3.048864 -1.407528
 F -6.255348 -3.635764 -1.576959
 C -6.782400 -0.949027 2.800614
 F -7.360649 0.231623 3.113332
 O -1.697387 0.541581 -0.709126
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 Pd 0.789825 -1.659767 -0.589119
 N 1.991528 -3.210557 -1.379492
 C 3.187896 -2.895785 -2.249695
 C 4.263838 -2.104867 -1.474753
 O 0.238355 1.601930 0.582860
 C 3.695161 2.419223 3.951718
 F 2.947977 1.462009 4.548613
 C 6.540145 0.512477 0.283797
 F 7.625726 0.990719 0.929663
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 C -1.509262 -1.415686 2.321443
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 C -1.144579 -2.919065 -1.753240
 C -0.684585 -4.240447 -1.698460
 C 0.489132 -4.695140 -2.298209
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 C 1.720733 -3.791184 2.964446
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 C 3.824489 -4.208584 -2.763366
 C 2.746760 -2.052319 -3.457517
 C 4.022209 -2.957617 2.350354
 C 2.207137 -1.317426 2.832842
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 H 3.133849 -4.763514 -3.406175

H 3.617494 -1.829378 -4.084974
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 H 2.304761 -1.102538 -3.137821
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 H 4.598698 -2.177484 1.841776
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 H 1.291456 -6.576471 -2.993409
 H -1.199487 -4.914526 -1.016470
 H -1.106059 -0.899232 -2.477895
 H 1.862290 -6.064672 -1.391055
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 H 2.959730 4.185486 -4.351425
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 H -1.907509 3.844675 -3.382529
 H 1.299576 4.984491 -6.006705
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 H -0.778841 5.486780 -1.128921
 H -5.578711 5.298463 0.156103
 H -4.457790 7.484780 -0.167310
 H -2.041876 7.556553 -0.783818
 H -1.174747 -1.579606 3.352619
 H -2.689039 0.998098 2.781198
 H -2.601656 -1.527477 2.285841
 H -1.050980 -2.180272 1.688897
 H -1.259396 1.970366 2.344506
 H -1.195024 0.878105 3.742395
 H 1.994367 2.856889 1.922164
 H 4.413586 1.228711 -1.234472
 H 5.908599 1.322345 2.790540
 H -3.813108 -0.642413 -1.669952
 H -5.327819 1.143449 1.934122
 H -6.507701 -2.841671 0.854508

XIII-re

E0 = -4223.8380064
 E0+ZPE = -4222.810863
 E298 = -4222.737013
 H298 = -4222.736068
 G298 = -4222.924595
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 C -6.049152 -0.695532 0.940177
 C -5.880558 -1.681166 -0.027609
 C -4.934343 -1.481819 -1.037635

C -3.546247 1.939356 -0.154144
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 C -1.460722 3.131412 -0.715008
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 C -2.103112 6.817686 -0.274195
 C -1.440878 5.638762 -0.540362
 C -0.079356 3.070143 -1.273463
 C 0.929812 2.407859 -0.590049
 C 2.295552 2.460445 -1.010512
 C 2.580353 3.093918 -2.205334
 C 1.571895 3.667953 -3.015806
 C 0.217786 3.665082 -2.550569
 C 1.882994 4.253594 -4.272873
 C 0.894464 4.791108 -5.063932
 C -0.450103 4.759068 -4.624763
 C -0.780229 4.215561 -3.402205
 C 3.413917 1.938171 -0.183460
 C 3.513427 2.249283 1.183533
 C 4.615203 1.833375 1.924272
 C 5.647345 1.104543 1.324193
 C 5.552268 0.790656 -0.026949
 C 4.444668 1.201209 -0.774925
 C 4.721641 2.159528 3.390635
 F 5.686046 3.076315 3.628741
 C 6.626694 -0.003758 -0.721792
 F 6.113449 -1.109291 -1.311094
 O 0.625121 1.714988 0.572644
 P -0.215515 0.252094 0.495962
 Pd 0.598951 -1.755637 -0.445084
 N 0.979034 -3.750419 -1.061576
 C -0.100017 -4.797590 -0.910706
 C -1.369592 -4.333477 -1.639554
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 C -6.990316 -0.911378 2.095496
 F -7.915400 -1.855347 1.830108
 C -4.801295 -2.521369 -2.121130
 F -3.675410 -2.357910 -2.849158
 N -0.760165 0.215452 2.083121
 C -1.061336 1.477745 2.832654
 C -2.463328 1.528142 3.455729
 C -1.050128 -1.149331 2.633934
 C -2.493118 -1.620499 2.385513
 C -0.649769 -1.335365 4.103677
 F -7.644687 0.225165 2.422950
 F -6.318455 -1.307081 3.202767
 F -5.843517 -2.474026 -2.980547
 F -4.776400 -3.770641 -1.605167
 F 5.040205 1.062621 4.114767
 F 3.567466 2.653896 3.889603
 F 7.598069 -0.402569 0.120904
 F 7.211368 0.719934 -1.704951
 C -0.066249 -1.243644 -2.515779

C 1.306742 -1.139331 -2.846298
C 2.214638 -2.173384 -3.122976
C 1.889337 -3.527004 -3.167758
C 2.949876 -4.578760 -3.329927
N 2.085632 -2.845027 0.665090
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C 2.600566 -3.730751 2.922063
C 2.054157 -3.941121 -0.101469
O 2.754574 -4.963284 -0.083195
C 0.362426 -6.139969 -1.523930
C -0.454932 -5.028828 0.576290
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H -1.733026 -3.383803 -1.237008
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H -1.272112 -5.755956 0.649824
H 0.400414 -5.419137 1.133645
H -0.785712 -4.098299 1.049558
H 5.127715 -2.771812 2.238325
H 4.590085 -3.980705 1.042437
H 4.729473 -2.277376 0.578263
H 3.253109 -3.626908 3.798026
H 1.565815 -3.571373 3.247738
H 2.692214 -4.752096 2.541572
H 3.543299 -1.119687 3.202443
H 3.115420 -0.571112 1.569224
H 1.845521 -1.072852 2.687872
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H 3.060980 -5.154307 -2.403735
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H 2.695847 -5.277694 -4.136282
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H 2.919172 4.257043 -4.602062
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H -1.817304 4.192012 -3.089805
H 1.139984 5.229178 -6.027097
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H -0.387667 5.658341 -0.796205
H -5.206706 5.603160 0.435039
H -3.985700 7.752702 0.270765
H -1.564373 7.759743 -0.326504
H -1.032035 2.265992 2.079694
H -0.401688 -1.817027 2.053267
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H -3.424413 -0.198122 -1.853330
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H 2.726967 2.817078 1.664036

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 H 6.497477 0.769690 1.906806
 H -0.127740 2.865942 4.202491
 H -0.006823 1.191237 4.746552
 H 1.023618 1.766786 3.424820
 H -1.295513 -0.782273 4.791821
 H -0.746742 -2.397929 4.352900
 H 0.386569 -1.043546 4.286412
 H -2.634738 2.537515 3.847414
 H -3.238230 1.318363 2.715503
 H -2.583069 0.831780 4.290168
 H -2.758558 -1.518146 1.329352
 H -2.576868 -2.681202 2.651377
 H -3.230207 -1.073200 2.979755

XIII-si

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 E0+ZPE = -4222.810035
 E298 = -4222.736408
 H298 = -4222.735464
 G298 = -4222.922322
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 C 3.470959 2.050352 1.487052
 C 4.499616 1.611166 2.320928
 C 5.614067 0.954573 1.798486
 C 5.675403 0.729823 0.423517
 C 2.474634 2.345499 -0.811614
 C 1.079681 2.326136 -0.492715
 C 0.130010 2.956268 -1.283174
 C 0.529427 3.488914 -2.559846
 C 1.916994 3.478996 -2.911374
 C 2.854465 2.935956 -2.002252
 C -0.395487 3.992504 -3.516087
 C 0.033954 4.483803 -4.729753
 C 1.410563 4.508386 -5.055617
 C 2.330935 4.012742 -4.162044
 C -1.291173 3.053645 -0.838950
 C -1.947333 4.328738 -0.726222
 C -3.356382 4.362971 -0.471714
 C -4.062920 3.143829 -0.334914
 C -3.427584 1.916357 -0.350246
 C -2.009034 1.902695 -0.545377
 C -1.255468 5.568086 -0.821595
 C -1.924465 6.766195 -0.695652
 C -3.322583 6.795385 -0.478068
 C -4.020818 5.615283 -0.368029
 C -4.226029 0.670744 -0.200985
 C -3.999836 -0.456604 -1.010970
 C -4.786000 -1.598060 -0.870172
 C -5.809057 -1.651425 0.080824
 C -6.042298 -0.537188 0.881356
 C -5.264782 0.614174 0.737083
 C -4.573102 -2.791329 -1.767349
 F -5.539189 -2.879381 -2.708567

C -7.069926 -0.588084 1.980278
 F -7.711584 0.593641 2.117603
 O -1.354975 0.687311 -0.501845
 P -0.194371 0.263985 0.654577
 Pd 0.753618 -1.827247 0.071720
 N 1.208489 -3.834440 -0.398319
 C 0.194661 -4.899945 -0.061607
 C -1.149065 -4.646374 -0.779887
 O 0.682760 1.705355 0.682623
 C 4.352552 1.820385 3.804793
 F 3.363200 1.037713 4.308218
 C 6.862493 0.034938 -0.191514
 F 7.685412 -0.489809 0.737159
 N -0.860645 0.386658 2.197625
 C -1.129691 1.717546 2.831666
 C -0.080855 2.098237 3.893358
 C -1.243231 -0.904951 2.848793
 C -0.808924 -1.015893 4.317347
 C -2.718798 -1.299427 2.668505
 C 1.905555 -2.022328 1.984535
 C 3.093952 -1.889119 1.229365
 C 3.777274 -2.862062 0.484118
 C 3.400838 -4.194648 0.380941
 C 4.094655 -5.134310 -0.560307
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 C 0.664897 -1.766693 -3.380725
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 C 1.268987 -3.574390 -1.829608
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 C -0.058554 -4.906144 1.455520
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 C 0.058731 -0.365837 -3.267243
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 F 6.473025 -0.972259 -1.009888
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 H -0.061026 0.077143 -4.262889
 H -0.920293 -0.402472 -2.781672
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 H 3.486105 -0.878883 1.148016
 H 2.811062 -4.634454 1.174430
 H 5.028656 -4.697441 -0.930359
 H 4.317522 -6.094146 -0.079246
 H 4.575202 -2.509006 -0.165474
 H 1.678252 -1.205637 2.663631
 H 3.454666 -5.326661 -1.430438
 H 3.910068 2.998310 -2.251905
 H 3.390776 4.006427 -4.404238
 H -0.694553 4.851358 -5.447094
 H -1.455030 3.972681 -3.291998
 H 1.734097 4.905231 -6.013572
 H -5.143089 3.182851 -0.221174
 H -0.183502 5.564841 -0.981411
 H -5.092999 5.621015 -0.187399
 H -3.837427 7.747739 -0.389230
 H -1.371494 7.699135 -0.761254
 H -0.666341 -1.656913 2.299198
 H -1.024945 2.440579 2.022803
 H 2.627493 2.578875 1.913532
 H 4.689734 0.929544 -1.474859
 H 6.410254 0.616162 2.449237
 H -3.208263 -0.442722 -1.748693
 H -5.457292 1.466601 1.379869
 H -6.406666 -2.548242 0.197028
 H -2.688138 2.925918 3.691486
 H -3.305900 1.655024 2.624785
 H -2.739279 1.256936 4.259396
 H -2.855830 -2.330061 3.018075
 H -3.409918 -0.668143 3.232256
 H -3.003028 -1.264432 1.613983
 H -1.404709 -0.382312 4.981639
 H -0.951813 -2.051579 4.645793
 H 0.246088 -0.762109 4.450856
 H 0.932797 1.884027 3.547223
 H -0.151913 3.172658 4.101791
 H -0.233111 1.570887 4.838762

XIV-re

E0 = -2992.4029794
 E0+ZPE = -2991.329640
 E298 = -2991.268746
 H298 = -2991.267802
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 C 2.649629 4.420797 2.327907
 C 1.797491 4.002941 1.305379
 C 0.538553 3.454706 1.598500
 C 0.160356 3.330283 2.945072
 C 1.014952 3.742139 3.967147

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 C -2.512000 2.904900 -1.437838
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 C -0.692150 4.184419 -0.406889
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 C 0.144456 -2.986257 1.582105
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 C -5.514147 -0.196756 -0.163535
 C -4.997276 -1.459961 -0.541355
 C -3.648988 -1.679202 -0.748806
 C -2.757251 -0.572664 -0.564644
 C -6.895946 -0.013170 0.112510
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 C 0.321969 -3.322356 0.086051
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 C 4.964303 1.515676 1.991694
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 H 2.158535 -2.595509 -2.619239
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 H -1.414006 -4.446246 -3.767476
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 H 2.926218 4.616546 4.458463

(XIV-re)₁

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 C 1.925284 3.923252 1.304227
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 C -1.822413 5.105818 -2.268263
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 Pd 1.842613 -0.373102 -0.654436
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 C 3.643410 1.284601 -3.139903
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 C 4.436789 -2.863532 -1.291232
 C 3.067803 -2.304552 -3.300780
 H 3.417348 -3.238806 -3.755539
 H 2.132192 -2.513297 -2.772384
 H 2.857989 -1.607108 -4.118860
 H 5.781317 -2.488884 -3.579324
 H 5.277217 -0.845931 -3.991453
 H 6.227482 -1.127766 -2.516725
 H 4.719920 -3.793060 -1.799468
 H 5.260145 -2.573057 -0.634431
 H 3.555131 -3.066749 -0.678380
 H 5.256355 1.320101 3.156731
 H 5.854977 1.185940 1.480913
 H 4.362161 2.083910 1.828197
 H 5.351778 -1.238947 3.319355
 H 4.425021 -2.233092 2.176808
 H 5.872041 -1.358498 1.624866
 H 3.233078 0.071279 3.895263
 H 2.285580 0.843680 2.605581
 H 2.298577 -0.920364 2.756461
 H 1.314936 -0.446939 -3.267675
 H 0.616948 2.198264 -1.863909
 H 3.415257 0.479954 -3.826139
 H 5.013848 2.932124 -2.946409
 H 5.691401 1.360890 -2.501492
 H 2.812255 2.999780 -2.193984
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 H 5.457016 1.762456 -4.214238
 H -0.053131 5.093283 -0.243007
 H -1.186765 5.986614 -2.219321
 H -4.349860 3.735923 -4.071365
 H -4.057582 1.932139 -2.439279
 H -2.936946 5.788990 -3.963128
 H -5.772883 -2.128923 -0.859789

H -4.367774 3.049348 0.552120
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 H 0.174449 -1.702151 4.777290
 H -0.146423 0.491901 3.720981
 H -1.823693 0.813576 3.236442
 H -1.485335 0.098323 4.809735
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 H 1.478288 -3.194981 3.318661
 H 0.816906 -4.735552 2.772716
 H 0.920221 -2.882279 -0.312973
 H 2.057183 -2.539506 1.008376
 H 1.524676 -4.198027 0.683562
 H -0.738199 -4.903543 0.903183
 H -1.961539 -4.006008 1.796710
 H -1.468150 -3.464796 0.191291
 H -0.041673 -4.105536 5.050009
 H -1.365356 -4.194790 3.898239
 H -4.684118 -4.089538 -0.187130
 H -1.836200 -2.128662 -2.744170
 H -4.151089 -6.253307 -1.249970
 H -1.292724 -4.290858 -3.796518
 H -2.439888 -6.372072 -3.055275
 H -0.643913 2.860724 3.256108
 H 2.204865 4.030370 0.260119
 H 0.949830 3.504657 5.028990
 H 3.786951 4.717195 2.031813
 H 3.171866 4.452779 4.428164

(XIV-re)₂

E0 = -2992.4053652
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 H298 = -2991.270351
 G298 = -2991.423247
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 C -0.413703 -3.457913 1.669525
 C -1.623051 -4.150739 1.498110
 C -2.374130 -4.562608 2.599089
 C 0.465211 -3.171788 0.504533
 C 1.200352 -1.953297 0.346372
 C 2.257408 -1.842703 -0.547430
 C 2.441708 -2.871187 -1.536031
 C 1.625958 -4.045164 -1.475151
 C 0.697876 -4.179085 -0.414479
 C 3.376400 -2.758308 -2.602584
 C 3.502070 -3.756739 -3.543983
 C 2.710912 -4.927507 -3.465645
 C 1.792535 -5.065541 -2.450565

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 C 0.925656 3.787357 3.799755
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 C 1.399119 1.339099 3.038717
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 C 5.496505 0.206157 -0.262332
 C 4.980970 1.488703 -0.572166
 C 3.631908 1.718752 -0.763518
 C 2.745396 0.603197 -0.635965
 C 6.881277 0.008623 -0.010979
 C 7.372941 -1.239380 0.295026
 C 6.490423 -2.343154 0.364709
 C 5.145032 -2.186661 0.110340
 C 3.173147 3.075778 -1.163582
 C 3.614798 4.210792 -0.464186
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 C 2.696708 0.534135 2.794796
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 C -2.705137 -1.798866 -2.760596
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 O -5.729945 -0.127710 -0.526634
 N -3.749614 0.591912 -1.583612
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 C -4.873206 -1.848735 1.774912
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 C -5.128868 0.557763 2.497372
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 H -2.229674 -1.355798 2.415017
 H -2.451571 0.294263 3.024493
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 H 0.122982 0.168081 -2.528849
 H -5.587265 -1.329117 -4.317285
 H 0.172853 -5.123523 -0.301396
 H 1.171919 -5.955758 -2.382381
 H 4.213718 -3.642124 -4.356986
 H 3.983909 -1.864230 -2.681695
 H 2.825534 -5.709457 -4.211098
 H 5.677293 2.315871 -0.683410
 H 4.483797 -3.042729 0.176763
 H 7.544851 0.868869 -0.057963
 H 8.432343 -1.378949 0.491278
 H 6.876706 -3.324825 0.625097
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 H 1.413185 4.392154 1.801968
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 H -0.953002 2.756621 -0.423389
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 H -2.173720 2.018126 1.702097
 H -1.592492 2.506325 3.301386
 H 2.797701 2.987722 3.170145
 H 2.262536 2.345658 4.718205
 H 2.524084 -0.511623 2.557379
 H 3.292598 0.985306 1.997818
 H 3.292161 0.573095 3.714431
 H 1.083252 0.267360 4.903013
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 H 0.098813 -0.341417 3.561805
 H 1.399152 4.655607 4.275097
 H 0.055007 3.531072 4.415823
 H 4.233177 4.082167 0.420273
 H 2.023077 2.396334 -2.857935
 H 3.606940 6.358881 -0.325353
 H 1.402398 4.666488 -3.609546
 H 2.184883 6.662455 -2.345634
 H 0.960261 -2.668015 3.134322
 H -1.980784 -4.357794 0.493435
 H -0.380285 -3.373614 5.082213
 H -3.309973 -5.091705 2.442934
 H -2.517695 -4.606133 4.751446

(XIV-re)₃

E0 = -2992.4005292
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H298 = -2991.265156
G298 = -2991.418651
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C -3.882724 -4.143184 -0.889120
C -3.550781 -5.402142 -1.388979
C -3.667215 -1.644219 -0.875404
C -5.015314 -1.371607 -0.736033
C -5.499678 -0.100316 -0.343660
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C 0.074320 -3.076412 1.732544
C -2.201427 1.861719 -0.416059
C -1.142502 1.920131 0.480346
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C -1.540676 4.097101 -1.246772
C -2.368838 2.935615 -1.361283
C -3.298194 2.881249 -2.437469
C -3.411237 3.923523 -3.331615
C -2.612013 5.083312 -3.195307
C -1.695213 5.164170 -2.173001
O -0.861508 0.812218 1.273921
C 0.548291 3.324909 1.822720
C 1.818713 3.885750 1.618354
C 2.630001 4.229084 2.700457
C 2.188237 4.011831 4.006509
C 0.928097 3.450314 4.222903
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C -0.588021 -0.437193 4.028659
C -0.950375 -4.089446 1.175861
C 1.287989 -3.146202 0.790140
Pd 1.842948 -0.363885 -0.675474
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C 2.576977 2.048406 -2.605703

C 3.634251 1.323339 -3.155614
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 C 3.080756 -2.281373 -3.314001
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 H 1.102601 -4.454933 3.025408
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 H -1.166722 -4.472392 -3.626389
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XIV-si

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 C -4.948568 -4.317799 -1.373422
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 C -1.997639 3.596655 -2.326789
 C -1.688278 4.665568 -3.140145
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 C 0.160636 5.274560 -1.711193
 O -0.689390 0.667716 1.362455
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 H -0.021028 -1.616122 4.225773
 H -0.395742 -0.006171 3.604988
 H -1.410936 -0.725396 4.868082
 H -0.738760 -3.159613 -0.841901
 H 0.920523 -3.194627 -0.185689
 H -0.050935 -4.668345 -0.242641
 H 0.132803 -3.817603 3.369852
 H 0.520086 -5.001171 2.122051
 H 1.352540 -3.443889 2.156034
 H 3.094104 3.214540 1.611011
 H -0.631728 2.267007 3.529661
 H 4.213766 3.270004 3.806611
 H 0.489559 2.297480 5.726907
 H 2.923441 2.801270 5.883967
 H -2.368503 -1.854913 -2.884867
 H -5.554940 -2.677846 -0.118887
 H -2.481651 -4.178307 -3.707532
 H -5.675717 -5.003550 -0.946562
 H -4.133876 -5.771853 -2.744753

(XIV-si)₁

E0+ZPE = -2991.321652
 E298 = -2991.261404
 H298 = -2991.260459
 G298 = -2991.413553
 NImag = 1, (-214.5629)
 C -3.800941 -4.761946 -2.810372
 C -4.645632 -4.565546 -1.716562
 C -4.680990 -3.329127 -1.070592
 C -3.869104 -2.267389 -1.501216
 C -3.026739 -2.476546 -2.607238

C -2.994360 -3.711157 -3.254684
 C -3.977447 -0.927012 -0.865506
 C -5.229359 -0.376559 -0.674595
 C -5.415329 0.932293 -0.167489
 C -4.267210 1.757062 0.053365
 C -2.957447 1.218592 -0.210771
 C -2.833952 -0.128764 -0.524475
 C -6.713128 1.448463 0.092712
 C -6.881446 2.725138 0.577859
 C -5.748415 3.535930 0.822551
 C -4.477846 3.068572 0.563343
 O -1.587433 -0.711325 -0.609419
 P -0.328041 -0.695410 0.551951
 N -0.608104 -1.926680 1.708834
 C -1.507941 -1.814251 2.960644
 C -1.074729 -2.870378 4.016298
 C -0.878312 -4.291927 3.520436
 C 0.144653 -4.250072 2.398074
 C -0.283361 -3.358320 1.212416
 C -1.768167 2.117092 -0.153122
 C -0.743154 1.881685 0.748140
 C 0.247841 2.867105 1.061017
 C 0.278019 3.999181 0.267027
 C -0.620649 4.203135 -0.808443
 C -1.682600 3.266110 -1.014322
 C -2.581155 3.495174 -2.092705
 C -2.440582 4.594958 -2.911301
 C -1.404386 5.532689 -2.689459
 C -0.515241 5.338206 -1.657420
 O -0.734964 0.663172 1.424424
 C 1.131277 2.798366 2.256894
 C 2.468009 3.223731 2.188130
 C 3.268056 3.268964 3.330019
 C 2.745113 2.896748 4.569558
 C 1.412810 2.488311 4.656282
 C 0.614335 2.442137 3.513647
 C -3.006786 -1.958673 2.625562
 C -1.336716 -0.480885 3.723856
 C 0.897196 -3.384896 0.225004
 C -1.475420 -4.007714 0.479591
 Pd 1.708652 -0.332629 -0.721587
 C 0.631258 -0.148840 -2.642783
 C 0.933242 -1.507465 -2.919272
 C 2.152615 -2.050092 -3.338746
 C 3.297480 -1.302083 -3.630896
 C 4.608032 -1.987443 -3.908751
 N 3.518327 -0.813155 0.361145
 C 4.304436 -0.735231 -0.717079
 O 5.471334 -1.110415 -0.902105
 N 3.530185 -0.060746 -1.763798
 C 4.119188 1.308886 -2.053731
 C 5.379721 1.178786 -2.942466
 C 4.053275 -1.197690 1.688641
 C 5.240594 -0.290726 2.082491
 C 2.940442 -1.014990 2.729583
 C 4.527989 -2.668752 1.673047

C 3.094236 2.195592 -2.780379
 C 4.527038 2.029406 -0.751457
 H 4.816923 3.062610 -0.978899
 H 3.696266 2.043107 -0.043596
 H 5.376541 1.537067 -0.272529
 H 5.822773 2.173009 -3.079862
 H 6.113264 0.523127 -2.472031
 H 5.139573 0.785695 -3.935083
 H 3.543674 3.176014 -2.977200
 H 2.795802 1.782851 -3.750012
 H 2.196931 2.349590 -2.172994
 H 5.624957 -0.580911 3.068403
 H 6.050747 -0.378185 1.354757
 H 4.921688 0.755527 2.138440
 H 4.914847 -2.953919 2.659999
 H 3.705276 -3.347216 1.424295
 H 5.320192 -2.800632 0.932291
 H 3.314176 -1.266741 3.729615
 H 2.593302 0.023113 2.744227
 H 2.079661 -1.654677 2.516505
 H 1.203217 0.620845 -3.143208
 H 0.149586 -2.224926 -2.677036
 H 3.164594 -0.314514 -4.051614
 H 4.476715 -3.074338 -3.950546
 H 5.040812 -1.649933 -4.858750
 H 2.263737 -3.130728 -3.264990
 H -0.409189 0.103324 -2.473764
 H 5.327813 -1.772019 -3.111409
 H 0.998325 4.780344 0.493561
 H 0.290714 6.046230 -1.479958
 H -3.130985 4.741783 -3.737362
 H -3.376056 2.782643 -2.280560
 H -1.309707 6.398905 -3.338359
 H -6.106389 -0.957504 -0.947623
 H -3.622661 3.702647 0.765864
 H -7.572649 0.808674 -0.093146
 H -7.877471 3.109044 0.780011
 H -5.880044 4.537648 1.222563
 H 1.101850 -3.885455 2.793211
 H 0.327816 -5.254275 1.997616
 H -0.521356 -4.926065 4.341588
 H -1.823509 -4.731187 3.178486
 H -0.129474 -2.529538 4.459471
 H -1.825395 -2.838006 4.815063
 H 0.640743 -2.987726 -0.757430
 H 1.771728 -2.848280 0.589433
 H 1.178473 -4.433716 0.075916
 H -2.331555 -4.206542 1.124113
 H -1.812860 -3.382563 -0.346154
 H -1.154752 -4.970027 0.063135
 H -3.595429 -1.770941 3.531786
 H -3.311498 -1.222395 1.877781
 H -3.277952 -2.949389 2.257824
 H -0.286379 -0.193159 3.793409
 H -1.901498 0.337138 3.281778
 H -1.716241 -0.632833 4.740888

H 2.886157 3.514001 1.230599
 H -0.426753 2.154551 3.599539
 H 4.302067 3.592645 3.247646
 H 0.987777 2.214046 5.618253
 H 3.367749 2.929683 5.459374
 H -5.330890 -3.186456 -0.211456
 H -2.405126 -1.663029 -2.966936
 H -5.276528 -5.376349 -1.361791
 H -2.342844 -3.849918 -4.113500
 H -3.772879 -5.724113 -3.314479

(XIV-si)₂

E0 = -2992.400157
 E0+ZPE = -2991.326551
 E298 = -2991.265904
 H298 = -2991.264960
 G298 = -2991.417924
 NImag = 1, (-169.5783)
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 C 1.083078 2.775084 4.563908
 C 0.417122 2.631399 3.347119
 C 1.059666 2.926883 2.132587
 C 2.387849 3.382271 2.180335
 C 3.053231 3.528096 3.397711
 C 0.298180 2.917831 0.853366
 C -0.658502 1.907487 0.507071
 C -1.633475 2.124594 -0.457508
 C -1.478171 3.232403 -1.361156
 C -0.423484 4.171181 -1.131029
 C 0.389572 4.015655 0.017391
 C -0.251773 5.263445 -2.023700
 C -1.072843 5.416291 -3.117481
 C -2.104898 4.478677 -3.359132
 C -2.307819 3.419434 -2.501089
 O -0.670366 0.721672 1.236382
 P -0.410102 -0.752493 0.483545
 O -1.507462 -0.666331 -0.800139
 C -2.761347 -0.091543 -0.737337
 C -2.856836 1.272333 -0.518628
 C -4.155792 1.858551 -0.314656
 C -5.316888 1.033608 -0.464243
 C -5.154743 -0.327439 -0.820834
 C -3.911316 -0.911686 -0.963909
 C -6.607922 1.594525 -0.269219
 C -6.758431 2.914475 0.088027
 C -5.613461 3.725416 0.269481
 C -4.348856 3.214659 0.071490
 C -3.822557 -2.327708 -1.410992
 C -3.079892 -2.681104 -2.549829
 C -3.070206 -3.996324 -3.013273
 C -3.800551 -4.983897 -2.347187
 C -4.545332 -4.644980 -1.216128
 C -4.558187 -3.327426 -0.754358
 Pd 1.761933 -0.743856 -0.666413
 N 3.557775 -0.558857 0.564355
 C 4.378264 -0.536018 -0.485990

O 5.606961 -0.689153 -0.570117
N 3.557570 -0.286887 -1.669380
C 3.767845 1.114026 -2.200300
C 2.655202 1.472224 -3.200624
C 3.744194 2.159751 -1.065754
C 5.133326 1.210534 -2.922108
C 0.948490 -1.489071 -2.607819
C 1.692169 -2.690530 -2.519953
C 3.050686 -2.903285 -2.787314
C 3.928281 -1.941448 -3.272221
C 5.401965 -2.208874 -3.362824
C 4.073172 -0.700908 1.945152
C 2.914385 -0.460092 2.918790
C 4.645386 -2.122261 2.138592
C 5.175810 0.342717 2.235364
N -1.092075 -1.803548 1.657944
C -1.778452 -1.346656 2.957128
C -2.574467 -2.506920 3.612992
C -1.846659 -3.836873 3.695778
C -1.536824 -4.245884 2.267689
C -0.614960 -3.261023 1.513983
C -0.731668 -0.830170 3.964912
C -2.858168 -0.266379 2.716112
C 0.833879 -3.440710 2.007674
C -0.696831 -3.697335 0.041513
H 3.808553 3.166472 -1.496645
H 2.817097 2.084446 -0.493086
H 4.586078 2.025531 -0.381296
H 5.289407 2.244286 -3.254516
H 5.944782 0.921403 -2.253111
H 5.166931 0.569882 -3.808777
H 2.829554 2.480616 -3.593447
H 2.634069 0.791650 -4.058900
H 1.670625 1.463278 -2.723354
H 5.524665 0.240439 3.270807
H 6.023401 0.209398 1.560799
H 4.780769 1.356909 2.112322
H 5.008576 -2.256926 3.165821
H 3.876564 -2.878857 1.946178
H 5.476818 -2.289391 1.448558
H 3.261784 -0.549206 3.955237
H 2.497464 0.540698 2.780576
H 2.114751 -1.186250 2.765058
H 1.293293 -0.708371 -3.275180
H 1.168795 -3.551298 -2.108292
H 3.531838 -1.135532 -3.874401
H 5.611812 -3.277823 -3.244388
H 5.817568 -1.869909 -4.319059
H 3.475424 -3.848068 -2.451565
H -0.130292 -1.564971 -2.527655
H 5.920610 -1.679155 -2.553717
H -2.871047 -2.153576 4.607785
H -0.934510 -3.763051 4.300708
H -3.502380 -2.660558 3.045376
H -2.483686 -4.586946 4.181002
H 1.087653 4.809235 0.268425

H 0.548766 5.972911 -1.828373
 H -2.741744 4.593037 -4.232047
 H -3.097046 2.704288 -2.703727
 H -0.928285 6.250086 -3.798864
 H -6.042396 -0.926723 -1.006806
 H -3.485925 3.851590 0.224891
 H -7.476650 0.953809 -0.400904
 H -7.749469 3.332873 0.240097
 H -5.731364 4.762382 0.572057
 H -2.483105 -4.339165 1.718195
 H -1.050273 -5.227591 2.225382
 H 1.140247 -4.486610 1.883787
 H 1.524614 -2.823696 1.427673
 H 0.950156 -3.182645 3.063549
 H -0.017260 -3.134237 -0.594799
 H -0.409932 -4.753270 -0.030788
 H -1.709805 -3.586469 -0.345151
 H -1.236568 -0.426175 4.851504
 H -0.063205 -1.628086 4.300465
 H -0.120139 -0.038249 3.532699
 H -2.453168 0.717612 2.497615
 H -3.526713 -0.560599 1.902541
 H -3.462311 -0.183633 3.627195
 H -2.520453 -1.917035 -3.080625
 H -5.134338 -3.067914 0.129851
 H -2.494821 -4.248870 -3.899936
 H -5.117186 -5.405509 -0.690907
 H -3.790438 -6.008588 -2.708538
 H -0.619597 2.312527 3.339869
 H 2.907361 3.613670 1.256402
 H 0.562540 2.545132 5.489852
 H 4.083184 3.874093 3.407026
 H 2.923683 3.334813 5.543562

(XIV-*re*)₃

E0+ZPE = -2991.327070
 E298 = -2991.266468
 H298 = -2991.265524
 G298 = -2991.418951
 NImag = 1, (-208.3743)
 C -4.108062 -4.636675 -2.656674
 C -4.936039 -4.297818 -1.585589
 C -4.880106 -3.016670 -1.034318
 C -3.992256 -2.052076 -1.537866
 C -3.163076 -2.406663 -2.616073
 C -3.223905 -3.684537 -3.171073
 C -4.007624 -0.666580 -0.995085
 C -5.211247 -0.003757 -0.864190
 C -5.296547 1.325322 -0.382591
 C -4.089865 2.041215 -0.097112
 C -2.822424 1.386234 -0.304651
 C -2.813185 0.040064 -0.638662
 C -6.553776 1.957839 -0.187343
 C -6.631592 3.241893 0.300669
 C -5.443984 3.941991 0.616437
 C -4.209244 3.361409 0.420357

O -1.624543 -0.646419 -0.705519
 P -0.394545 -0.790621 0.459190
 N -0.818827 -2.047717 1.516397
 C -1.695770 -1.880376 2.772702
 C -2.269854 -3.241143 3.238627
 C -1.246833 -4.367211 3.431394
 C -0.067755 -4.231539 2.455984
 C -0.394788 -3.473268 1.150529
 C -1.556622 2.157401 -0.122657
 C -0.627428 1.795797 0.842709
 C 0.384444 2.698483 1.304776
 C 0.567851 3.864241 0.585017
 C -0.203906 4.181099 -0.559530
 C -1.305591 3.336971 -0.908413
 C -2.081041 3.682597 -2.049419
 C -1.785480 4.803554 -2.795113
 C -0.709676 5.648394 -2.433334
 C 0.062106 5.341065 -1.336186
 O -0.723287 0.535838 1.433723
 C 1.120452 2.514449 2.585256
 C 2.483038 2.838806 2.691520
 C 3.138351 2.787494 3.922099
 C 2.444540 2.413862 5.074064
 C 1.087408 2.098220 4.985183
 C 0.432072 2.151025 3.755318
 C -2.934862 -0.997129 2.524727
 C -0.834441 -1.296291 3.909739
 C -1.488415 -4.191336 0.328193
 C 0.884759 -3.524241 0.297960
 Pd 1.657645 -0.459385 -0.794249
 C 0.631767 -0.446601 -2.756889
 C 1.076175 -1.772293 -2.993764
 C 2.353247 -2.194049 -3.379275
 C 3.417034 -1.337085 -3.672119
 C 4.797795 -1.881875 -3.912177
 N 3.486572 -0.799238 0.323673
 C 4.276533 -0.653826 -0.742911
 O 5.472941 -0.933406 -0.913305
 N 3.465107 -0.049519 -1.803117
 C 3.913597 1.374341 -2.072434
 C 5.241596 1.380147 -2.866913
 C 4.035008 -1.206414 1.638812
 C 5.174772 -0.256568 2.071960
 C 2.914294 -1.121081 2.683176
 C 4.582553 -2.650098 1.565278
 C 2.852615 2.132671 -2.888403
 C 4.129771 2.149121 -0.754675
 H 4.357590 3.197736 -0.981712
 H 3.227967 2.112279 -0.138338
 H 4.961837 1.736576 -0.179190
 H 5.570510 2.417354 -3.006194
 H 6.013913 0.826433 -2.332367
 H 5.117808 0.937651 -3.860475
 H 3.209153 3.151156 -3.081216
 H 2.666090 1.670855 -3.863714
 H 1.905522 2.206161 -2.345576

H 5.562728 -0.555542 3.053877
 H 5.993944 -0.282864 1.349992
 H 4.804290 0.770662 2.154066
 H 4.975763 -2.959224 2.542426
 H 3.796527 -3.356534 1.277956
 H 5.385977 -2.709303 0.827271
 H 3.293565 -1.414116 3.669557
 H 2.526360 -0.101058 2.755551
 H 2.079305 -1.780366 2.431528
 H 1.138092 0.366502 -3.259872
 H 0.365994 -2.563891 -2.753784
 H 3.191308 -0.370884 -4.102544
 H 4.778294 -2.975463 -3.976440
 H 5.230186 -1.483086 -4.838008
 H 2.573764 -3.256136 -3.285328
 H -0.431411 -0.296595 -2.613820
 H 5.459708 -1.611034 -3.081460
 H -2.786996 -3.044329 4.184893
 H 0.767100 -3.711218 2.938581
 H -0.867338 -4.370636 4.459558
 H -3.051007 -3.551906 2.539346
 H -1.750781 -5.330757 3.292397
 H 0.308742 -5.223770 2.182246
 H -2.690891 0.046119 2.339559
 H -3.516699 -1.376010 1.679715
 H -3.575216 -1.037438 3.413664
 H -1.169775 -5.220394 0.120726
 H -2.456796 -4.238335 0.825370
 H -1.638106 -3.687553 -0.629904
 H -0.036094 -1.984548 4.201680
 H -0.372213 -0.356237 3.614046
 H -1.459920 -1.112806 4.792665
 H 0.737652 -3.137173 -0.710731
 H 1.717710 -2.984741 0.746295
 H 1.175607 -4.576097 0.196171
 H 1.310997 4.580531 0.924351
 H 0.896049 5.977504 -1.050275
 H -2.383253 5.038925 -3.671410
 H -2.903764 3.040888 -2.343733
 H -0.492506 6.532681 -3.025987
 H -6.127756 -0.513469 -1.149884
 H -3.313698 3.913618 0.678913
 H -7.456653 1.399222 -0.422810
 H -7.597901 3.714478 0.453038
 H -5.504239 4.948245 1.022192
 H 3.036244 3.122427 1.802321
 H -0.630130 1.935375 3.703819
 H 4.195083 3.034416 3.976929
 H 0.532232 1.819424 5.876925
 H 2.955418 2.372404 6.032111
 H -5.523726 -2.760072 -0.196910
 H -2.482073 -1.671097 -3.031919
 H -5.626822 -5.030383 -1.176271
 H -2.583650 -3.934915 -4.012984
 H -4.152264 -5.632421 -3.089392

XIV-si-c

E0+ZPE = -2991.327555
E298 = -2991.267168
H298 = -2991.266224
G298 = -2991.418638
NImag = 1, (-177.8758)
C 2.274534 4.307863 3.862173
C 2.639895 4.582893 2.542664
C 1.815512 4.188296 1.488607
C 0.604590 3.516180 1.731818
C 0.244378 3.256200 3.064486
C 1.073274 3.643236 4.118046
C -0.326169 3.221872 0.610154
C -1.070163 2.004238 0.476805
C -2.121017 1.883559 -0.422390
C -2.315156 2.908722 -1.414976
C -1.512880 4.090422 -1.355757
C -0.572674 4.225418 -0.308695
C -1.690396 5.112620 -2.327013
C -2.606525 4.967457 -3.342542
C -3.379978 3.785493 -3.425304
C -3.243017 2.785920 -2.486701
O -0.780151 0.942601 1.333131
P -0.188737 -0.512990 0.740334
O -1.183693 -0.763631 -0.600379
C -2.554026 -0.569054 -0.597191
C -3.043545 0.711524 -0.396356
C -4.455559 0.898875 -0.200836
C -5.328524 -0.223670 -0.362213
C -4.779152 -1.470981 -0.746848
C -3.417741 -1.678057 -0.874908
C -6.726704 -0.057216 -0.169174
C -7.249008 1.162499 0.195309
C -6.386275 2.268526 0.381740
C -5.028090 2.142866 0.184057
C -2.929259 -2.983953 -1.393586
C -3.499377 -4.188393 -0.946284
C -3.113506 -5.412614 -1.493762
C -2.150883 -5.456916 -2.503753
C -1.581227 -4.267048 -2.962762
C -1.965372 -3.043325 -2.415252
Pd 2.116087 -0.502434 0.046695
N 2.506927 0.040455 -2.019666
C 3.832734 -0.036475 -1.891903
O 4.747804 0.369111 -2.626505
N 4.106178 -0.722954 -0.633638
C 4.662107 -2.107489 -0.867153
C 4.631627 -2.910997 0.444680
C 3.850242 -2.879552 -1.933134
C 6.130933 -2.017237 -1.346767
C 2.865997 -0.373663 2.132063
C 3.247770 0.967765 1.885281
C 4.392500 1.440845 1.232308
C 5.405983 0.637699 0.720463
C 6.514919 1.219240 -0.108299
C 1.888025 0.647757 -3.218589

C 0.369542 0.485748 -3.121287
 C 2.238723 2.150615 -3.278497
 C 2.377804 -0.063722 -4.499808
 N -0.722572 -1.574514 1.971287
 C -1.495152 -1.163496 3.233206
 C -1.912598 -2.424129 4.041321
 C -2.464024 -3.533792 3.158739
 C -1.400381 -4.000711 2.151522
 C -0.215264 -3.016228 1.906131
 C -2.807381 -0.420570 2.893558
 C -0.615786 -0.292473 4.150353
 C 0.338014 -3.398103 0.516203
 C 0.941219 -3.266868 2.905454
 H 4.231021 -3.905116 -2.011119
 H 2.788743 -2.923848 -1.671542
 H 3.938693 -2.408592 -2.915836
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 H 6.203673 -1.426232 -2.260224
 H 6.770052 -1.559256 -0.585232
 H 5.064094 -3.904074 0.275537
 H 5.220572 -2.431290 1.234124
 H 3.609752 -3.047096 0.810277
 H 1.902037 0.377455 -5.384827
 H 3.461389 0.023914 -4.601126
 H 2.112387 -1.127369 -4.467692
 H 1.752726 2.626618 -4.139989
 H 1.890519 2.653405 -2.368442
 H 3.319725 2.285775 -3.364061
 H -0.113796 0.886552 -4.020326
 H 0.104123 -0.571313 -3.020972
 H -0.029603 1.014119 -2.252883
 H 3.629484 -1.144296 2.156108
 H 2.519549 1.722568 2.165916
 H 5.583441 -0.326745 1.177389
 H 6.541874 2.310386 -0.009747
 H 7.491961 0.814259 0.180424
 H 4.405060 2.497405 0.972673
 H 2.064622 -0.516062 2.849695
 H 6.343586 0.988250 -1.167003
 H -2.634226 0.551481 2.441032
 H -3.432310 -1.005534 2.213521
 H -3.372490 -0.262377 3.819443
 H 0.526027 -4.478088 0.520817
 H -0.370442 -3.192171 -0.286444
 H 1.286977 -2.904056 0.285859
 H 0.277357 -0.838505 4.470716
 H -0.297453 0.624409 3.654311
 H -1.178171 -0.015964 5.051270
 H 1.813471 -2.671757 2.632555
 H 0.690213 -3.041644 3.942464
 H 1.232724 -4.323002 2.861881
 H -0.040923 5.167537 -0.210283
 H -1.077154 6.007711 -2.256882
 H -4.086343 3.661400 -4.241534
 H -3.835715 1.883625 -2.576006
 H -2.730009 5.749588 -4.086376

H -5.459884 -2.285695 -0.978650
 H -4.380979 2.999027 0.336709
 H -7.376315 -0.918103 -0.308722
 H -8.318649 1.277999 0.346634
 H -6.798448 3.226876 0.685660
 H -1.879276 -4.209599 1.191184
 H -0.954944 -4.946868 2.482625
 H -1.075843 -2.803359 4.634609
 H -2.666039 -2.098756 4.767511
 H -3.349330 -3.168652 2.625978
 H -2.804725 -4.373677 3.775750
 H -4.242620 -4.163876 -0.153740
 H -1.524650 -2.125740 -2.788920
 H -3.563475 -6.331421 -1.126935
 H -0.838075 -4.288006 -3.755312
 H -1.848727 -6.409216 -2.930893
 H 2.117798 4.384330 0.463858
 H -0.703893 2.773997 3.275531
 H 3.573374 5.097506 2.331284
 H 0.772493 3.435208 5.141441
 H 2.918824 4.610240 4.683026

(XIV-si-c)₁

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 E0+ZPE = -2991.327714
 E298 = -2991.267060
 H298 = -2991.266115
 G298 = -2991.420261
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 C 2.310981 4.623479 2.981269
 C 1.554961 4.278882 1.861234
 C 0.416023 3.460155 1.977133
 C 0.060192 3.001143 3.257169
 C 0.820283 3.341692 4.376545
 C -0.439289 3.201832 0.788139
 C -1.120365 1.964534 0.537950
 C -2.120393 1.861617 -0.420991
 C -2.291583 2.930886 -1.369830
 C -1.545349 4.137233 -1.195685
 C -0.681244 4.249198 -0.082705
 C -1.706000 5.204327 -2.120620
 C -2.549211 5.079479 -3.200057
 C -3.264927 3.874494 -3.395605
 C -3.145089 2.831017 -2.503596
 O -0.827076 0.869485 1.347518
 P -0.201583 -0.552992 0.721271
 O -1.155950 -0.777013 -0.647112
 C -2.526714 -0.593278 -0.675491
 C -3.031629 0.682089 -0.481247
 C -4.452733 0.856893 -0.335894
 C -5.310329 -0.272884 -0.529412
 C -4.737599 -1.519640 -0.879981
 C -3.371443 -1.713148 -0.960995
 C -6.716213 -0.119773 -0.387523
 C -7.263028 1.093742 -0.039612

C -6.417036 2.205647 0.184038
 C -5.051495 2.092889 0.036193
 C -2.852634 -3.030069 -1.417712
 C -3.369879 -4.222154 -0.883567
 C -2.954167 -5.463727 -1.367241
 C -2.016169 -5.535579 -2.398547
 C -1.498771 -4.357234 -2.942308
 C -1.911074 -3.116446 -2.457359
 Pd 2.118528 -0.427225 0.026609
 N 2.473111 0.106868 -2.059492
 C 3.800979 0.054101 -1.950618
 O 4.697863 0.444196 -2.716325
 N 4.109480 -0.582776 -0.675901
 C 4.718098 -1.951028 -0.874635
 C 4.700906 -2.723082 0.455266
 C 3.944746 -2.774623 -1.930520
 C 6.187383 -1.821059 -1.343228
 C 2.899310 -0.158489 2.094234
 C 3.226416 1.181703 1.776715
 C 4.342561 1.665844 1.085423
 C 5.378584 0.876397 0.596869
 C 6.458030 1.460201 -0.268534
 C 1.835264 0.652305 -3.279390
 C 0.318232 0.503418 -3.151822
 C 2.185555 2.150330 -3.420465
 C 2.303679 -0.124555 -4.529996
 N -0.755099 -1.682472 1.890731
 C -1.652266 -1.363354 3.101160
 C -2.397205 -2.635951 3.599058
 C -1.586281 -3.916711 3.687911
 C -0.993394 -4.167959 2.312056
 C -0.034316 -3.047609 1.854011
 C -0.812512 -0.755278 4.245925
 C -2.820565 -0.398182 2.788793
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 C 0.385116 -3.430034 0.418832
 H 4.362701 -3.787206 -1.982644
 H 2.883236 -2.852318 -1.677299
 H 4.026656 -2.321468 -2.922023
 H 6.601495 -2.823400 -1.508907
 H 6.247982 -1.248192 -2.268948
 H 6.804358 -1.327340 -0.585865
 H 5.176082 -3.701538 0.318231
 H 5.256817 -2.199417 1.240741
 H 3.679318 -2.890841 0.807169
 H 1.817367 0.273598 -5.429642
 H 3.386040 -0.046928 -4.651505
 H 2.034272 -1.183957 -4.440670
 H 1.683293 2.581320 -4.296179
 H 1.852629 2.698059 -2.530845
 H 3.264382 2.281824 -3.531485
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 H 0.046552 -0.545662 -3.002434
 H -0.063035 1.072138 -2.300783
 H 3.691970 -0.898012 2.145516
 H 2.474913 1.920111 2.033916

H 5.595116 -0.059357 1.095271
 H 6.454131 2.554447 -0.207524
 H 7.450450 1.093718 0.018610
 H 4.314054 2.709698 0.777921
 H 2.116430 -0.292996 2.834861
 H 6.278450 1.188184 -1.316099
 H -2.834664 -2.379105 4.571534
 H -0.802889 -3.847862 4.452536
 H -3.238337 -2.819150 2.917262
 H -2.238201 -4.747465 3.986274
 H -0.206843 5.208018 0.104595
 H -1.137210 6.117676 -1.964066
 H -3.912182 3.768054 -4.261787
 H -3.691216 1.911417 -2.677110
 H -2.658525 5.895975 -3.908302
 H -5.401300 -2.347510 -1.115281
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 H -7.351671 -0.986747 -0.552133
 H -8.338542 1.199359 0.072139
 H -6.848006 3.158871 0.477851
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 H -0.427808 -5.107178 2.288509
 H 1.665230 -4.088522 2.703735
 H 1.977751 -2.385163 2.365263
 H 1.032347 -2.846019 3.783808
 H 1.187344 -2.798536 0.023403
 H 0.769202 -4.456247 0.439475
 H -0.457235 -3.400026 -0.271864
 H -1.474309 -0.410258 5.050053
 H -0.113852 -1.472779 4.683362
 H -0.239551 0.104854 3.889226
 H -2.519965 0.640334 2.685502
 H -3.353452 -0.703645 1.886977
 H -3.527478 -0.456658 3.624493
 H -4.095948 -4.171711 -0.076419
 H -1.508949 -2.207347 -2.891525
 H -3.362451 -6.373803 -0.935546
 H -0.773769 -4.401850 -3.750519
 H -1.691596 -6.501155 -2.776712
 H 1.862535 4.626718 0.879377
 H -0.828634 2.392786 3.379325
 H 3.190750 5.250249 2.863136
 H 0.521791 2.978609 5.356499
 H 2.539462 4.416696 5.118111

(XIV-si-c)₂

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 E0+ZPE = -2991.321862
 E298 = -2991.261280
 H298 = -2991.260336
 G298 = -2991.414263
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 C -3.350021 -4.260394 -1.394253
 C -2.822023 -2.976618 -1.617969

C -1.819527 -2.834259 -2.593150
 C -1.359271 -3.937768 -3.311635
 C -3.385683 -1.791220 -0.913112
 C -2.586079 -0.673386 -0.495656
 C -3.158640 0.555087 -0.191151
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 C -5.372310 -0.542883 -0.188290
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 C -1.912414 4.032586 -1.222790
 C -2.679952 2.825035 -1.205953
 C -2.340784 1.801604 -0.250077
 C -2.230713 5.058555 -2.153505
 C -3.248974 4.894552 -3.062963
 C -3.985312 3.686569 -3.077961
 C -3.712210 2.681767 -2.175575
 C 0.623852 3.487141 1.539506
 C 1.840244 4.016537 1.077324
 C 2.820519 4.444407 1.973969
 C 2.608877 4.340946 3.350303
 C 1.404668 3.813356 3.822340
 C 0.420029 3.396280 2.925807
 Pd 2.097413 -0.432450 0.002328
 N 2.429984 0.350824 -1.986890
 C 3.756694 0.211457 -1.931923
 O 4.653459 0.669015 -2.657755
 N 4.052078 -0.635647 -0.780147
 C 4.547418 -1.995231 -1.217045
 C 4.581314 -2.959715 -0.018346
 C 3.634924 -2.609129 -2.303920
 C 5.983282 -1.886201 -1.785462
 C 2.905993 -0.676751 2.051122
 C 3.329222 0.675570 2.008914
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 C 1.777161 1.051532 -3.113785
 C 0.261625 0.967589 -2.922537
 C 2.205349 2.535858 -3.135323
 C 2.150060 0.379477 -4.454090
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 C -0.345817 -2.031497 4.574062
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 C -1.747897 -3.719444 1.624662

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 C -0.740315 0.275902 3.939084
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 H 2.595021 -2.657535 -1.965805
 H 3.666480 -2.023099 -3.225958
 H 6.315779 -2.878729 -2.113855
 H 6.016490 -1.195975 -2.628604
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 H 5.231905 -2.599315 0.785616
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 H 2.641507 1.409728 2.425452
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 H 2.106172 -0.926003 2.742156
 H 6.325353 1.061249 -1.131375
 H 0.452371 -4.809097 2.706857
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 H 1.431390 -3.364844 2.961647
 H 0.374066 -3.992440 5.095842
 H -0.309969 5.128893 -0.285298
 H -1.641056 5.971907 -2.139434
 H -4.772499 3.545846 -3.813637
 H -4.281500 1.761603 -2.216597
 H -3.480597 5.680460 -3.776369
 H -5.388721 -2.509396 -1.071543
 H -4.613230 2.653250 0.803831
 H -7.364961 -1.382842 -0.137116
 H -8.423070 0.660568 0.781501
 H -7.027757 2.671274 1.262480
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 H -2.957604 -0.904583 4.515246
 H -3.071891 -0.766045 2.753473
 H -2.936417 -2.357100 3.517329
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 H -2.425176 -3.089489 1.050927
 H -0.055482 -2.958781 -0.389209
 H 1.440581 -2.871928 0.565407

H 0.553064 -4.394068 0.422127
 H 2.018573 4.085015 0.008210
 H -0.527237 3.027458 3.302658
 H 3.751508 4.856983 1.594185
 H 1.222752 3.741380 4.891456
 H 3.372658 4.672285 4.048469
 H -4.114261 -4.398593 -0.634466
 H -1.408149 -1.853057 -2.800515
 H -3.310567 -6.346045 -1.915894
 H -0.587453 -3.800174 -4.064111
 H -1.529091 -6.065770 -3.634412

(XIV-si-c)₃

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 E298 = -2991.264255
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 C -1.823350 -2.961720 -2.484646
 C -1.379374 -4.105364 -3.148426
 C -3.396261 -1.812254 -0.880392
 C -2.582157 -0.692215 -0.501524
 C -3.132222 0.555242 -0.240653
 C -4.548209 0.655102 -0.012845
 C -5.367657 -0.496120 -0.237991
 C -4.765042 -1.678407 -0.732738
 C -6.767616 -0.413721 -0.008839
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 C -6.530584 1.885119 0.691839
 C -5.172583 1.842054 0.460043
 O -1.206055 -0.844252 -0.499475
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 C -2.284443 1.782624 -0.292068
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 C -3.797653 3.652484 -3.200844
 C -3.570802 2.656420 -2.276046
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 C 1.834564 3.988545 1.250362
 C 2.755657 4.405485 2.212816
 C 2.450193 4.301674 3.571505
 C 1.211622 3.786694 3.960824
 C 0.286311 3.380251 2.998753
 Pd 2.082431 -0.468530 -0.038350
 N 2.382175 0.313378 -2.043160
 C 3.712579 0.239652 -1.968138

O 4.599740 0.765630 -2.658543
N 4.031801 -0.626669 -0.835072
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C 4.609743 -2.953430 -0.119939
C 3.621452 -2.585419 -2.383445
C 5.963598 -1.823811 -1.892812
C 2.919098 -0.722267 1.994740
C 3.317549 0.638666 1.973818
C 4.446881 1.192247 1.355834
C 5.411668 0.466700 0.663319
C 6.498771 1.160574 -0.107251
C 1.714425 1.046622 -3.140752
C 0.207403 0.799004 -3.042138
C 2.001256 2.558187 -3.010464
C 2.204772 0.538175 -4.515739
N -0.542300 -1.548530 2.107399
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C 0.524837 -3.606967 3.084543
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H 3.279066 0.696443 -4.628308
H 1.993963 -0.532655 -4.622632
H 1.503173 3.117373 -3.813028
H 1.625757 2.933102 -2.051441
H 3.076942 2.743900 -3.066648
H -0.322307 1.337689 -3.836646
H -0.011725 -0.269530 -3.140900
H -0.182121 1.133293 -2.079059
H 3.672448 -1.489308 1.851965
H 2.621941 1.352357 2.412438
H 5.586527 -0.562894 0.943763
H 6.562428 2.217253 0.176659
H 7.475730 0.691826 0.059697
H 4.478621 2.276364 1.277568
H 2.134492 -0.995732 2.692384
H 6.275119 1.120077 -1.180372
H -1.303670 -1.814389 5.454398
H 1.573974 -3.355510 2.895583
H 0.941519 -2.526973 4.921941
H -2.024737 -2.902073 4.305495
H -0.022292 -3.962077 5.171831

H 0.460059 -4.700362 3.027111
 H -2.649723 0.329433 2.740799
 H -3.193217 -1.354130 2.789830
 H -3.015835 -0.436212 4.294890
 H -2.264869 -3.780144 2.713167
 H -2.281919 -3.331761 1.008720
 H -1.499474 -4.827387 1.522184
 H 0.732464 -0.410667 4.382451
 H -0.072130 0.841768 3.434001
 H -0.729684 0.367338 4.999993
 H -0.091011 -3.114250 -0.284584
 H 1.436121 -2.894939 0.596885
 H 0.614510 -4.459920 0.604570
 H -0.243510 5.105931 -0.257467
 H -1.477412 5.931707 -2.189948
 H -4.554563 3.509291 -3.967167
 H -4.145098 1.739904 -2.329641
 H -3.247425 5.633610 -3.900660
 H -5.411157 -2.497156 -1.036913
 H -4.563501 2.717685 0.655502
 H -7.377342 -1.294629 -0.195371
 H -8.411143 0.800966 0.629042
 H -6.983285 2.799031 1.066725
 H 2.084291 4.056835 0.195505
 H -0.689651 3.019513 3.307988
 H 3.714401 4.809721 1.898852
 H 0.957596 3.715032 5.015087
 H 3.168576 4.624209 4.320148
 H -4.194305 -4.386341 -0.509337
 H -1.379927 -2.001146 -2.720086
 H -3.417171 -6.404576 -1.693382
 H -0.590311 -4.018693 -3.890587
 H -1.598877 -6.239807 -3.388352

XVI-re

E0 = -3228.2916341
 E0+ZPE = -3227.051293
 E298 = -3226.980473
 H298 = -3226.979529
 G298 = -3227.153542
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 C -3.923155 -2.288474 -0.321553
 C -4.395509 -3.032161 0.783863
 C -4.395085 -4.431335 0.718717
 C -3.961707 -5.122396 -0.413759
 C -3.542271 -4.368934 -1.513758
 C -3.955433 -0.790361 -0.303094
 C -5.178347 -0.150942 -0.243170
 C -5.306916 1.259314 -0.251055
 C -4.135918 2.061960 -0.430221
 C -2.865308 1.406751 -0.600966
 C -2.788046 0.033507 -0.420099
 C -6.572550 1.885970 -0.092306
 C -6.684831 3.256911 -0.078257
 C -5.525604 4.055708 -0.220694

C -4.287711 3.476700 -0.397250
 C -1.664389 2.208288 -0.981208
 C -0.526590 2.259280 -0.181528
 C 0.458844 3.287367 -0.332157
 C 0.344903 4.119828 -1.429930
 C -0.669442 3.968875 -2.405496
 C -1.701332 3.005040 -2.179830
 C -0.698206 4.769269 -3.579739
 C -1.691570 4.608654 -4.517623
 C -2.698229 3.634676 -4.314173
 C -2.708724 2.859921 -3.174964
 C 1.514796 3.611746 0.683000
 C 1.135335 4.204483 1.909559
 C 2.126812 4.624728 2.802486
 C 3.486864 4.505108 2.509996
 C 3.840774 3.956034 1.275791
 C 2.885862 3.503001 0.358615
 C 4.541865 4.944985 3.497743
 C -0.314303 4.458143 2.259409
 C 3.357572 2.882570 -0.937160
 O -0.393599 1.364205 0.877669
 P -0.259979 -0.283400 0.604831
 Pd 1.711806 -1.072533 -0.595197
 N 3.315497 -2.066495 -1.553788
 C 3.317750 -3.580128 -1.615577
 C 2.032117 -4.080238 -2.297303
 O -1.544486 -0.567801 -0.461549
 C -4.934128 -2.374634 2.036977
 C -3.939003 -6.632725 -0.448796
 C -3.106833 -2.228762 -2.743338
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 C -0.317327 -2.371997 2.346243
 C -1.181896 -3.040276 3.436919
 C -1.245281 -2.244980 4.730066
 C -1.914991 -0.922267 4.400692
 C -1.232795 -0.056367 3.303339
 C -0.544003 -3.215376 1.073132
 C 1.163153 -2.472277 2.757612
 C -2.344916 0.937151 2.896749
 C -0.048555 0.708982 3.930201
 C 0.711208 -0.894215 -2.562839
 C 1.563600 0.186145 -2.900606
 C 2.882197 0.125210 -3.368362
 C 3.584756 -1.053800 -3.606804
 C 5.049650 -1.030233 -3.939005
 N 3.699779 -0.918941 0.352223
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 C 5.031226 -1.612895 2.333439
 C 4.328276 -1.571981 -0.629697
 O 5.537237 -1.782161 -0.821666
 C 4.527064 -4.095835 -2.433026
 C 3.388361 -4.201205 -0.201859
 C 5.605485 0.503889 1.098091
 C 3.489615 0.375553 2.423086
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 H 1.137482 -3.768527 -1.750369

H 1.948305 -3.725666 -3.330413
 H 4.506240 -5.192668 -2.446551
 H 4.484349 -3.752609 -3.471515
 H 5.463919 -3.757023 -1.991349
 H 3.337006 -5.293771 -0.280053
 H 4.323909 -3.939904 0.298731
 H 2.555166 -3.864753 0.421286
 H 6.109246 0.909307 1.985075
 H 6.329545 -0.039774 0.490375
 H 5.219495 1.343536 0.513359
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 H 5.736882 -2.176311 1.716430
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 H 3.024844 1.189365 1.860342
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 H 5.633960 -1.408455 -3.091406
 H 3.443372 1.057136 -3.390071
 H -0.332491 -0.658828 -2.400388
 H 5.273155 -1.654697 -4.812462
 H 1.064301 4.926004 -1.548507
 H 0.089472 5.504340 -3.726612
 H -3.469700 3.493833 -5.066271
 H -3.483606 2.114239 -3.039942
 H -1.701038 5.218077 -5.416976
 H -6.082093 -0.751616 -0.182430
 H -3.411801 4.106753 -0.497085
 H -7.451105 1.256834 0.029933
 H -7.655422 3.727469 0.051701
 H -5.611414 5.138441 -0.187523
 H -0.764700 -4.040488 3.603167
 H -2.200062 -3.182357 3.053260
 H -1.577713 -3.148833 0.730547
 H 0.115442 -2.930179 0.247019
 H -0.324550 -4.263024 1.309022
 H 1.431623 -3.523950 2.916330
 H 1.817169 -2.075635 1.979053
 H 1.373277 -1.933605 3.684802
 H -2.942440 -1.139878 4.083514
 H -1.994451 -0.285002 5.289528
 H -1.988817 1.771813 2.301983
 H -3.134593 0.428495 2.337775
 H -2.792471 1.343008 3.811550
 H -0.413979 1.375384 4.721326
 H 0.679106 0.028596 4.382020
 H 0.471821 1.319036 3.189898
 H -1.833670 -2.782344 5.484438
 H -0.247022 -2.099928 5.160241
 H -4.750743 -4.994030 1.579942
 H -3.235498 -4.882447 -2.423003
 H 1.823176 5.081541 3.742506
 H 4.893586 3.868870 1.017031

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 H -0.857777 3.529847 2.462115
 H -0.390226 5.084661 3.153681
 H 2.854662 3.304134 -1.812572
 H 4.434099 3.030958 -1.065475
 H 3.170751 1.802538 -0.941170
 H 4.870519 4.105666 4.125323
 H 5.430702 5.333814 2.988788
 H 4.165068 5.724880 4.168308
 H -5.986054 -2.083057 1.920233
 H -4.885645 -3.064775 2.885780
 H -4.382621 -1.468842 2.298945
 H -3.812589 -1.426689 -2.987519
 H -2.120896 -1.768769 -2.628310
 H -3.059677 -2.909383 -3.599096
 H -4.148823 -7.013510 -1.454401
 H -2.955260 -7.022690 -0.154470
 H -4.677148 -7.061567 0.237357

(XV-re)₁

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 E0+ZPE = -3227.051052
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 H298 = -3226.978584
 G298 = -3227.154950
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 C -4.593547 -4.312314 0.824400
 C -4.088751 -5.066199 -0.234154
 C -3.545963 -4.375381 -1.322378
 C -3.942428 -0.733746 -0.303992
 C -5.152852 -0.070625 -0.348846
 C -5.253852 1.338607 -0.432325
 C -4.058320 2.107971 -0.585627
 C -2.793031 1.422309 -0.658181
 C -2.747412 0.058491 -0.391674
 C -6.513128 1.994672 -0.376009
 C -6.597733 3.366434 -0.435960
 C -5.415584 4.135280 -0.550523
 C -4.182259 3.525313 -0.628609
 C -1.570136 2.192600 -1.028483
 C -0.475695 2.269015 -0.177531
 C 0.524175 3.283215 -0.308995
 C 0.481834 4.071689 -1.442956
 C -0.481012 3.885869 -2.465871
 C -1.536181 2.942117 -2.257393
 C -0.439234 4.636174 -3.672331
 C -1.384504 4.446559 -4.653783
 C -2.413234 3.493303 -4.464123
 C -2.492837 2.767005 -3.296013
 C 1.497569 3.630340 0.776679
 C 2.886942 3.459906 0.594741
 C 3.761720 3.894357 1.597650
 C 3.306561 4.495748 2.773098

C 1.929911 4.684074 2.918781
 C 1.017834 4.273330 1.941474
 C 4.271302 4.921073 3.855245
 C 3.457294 2.813054 -0.647150
 C -0.452032 4.581513 2.131104
 O -0.417021 1.408506 0.917033
 P -0.178415 -0.227525 0.651203
 Pd 1.707681 -1.029442 -0.631883
 N 3.242430 -2.074137 -1.653669
 C 3.146006 -3.576346 -1.815033
 C 1.822204 -3.943929 -2.508236
 O -1.527157 -0.581851 -0.335009
 C -5.189114 -2.193572 2.004507
 C -4.121833 -6.576491 -0.210411
 C -2.909105 -2.313544 -2.590429
 N -0.481279 -0.828040 2.211090
 C -0.918356 0.019790 3.415701
 C -1.005536 -0.849862 4.696911
 C -1.810290 -2.147990 4.583401
 C -1.645078 -2.795576 3.199402
 C -0.403064 -2.346945 2.397312
 C 0.130094 1.101022 3.749564
 C -2.303704 0.650284 3.169300
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 C 0.922952 -2.769272 3.064396
 C 0.711426 -0.656556 -2.580951
 C 1.640868 0.377756 -2.850152
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 C 3.579666 -0.946507 -3.635536
 C 5.044159 -0.996886 -3.967771
 N 3.674772 -1.096743 0.329588
 C 4.425338 -0.738508 1.554760
 C 4.936982 -2.012117 2.262532
 C 4.276256 -1.710382 -0.694277
 O 5.473149 -1.974022 -0.892604
 C 4.311946 -4.107841 -2.683376
 C 3.197289 -4.299573 -0.449348
 C 5.629573 0.170434 1.215470
 C 3.480357 0.028945 2.485858
 H 1.760293 -5.032775 -2.618996
 H 0.955678 -3.612478 -1.927802
 H 1.750603 -3.513460 -3.513191
 H 4.223521 -5.197762 -2.772247
 H 4.282118 -3.690054 -3.694463
 H 5.271957 -3.859065 -2.230844
 H 3.048879 -5.375799 -0.598778
 H 4.164583 -4.155656 0.038403
 H 2.414025 -3.938229 0.222505
 H 6.133967 0.479980 2.139978
 H 6.341254 -0.354368 0.576679
 H 5.291895 1.071517 0.694690
 H 5.475845 -1.752841 3.182692
 H 4.104177 -2.671030 2.532624
 H 5.618492 -2.561923 1.607400
 H 3.991691 0.285443 3.421924
 H 3.139403 0.958084 2.019485

H 2.601077 -0.571545 2.727946
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 H 1.326625 1.383778 -2.578332
 H 2.967970 -1.771108 -3.976374
 H 5.446354 0.012790 -4.106811
 H 5.601324 -1.463749 -3.146734
 H 3.578775 1.148524 -3.272617
 H -0.316583 -0.357322 -2.415012
 H 5.229487 -1.578453 -4.878938
 H -1.483311 -2.831952 5.375378
 H -2.874054 -1.958379 4.769532
 H 1.211375 4.870013 -1.552849
 H 0.363732 5.356650 -3.808356
 H -3.146528 3.330260 -5.249148
 H -3.283977 2.037050 -3.168791
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 H -3.289607 4.134432 -0.707078
 H -7.409801 1.388110 -0.272491
 H -7.563917 3.860576 -0.384407
 H -5.479567 5.219808 -0.573482
 H -2.516052 -2.575472 2.576564
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 H -1.400597 -2.926245 0.514405
 H 0.373042 -2.925231 0.411391
 H -0.456656 -4.194816 1.304080
 H 1.127435 -2.257337 4.005197
 H 0.903468 -3.846847 3.268847
 H 1.758415 -2.571499 2.387954
 H -1.437835 -0.207739 5.473005
 H 0.008236 -1.072903 5.038805
 H 1.094606 0.637079 3.973660
 H 0.279396 1.819810 2.949560
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 H -2.598526 1.243950 4.043006
 H -2.307829 1.307091 2.299585
 H -3.064340 -0.120683 3.016835
 H -5.042707 -4.824343 1.673475
 H -3.179254 -4.937957 -2.179003
 H 4.830857 3.755744 1.452258
 H 1.552732 5.181603 3.810252
 H -1.060022 3.674143 2.217178
 H -0.607330 5.169974 3.040651
 H -0.852285 5.156321 1.287236
 H 4.458839 4.102453 4.563116
 H 5.240229 5.213987 3.436550
 H 3.880395 5.766321 4.432070
 H 3.086272 3.279901 -1.565316
 H 4.548735 2.888351 -0.653247
 H 3.199824 1.748866 -0.695826
 H -3.527105 -1.467506 -2.911191
 H -1.901345 -1.928444 -2.408172
 H -2.852572 -3.024456 -3.420736
 H -4.719235 -1.230644 2.215869
 H -6.252626 -1.992438 1.818597
 H -5.135775 -2.810303 2.908082

H -4.832690 -6.950471 0.533673
H -4.405754 -6.986669 -1.186395
H -3.136357 -6.992493 0.038199

XV-si-c

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G298 = -3227.145373
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C -1.963932 -2.057609 4.789250
C -1.694703 -2.864722 3.530414
P -0.196513 -0.221805 0.834817
Pd 2.013297 -0.998175 0.049822
C 3.164823 -0.591509 1.939503
C 3.953174 0.360878 1.256790
C 5.058177 0.136906 0.425967
C 5.593082 -1.112571 0.133111
C 6.685833 -1.268592 -0.885814
C -0.492074 0.865375 4.142474
C -2.590874 1.120997 2.757633
C 0.749987 -2.360929 3.417269
C -0.501163 -3.130623 1.394857
O -0.374442 1.431868 1.035040
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C 0.447218 3.401328 -0.113478
C 0.329044 4.274008 -1.177981
C -0.628711 4.107479 -2.204124
C -1.593002 3.061489 -2.077118
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C -1.566324 4.760076 -4.350200
C -2.497879 3.699280 -4.251011
C -2.516634 2.878043 -3.145008
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C 2.864888 3.650707 0.553509
C 3.830350 4.056568 1.483295
C 3.489162 4.526491 2.753866
C 2.131745 4.617252 3.070449
C 1.131454 4.234141 2.170265
C 4.553303 4.918167 3.752266
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C -2.572778 -0.049264 -0.505525
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C -6.714989 2.878138 -0.517523
C -5.608801 3.759652 -0.471192

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C 3.499538 -1.671030 -2.054620
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C 2.463971 -4.215993 -1.356346
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C 2.943222 0.446510 -4.083676
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H 1.508730 -3.774282 -1.056908
H 2.595369 -4.052626 -2.429234
H 4.891617 -5.328217 -0.993403
H 5.122483 -3.968446 -2.126071
H 5.818348 -3.907247 -0.493935
H 3.487620 -5.093887 1.018574
H 4.319139 -3.623939 1.532106
H 2.554316 -3.624405 1.343162
H 1.091945 -1.231717 -5.287007
H 2.371485 -2.221977 -4.549545
H 0.728073 -2.238026 -3.870074
H 2.534658 0.888694 -5.001478
H 3.240102 1.264097 -3.416404
H 3.830002 -0.138897 -4.330762
H 0.208930 0.798568 -4.062408
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H 0.907477 1.291675 -2.509138
H 3.591635 -1.564875 2.160538
H 3.614807 1.390113 1.332369
H 5.466474 -1.911763 0.851346
H 7.140707 -0.298855 -1.117460
H 7.469310 -1.951262 -0.536977
H 5.423218 0.984910 -0.149550
H 2.506820 -0.201591 2.710204
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H -2.656192 -0.040730 5.196967
H -1.062653 -1.972700 5.407794
H -3.449452 -0.861394 3.863440
H -2.722850 -2.548277 5.411643
H 1.011467 5.117662 -1.237973
H 0.087421 5.752683 -3.412078
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 H -1.569420 5.405047 -5.224470
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 H 4.407270 3.081569 -0.842219
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 H 4.194004 5.691546 4.439859
 H 4.860938 4.058265 4.362564
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 H -6.031277 -2.401438 1.295621
 H -5.024278 -3.270990 2.448459
 H -4.572528 -1.639901 1.915952
 H -3.445066 -7.185486 -1.656000
 H -2.377882 -7.130552 -0.252438
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XVII-*re*

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 C 2.025033 4.726481 -2.341608
 C 2.554789 5.820482 -1.652931

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 C 3.658346 1.814667 -0.527488
 C 5.005960 1.567031 -0.342829
 C 5.516256 0.268424 -0.100603
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 C 3.227449 -0.609777 -0.396830
 C 2.765779 0.695837 -0.464735
 C 6.897618 0.052145 0.153387
 C 7.383619 -1.214287 0.384038
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 C 0.698980 -4.071371 -0.703474
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 C 2.490853 -2.691717 -1.652159
 C 1.851669 -4.793002 -2.770950
 C 2.799636 -4.577402 -3.744251
 C 3.600570 -3.411491 -3.699632
 C 3.455269 -2.496033 -2.680042
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 C -2.148406 -4.514613 3.432129
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 H 0.996632 4.281128 3.346780
 H 1.954301 3.829546 1.917786
 H 3.284590 1.219416 2.431295
 H 3.206927 0.266323 3.920691
 H 2.673869 -0.441432 2.396390

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 H -1.149306 2.728873 3.822293
 H 4.409019 4.140448 0.651090
 H 2.299202 6.832783 -1.953871
 H 1.938710 2.584208 -2.504405
 H 0.896050 -3.068814 2.974235
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(XVI-re)₁

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 C 3.677305 1.807565 -0.492688
 C 5.017680 1.568734 -0.253409
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 C 4.630083 -0.838075 0.012042
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 C 5.155376 -2.124249 0.317617
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 C 2.023899 -4.788044 -2.768082
 C 3.027589 -4.568910 -3.682903
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XVI-si

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 H 1.317664 -2.951185 0.176771
 H 0.679989 -4.587624 0.042554
 H -2.346697 -2.094472 -2.706602
 H -3.971396 -6.065663 -2.441210
 H -5.527538 -2.934162 0.060443
 H -0.634105 2.129663 3.563204
 H 2.946074 3.340568 1.519337
 H 2.972868 2.843733 5.786103

(XVI-si)₁

E0 = -2954.2757249

E0+ZPE = -2953.210176

E298 = -2953.149074
 H298 = -2953.148130
 G298 = -2953.303305
 NImag = 1, (-210.8728)
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 C -3.893245 -2.475205 -1.198264
 C -4.764060 -3.444365 -0.672397
 C -4.748265 -4.756320 -1.146776
 C -3.863268 -5.124727 -2.161422
 C -2.997165 -4.169347 -2.698924
 C -3.983170 -1.060961 -0.746739
 C -5.227323 -0.467940 -0.662427
 C -5.400230 0.893968 -0.318993
 C -4.241904 1.715963 -0.146959
 C -2.936116 1.127182 -0.306818
 C -2.831762 -0.247909 -0.475350
 C -6.694988 1.458925 -0.168105
 C -6.852916 2.783562 0.168758
 C -5.711330 3.593840 0.370967
 C -4.442767 3.077817 0.213984
 C -1.731629 2.007398 -0.271717
 C -0.761752 1.843567 0.703705
 C 0.214793 2.848140 0.992911
 C 0.311294 3.906781 0.109432
 C -0.518930 4.021937 -1.033110
 C -1.579829 3.078985 -1.219432
 C -0.349425 5.077245 -1.969881
 C -1.175377 5.188524 -3.064927
 C -2.210091 4.244203 -3.264948
 C -2.412209 3.221166 -2.363875
 C 1.006864 2.879093 2.253437
 C 0.364995 2.761207 3.497476
 C 1.079607 2.902895 4.686883
 C 2.450049 3.168925 4.657365
 C 3.096986 3.304869 3.427952
 C 2.380098 3.167652 2.238618
 O -0.787461 0.676752 1.469937
 P -0.338118 -0.732018 0.683640
 N -0.626110 -1.902118 1.904939
 C -0.362971 -3.361367 1.492860
 C 0.484156 -4.126848 2.544857
 O -1.597398 -0.858759 -0.472644
 Pd 1.693160 -0.391488 -0.647091
 C 0.569370 -0.170219 -2.536545
 C 0.857021 -1.524944 -2.844611
 C 2.055812 -2.067568 -3.319045
 C 3.191779 -1.321165 -3.642438
 C 4.484990 -2.007886 -3.987765
 N 3.489792 -0.133043 -1.744344
 C 4.273518 -0.861004 -0.742205
 O 5.410156 -1.293101 -0.982747
 N 3.527932 -0.914912 0.364135
 C 4.070534 -1.381494 1.657692
 C 3.030902 -1.067435 2.739789
 C 4.101598 1.231694 -2.001318
 C 3.076250 2.160780 -2.671691

C 4.565584 1.898182 -0.688652
 C 5.334146 1.100646 -2.928370
 C -1.375414 -1.567854 3.219441
 C -2.781289 -1.007600 2.912739
 C -1.592431 -2.757508 4.189485
 C -0.522693 -0.584474 4.050205
 C 0.441602 -3.441975 0.176393
 C -1.681949 -4.108224 1.202067
 C 4.344154 -2.900130 1.597321
 C 5.379935 -0.640966 2.011084
 H 4.874462 2.931093 -0.890315
 H 3.758077 1.905522 0.045669
 H 5.416297 1.368667 -0.252728
 H 5.801068 2.086790 -3.042902
 H 6.062059 0.408868 -2.502538
 H 5.056327 0.749867 -3.926860
 H 3.538452 3.138781 -2.850769
 H 2.744438 1.782511 -3.644560
 H 2.197612 2.311505 -2.037135
 H 5.754030 -0.984250 2.983861
 H 6.146703 -0.824668 1.255536
 H 5.202097 0.438021 2.079890
 H 4.731676 -3.262461 2.558417
 H 3.426392 -3.453214 1.370873
 H 5.080136 -3.117044 0.818537
 H 3.366220 -1.439161 3.716069
 H 2.870685 0.013157 2.819133
 H 2.069632 -1.529044 2.502890
 H 1.131678 0.606079 -3.038823
 H 0.082159 -2.245232 -2.588536
 H 3.049203 -0.321167 -4.029534
 H 4.334899 -3.088572 -4.088332
 H 4.905223 -1.623215 -4.925054
 H 2.161534 -3.150243 -3.271795
 H -0.465885 0.083268 -2.340002
 H 5.222020 -1.850018 -3.192489
 H 1.028829 4.697075 0.313192
 H 0.454200 5.791502 -1.807675
 H -2.850136 4.324723 -4.139243
 H -3.204813 2.501598 -2.534549
 H -1.031935 5.994158 -3.779589
 H -6.109033 -1.061254 -0.889793
 H -3.583375 3.715458 0.384045
 H -7.560756 0.817834 -0.316566
 H -7.846766 3.205749 0.288431
 H -5.834472 4.634870 0.657155
 H 0.561669 2.812878 5.638071
 H 4.162069 3.516969 3.390827
 H -2.313359 -4.442749 -3.498312
 H -5.425308 -5.491200 -0.719255
 H 1.028293 -4.934290 2.043711
 H 1.224683 -3.474738 3.013036
 H -0.117105 -4.594417 3.323735
 H -1.074901 -0.299622 4.954232
 H 0.407232 -1.069065 4.364343
 H -0.265213 0.320020 3.513027

H -3.307480 -0.799428 3.851619
 H -2.748826 -0.081787 2.341495
 H -3.372483 -1.739679 2.352431
 H -1.454024 -5.153926 0.962323
 H -2.381834 -4.112090 2.036920
 H -2.188125 -3.670176 0.341885
 H -0.658549 -3.135640 4.604599
 H -2.169797 -2.356679 5.029056
 H -2.167651 -3.587950 3.782523
 H -0.083801 -2.980336 -0.660952
 H 1.441483 -3.010383 0.251815
 H 0.551006 -4.502922 -0.072997
 H -2.345616 -2.119978 -2.657825
 H -3.849573 -6.146006 -2.532160
 H -5.445188 -3.168199 0.127982
 H -0.705239 2.581541 3.530954
 H 2.888835 3.280480 1.287963
 H 3.007101 3.275508 5.584155

XVI-si-c

E0 = -2954.2793384
 E0+ZPE = -2953.214097
 E298 = -2953.153069
 H298 = -2953.152124
 G298 = -2953.305766
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 C -0.229672 -3.401144 2.865057
 C -1.085731 -3.870607 3.861978
 C -2.281015 -4.507949 3.522002
 C -2.613659 -4.671256 2.175560
 C 0.407810 -3.176869 0.438061
 C 1.138169 -1.945281 0.408488
 C 2.211785 -1.747546 -0.448265
 C 2.454078 -2.703970 -1.497431
 C 1.670074 -3.898908 -1.539016
 C 0.698068 -4.114949 -0.534981
 C 3.411089 -2.498412 -2.530274
 C 3.592841 -3.433387 -3.526181
 C 2.837461 -4.629663 -3.543053
 C 1.893980 -4.853507 -2.567591
 C 3.103374 -0.557743 -0.323602
 C 4.514497 -0.722758 -0.103241
 C 5.362815 0.427663 -0.173800
 C 4.792669 1.681873 -0.501928
 C 3.430007 1.864204 -0.652425
 C 2.587186 0.721690 -0.455834
 C 5.107724 -1.973915 0.222261
 C 6.463036 -2.079413 0.449366
 C 7.302174 -0.944117 0.353226
 C 6.759180 0.282743 0.047554
 C 2.921512 3.182226 -1.119650
 C 1.977667 3.266074 -2.158594
 C 1.576340 4.504294 -2.659061
 C 2.108191 5.684606 -2.134498

C 3.050063 5.616016 -1.106409
 C 3.453158 4.377522 -0.606531
 O 1.212217 0.887776 -0.473245
 P 0.203394 0.530292 0.831218
 Pd -2.096671 0.496668 0.086662
 N -2.431328 -0.003177 -2.001562
 C -1.776479 -0.566829 -3.202688
 C -2.264678 0.156209 -4.478102
 O 0.807088 -0.951518 1.326720
 N 0.703227 1.528146 2.143399
 C 1.400069 0.969059 3.405022
 C 0.432153 0.028967 4.157788
 C 0.188034 2.979206 2.096731
 C 1.345817 3.993819 2.316701
 C -0.955709 3.227211 3.105799
 C -0.388414 3.347407 0.706395
 C -2.895073 0.336755 2.149808
 C -3.258448 -1.006205 1.881172
 C -4.383959 -1.478941 1.194916
 C -5.389464 -0.675880 0.666518
 C -6.474120 -1.255386 -0.195555
 N -4.070660 0.708487 -0.634990
 C -4.630609 2.093761 -0.859541
 C -4.644470 2.875586 0.465817
 C -3.760333 0.047730 -1.899589
 O -4.653701 -0.359806 -2.659121
 C -0.264848 -0.363924 -3.077614
 C -2.084057 -2.077100 -3.298467
 C -3.794247 2.891599 -1.886929
 C -6.084153 2.001181 -1.383338
 C 2.725291 0.248963 3.053646
 C 1.843411 2.038703 4.435043
 H -6.465748 3.013035 -1.568060
 H -6.126433 1.425390 -2.308407
 H -6.741859 1.526052 -0.648661
 H -5.083384 3.866440 0.300484
 H -5.249182 2.377641 1.231570
 H -3.634233 3.017278 0.860582
 H -4.179878 3.916082 -1.954989
 H -2.740966 2.937015 -1.594137
 H -3.851385 2.440286 -2.880984
 H -1.761774 -0.254707 -5.362678
 H -3.343519 0.041829 -4.600351
 H -2.028403 1.225675 -4.421742
 H -1.573318 -2.522402 -4.162044
 H -1.734630 -2.587830 -2.393417
 H -3.159824 -2.239457 -3.402143
 H 0.244843 -0.749233 -3.968783
 H -0.027450 0.699566 -2.971061
 H 0.131130 -0.884837 -2.203691
 H -3.667631 1.098432 2.160588
 H -2.533228 -1.760886 2.173096
 H -5.587327 0.280353 1.132191
 H -6.489205 -2.348451 -0.118357
 H -7.461768 -0.868265 0.081702
 H -4.382659 -2.531889 0.921975

H -2.114528 0.483467 2.888681
 H -6.285473 -1.002198 -1.246030
 H 0.175049 -5.066958 -0.517005
 H 1.293833 -5.760080 -2.574073
 H 4.321098 -3.246364 -4.310589
 H 3.991044 -1.583535 -2.543197
 H 2.996368 -5.360249 -4.331249
 H 5.458808 2.523299 -0.672383
 H 4.478023 -2.852325 0.305845
 H 7.390409 1.165464 -0.022642
 H 8.370017 -1.043303 0.527159
 H 6.891074 -3.044339 0.707027
 H -0.811109 -3.748424 4.906377
 H -3.541801 -5.164255 1.898963
 H 0.849668 4.544502 -3.466025
 H 3.470759 6.527052 -0.688849
 H -1.857714 2.691076 2.804507
 H -0.713621 2.929255 4.126674
 H -1.193723 4.297760 3.123894
 H 0.953531 -0.453211 4.994131
 H -0.409162 0.593707 4.574363
 H 0.034920 -0.756211 3.516407
 H 3.271112 0.043373 3.981755
 H 2.584888 -0.695407 2.537236
 H 3.354424 0.894692 2.433853
 H 1.099349 4.933013 1.811600
 H 1.521554 4.236456 3.363677
 H 2.274107 3.623572 1.876704
 H 1.049589 2.700755 4.775872
 H 2.193814 1.488410 5.314446
 H 2.682359 2.637763 4.077896
 H 0.351638 3.269960 -0.090280
 H -1.268491 2.757351 0.432589
 H -0.713741 4.391788 0.755827
 H 1.565399 2.356624 -2.581896
 H 1.792890 6.648318 -2.525078
 H 4.178798 4.335132 0.201269
 H 0.712532 -2.938489 3.139067
 H -2.037114 -4.306151 0.133674
 H -2.945913 -4.875488 4.298671

(XVI-si-c)₁

E0+ZPE = -2953.211652
 E298 = -2953.150318
 H298 = -2953.149374
 G298 = -2953.303923
 NImag = 1, (-184.1188)
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 C -0.289526 -3.615525 2.718395
 C -1.197616 -4.128059 3.645723
 C -2.431806 -4.624941 3.220888
 C -2.750748 -4.604059 1.861462
 C 0.413692 -3.167488 0.343504
 C 1.163681 -1.950296 0.398204
 C 2.263268 -1.723042 -0.414656

C 2.538137 -2.639422 -1.492254
 C 1.744507 -3.823349 -1.610870
 C 0.727660 -4.066055 -0.658419
 C 3.531454 -2.403016 -2.483734
 C 3.740486 -3.300233 -3.508529
 C 2.976435 -4.487501 -3.599486
 C 1.996425 -4.739003 -2.667988
 C 3.134458 -0.525815 -0.234810
 C 4.546485 -0.676371 -0.011052
 C 5.386112 0.478882 -0.095744
 C 4.806700 1.719426 -0.457264
 C 3.442003 1.891675 -0.603370
 C 2.604944 0.750799 -0.359406
 C 5.147454 -1.920500 0.325572
 C 6.502803 -2.013410 0.558459
 C 7.333256 -0.872432 0.454048
 C 6.782572 0.346942 0.131534
 C 2.927073 3.187411 -1.127457
 C 1.932004 3.224386 -2.119945
 C 1.522135 4.436150 -2.675716
 C 2.095876 5.637557 -2.254278
 C 3.088081 5.616170 -1.272253
 C 3.499168 4.404783 -0.717360
 O 1.231270 0.918998 -0.351195
 P 0.174443 0.483660 0.903572
 Pd -2.093528 0.506641 0.082921
 N -2.399067 -0.027318 -1.997338
 C -1.729446 -0.614291 -3.178224
 C -2.199084 0.083999 -4.474281
 O 0.830110 -0.991840 1.353263
 N 0.519214 1.415218 2.313379
 C 1.156158 0.808089 3.583943
 C 0.287129 -0.365834 4.094836
 C 0.260209 2.924867 2.188721
 C 1.592393 3.703791 2.221283
 C -0.715483 3.460140 3.271349
 C -0.408946 3.293343 0.839352
 C -2.924085 0.491511 2.132608
 C -3.308173 -0.859453 1.938206
 C -4.432307 -1.344487 1.256971
 C -5.408668 -0.550481 0.662018
 C -6.485742 -1.155761 -0.192614
 N -4.050258 0.744251 -0.677747
 C -4.581333 2.131601 -0.958564
 C -6.014654 2.046610 -1.537479
 C -3.729485 0.038931 -1.916706
 O -4.615093 -0.385683 -2.675404
 C -0.220026 -0.406766 -3.034020
 C -2.036781 -2.125636 -3.253063
 C -4.638965 2.952678 0.342053
 C -3.690148 2.890653 -1.968842
 C 2.612285 0.375938 3.305593
 C 1.214115 1.748268 4.815755
 H -4.057593 3.918120 -2.079841
 H -2.650403 2.929364 -1.629623
 H -3.709042 2.414944 -2.952759

H -6.374068 3.059231 -1.758718
H -6.031582 1.450383 -2.450266
H -6.707058 1.597111 -0.818507
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H -1.682404 -0.343057 -5.343047
H -3.275817 -0.034194 -4.610745
H -1.964811 1.154614 -4.435076
H -1.523687 -2.583665 -4.108530
H -1.689851 -2.624103 -2.340460
H -3.112426 -2.288097 -3.358155
H 0.307478 -0.824003 -3.899931
H 0.014649 0.660592 -2.964264
H 0.158166 -0.893712 -2.133248
H -3.684119 1.263729 2.088274
H -2.602960 -1.614327 2.280778
H -5.602205 0.430392 1.074378
H -6.508779 -2.245154 -0.076084
H -7.474472 -0.753573 0.058991
H -4.448358 -2.409642 1.039348
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H -6.284263 -0.941708 -1.249175
H 0.184714 -5.005976 -0.706000
H 1.387572 -5.637468 -2.731912
H 4.497615 -3.089324 -4.258809
H 4.119363 -1.494441 -2.442104
H 3.157046 -5.188193 -4.409825
H 5.468505 2.556316 -0.662281
H 4.522818 -2.802383 0.414167
H 7.408005 1.232986 0.051969
H 8.401102 -0.961536 0.633297
H 6.937618 -2.972368 0.826823
H -0.933110 -4.153270 4.699533
H -3.706386 -4.992634 1.519590
H 0.755950 4.437860 -3.446335
H 3.541194 6.543857 -0.932567
H -1.160247 4.395511 2.915099
H -1.531420 2.754590 3.449721
H -0.233598 3.687700 4.220939
H 0.790931 -0.848730 4.940987
H -0.675064 0.011249 4.458035
H 0.095098 -1.124957 3.345344
H 3.063404 -0.025160 4.221044
H 2.676952 -0.389375 2.535681
H 3.211104 1.235063 2.985709
H 1.391087 4.774085 2.093285
H 2.146465 3.585728 3.151751
H 2.236529 3.387715 1.401044
H 0.224563 2.006497 5.192795
H 1.712413 1.177489 5.606233
H 1.794881 2.658486 4.676300
H 0.163300 2.986491 -0.035663
H -1.422666 2.890645 0.760363
H -0.482331 4.385133 0.801105
H 1.486927 2.298480 -2.466304

H 1.773791 6.580533 -2.687574
H 4.259956 4.402901 0.058471
H 0.684236 -3.270754 3.051215
H -2.107612 -4.051054 -0.119143
H -3.136428 -5.029730 3.942125

XVII-re

E0 = -3190.1662936
E0+ZPE = -3188.934256
E298 = -3188.863039
H298 = -3188.862095
G298 = -3189.036760
NImag = 1, (-198.4380)
C 1.034546 4.269732 1.826090
C 1.472369 3.613390 0.652122
C 2.856325 3.471826 0.407873
C 3.766840 3.952328 1.356373
C 3.354364 4.569160 2.539422
C 1.982170 4.724357 2.748854
C 0.460492 3.232114 -0.386791
C -0.531223 2.217744 -0.200872
C -1.649264 2.115376 -1.019102
C -1.655566 2.834722 -2.265867
C -0.612449 3.778607 -2.527158
C 0.378927 3.992347 -1.538112
C -2.641562 2.631040 -3.271358
C -2.600592 3.330738 -4.457514
C -1.583056 4.284342 -4.699566
C -0.610335 4.501063 -3.751240
C -2.856792 1.346142 -0.596846
C -4.124731 2.022208 -0.497402
C -5.306288 1.245471 -0.282856
C -5.189506 -0.160501 -0.168651
C -3.971811 -0.812258 -0.153001
C -2.791272 -0.010718 -0.304703
C -4.263623 3.436858 -0.570808
C -5.499204 4.037561 -0.463588
C -6.668834 3.260987 -0.287755
C -6.569028 1.891943 -0.197580
C -3.964193 -2.308560 -0.067244
C -4.505443 -2.966200 1.060226
C -4.538292 -4.366942 1.086432
C -4.077056 -5.141700 0.022458
C -3.588793 -4.472846 -1.104486
C -3.527859 -3.078793 -1.173842
C -5.086462 -2.220770 2.244602
C -3.032762 -2.433688 -2.447792
C -4.099262 -6.651312 0.081919
O -1.557974 -0.631932 -0.282532
P -0.234166 -0.258532 0.716610
N -0.632896 -0.826246 2.286195
C -0.402777 -2.337098 2.500522
C -0.403932 -3.109890 1.156947
O -0.438810 1.390663 0.915776
C 3.386557 2.801352 -0.839254
C 4.359418 5.044644 3.562305

C -0.430524 4.545286 2.085218
Pd 1.700509 -1.062880 -0.545909
C 0.656517 -0.842589 -2.483633
C 1.538757 0.208850 -2.836627
C 2.844207 0.105977 -3.332317
C 3.502352 -1.094465 -3.591659
C 4.959797 -1.114270 -3.957787
N 3.247015 -2.107898 -1.548077
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N 3.695879 -1.020469 0.375653
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C -2.244327 0.933686 3.144624
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C 0.953816 -2.603178 3.179986
C -1.552983 -3.002796 3.303491
C 3.197799 -3.620921 -1.621659
C 3.297499 -4.260665 -0.217614
C 1.875841 -4.073381 -2.266699
C 4.364916 -4.164735 -2.481135
C 5.029491 -1.816450 2.313310
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H 1.008371 -3.741183 -1.688677
H 1.769933 -3.703809 -3.292500
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H 4.297401 -3.816996 -3.516692
H 5.324026 -3.851796 -2.068627
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H 6.349769 -0.202979 0.516804
H 5.268417 1.201245 0.600857
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H 4.218824 -2.482389 2.630269
H 5.710823 -2.378204 1.668206
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H 5.321918 -0.101505 -4.166776
H 5.552279 -1.511155 -3.124843
H 3.435902 1.018812 -3.359395
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H 1.100387 4.791215 -1.689029
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 H 4.609125 4.245663 4.273360
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 H -4.778792 -7.011815 0.861136
 H -4.417677 -7.085552 -0.872755
 H -3.102530 -7.056401 0.302211

(XVII-re)₁

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 C -1.356405 2.771211 -2.329055
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 C -2.165151 3.196060 -4.589413
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 C -3.930596 2.188723 -0.683210
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 C -4.748381 -6.393968 0.346960
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 C 4.381262 4.949437 3.784712
 C -0.299429 4.705625 1.930993
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 H -7.325242 4.160762 -0.761463
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 H -4.888409 -6.869167 -0.630356
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 H 1.240844 0.881131 4.024076

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 H -2.208690 1.412053 2.297897
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XVII-si

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 C -2.034449 1.539637 -1.287039
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 C -4.799132 4.368423 -2.976681
 C -3.441629 4.718990 -2.800425
 C -2.542369 3.823544 -2.261454
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 C 0.145417 1.983820 -0.122130
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(XVII-si)₁

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 C -0.366439 -1.947225 3.014874
 C 0.224192 -2.854324 1.912266
 O -1.572178 -0.682121 -0.076820
 C -3.339112 -2.591541 -2.334956
 C -4.565600 -6.386018 0.745222
 C -5.139667 -1.646054 2.347309
 Pd 1.721091 -1.047286 -0.553895
 N 3.314238 -1.926387 -1.675783
 C 4.106910 -2.158698 -0.463442
 O 5.063037 -2.948997 -0.452591
 N 3.597847 -1.383707 0.496848
 C 4.280387 -1.220852 1.799354
 C 4.230769 -2.546249 2.591540
 C 0.388843 -1.540574 -2.209852
 C 0.280299 -2.858033 -1.684812
 C 1.219725 -3.886045 -1.773675
 C 2.424258 -3.799866 -2.485611
 C 3.440067 -4.906635 -2.385731
 C 5.757941 -0.808445 1.608341
 C 3.568667 -0.098992 2.568596
 C -1.174360 0.582575 3.437915
 C -1.840249 0.062720 4.738743
 C -0.004623 1.499159 3.854522
 C -2.319055 1.401877 2.787617
 C -1.682473 -2.655363 3.419654
 C 0.654199 -1.974512 4.174063
 C 4.153980 -1.205888 -2.723021
 C 5.064287 -0.128802 -2.095410
 C 5.074708 -2.211610 -3.457013
 C 3.247759 -0.518503 -3.757504
 H 5.589692 0.407642 -2.894386
 H 4.484897 0.592333 -1.520920
 H 5.814958 -0.576471 -1.439901
 H 5.723697 -1.658094 -4.146639
 H 5.696432 -2.750834 -2.741381
 H 4.507047 -2.933532 -4.051016
 H 3.870856 0.014439 -4.485209
 H 2.640482 -1.234038 -4.322243
 H 2.581302 0.208518 -3.283235
 H 6.229914 -0.643345 2.585102
 H 6.312775 -1.583933 1.076345
 H 5.825782 0.125241 1.038828
 H 4.709100 -2.430445 3.572865
 H 3.198577 -2.871948 2.751847
 H 4.754543 -3.328310 2.035986
 H 3.952790 -0.029620 3.593589
 H 3.723764 0.869007 2.082793
 H 2.490725 -0.270197 2.612753
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 H -0.589448 -3.053515 -1.061016
 H 2.428461 -3.211861 -3.393555
 H 3.021496 -5.766758 -1.851362
 H 3.772342 -5.237542 -3.376921

H 1.083651 -4.742225 -1.115113
 H -0.498583 -0.919407 -2.190475
 H 4.319051 -4.565971 -1.827458
 H 1.543109 4.504243 -1.911844
 H 0.997822 4.553593 -4.314409
 H -2.405512 2.362650 -5.771192
 H -2.813358 1.457741 -3.525462
 H -0.509145 3.931014 -6.180309
 H -6.087385 -0.434286 -0.396734
 H -2.915490 3.988782 -1.495363
 H -7.254388 1.662770 -0.826272
 H -7.207339 4.072006 -1.413970
 H -5.013300 5.223295 -1.716590
 H 1.055092 5.793754 3.295096
 H 4.607509 3.806860 1.958169
 H -3.679811 -5.121964 -1.507501
 H -5.226589 -4.317986 2.403742
 H 0.354464 -1.399992 5.049308
 H 0.787546 -3.012510 4.500707
 H 1.625517 -1.602205 3.848914
 H -0.378415 2.324145 4.473364
 H 0.731168 0.943939 4.445102
 H 0.500862 1.930386 2.990741
 H -2.809487 1.994238 3.567812
 H -1.986091 2.086528 2.015937
 H -3.073548 0.739729 2.355465
 H -1.475365 -3.722398 3.559418
 H -2.119058 -2.297549 4.348660
 H -2.422985 -2.567280 2.621926
 H -1.231072 -0.602572 5.344830
 H -2.039972 0.947633 5.351627
 H -2.803243 -0.414309 4.544232
 H -0.459150 -2.960251 1.065674
 H 1.199352 -2.529240 1.548201
 H 0.355147 -3.852982 2.342110
 H -2.415147 -2.008527 -2.310247
 H -3.173040 -3.448483 -2.994897
 H -4.106591 -1.956376 -2.794796
 H -6.085594 -1.164025 2.070627
 H -5.310884 -2.188382 3.282640
 H -4.425272 -0.843096 2.546551
 H -5.308356 -6.597736 1.521603
 H -4.863128 -6.920838 -0.163718
 H -3.612983 -6.820363 1.077302
 H -0.825975 5.354706 0.387439
 H -1.307209 4.097608 1.521370
 H -0.913760 5.711573 2.120067
 H 3.077490 1.592998 -0.311135
 H 3.620171 3.020778 -1.193030
 H 4.602984 2.375400 0.128600
 H 3.623134 4.781159 4.829441
 H 4.742339 5.563157 3.710090
 H 3.278771 6.410646 4.242750

XVII-si-c

E0 = -3190.1621501

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 H298 = -3188.857980
 G298 = -3189.033223
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 C -3.122436 3.094013 1.358331
 C -3.136186 4.491398 1.368161
 C -3.747667 5.238969 0.357752
 C -4.386677 4.540425 -0.666208
 C -3.799899 0.902386 0.284369
 C -5.045345 0.303649 0.330390
 C -5.227644 -1.098744 0.325340
 C -4.076229 -1.941100 0.403349
 C -2.774304 -1.332621 0.501410
 C -2.652729 0.038142 0.304514
 C -6.523162 -1.678971 0.250856
 C -6.682548 -3.044749 0.216488
 C -5.543474 -3.883810 0.254468
 C -4.277275 -3.349351 0.353008
 C -1.605093 -2.185251 0.861749
 C -0.476697 -2.277837 0.057544
 C 0.499623 -3.309547 0.235375
 C 0.362505 -4.134793 1.334466
 C -0.657755 -3.962243 2.298843
 C -1.659990 -2.969460 2.069693
 C -0.706340 -4.757588 3.475606
 C -1.688160 -4.560924 4.418249
 C -2.660067 -3.552232 4.216742
 C -2.651865 -2.783318 3.073514
 C 1.590354 -3.625969 -0.742326
 C 2.945942 -3.489599 -0.366469
 C 3.943104 -3.897826 -1.260886
 C 3.643928 -4.439819 -2.513843
 C 2.297431 -4.601255 -2.848808
 C 1.266339 -4.220554 -1.982837
 C 3.350238 -2.919372 0.976027
 C -0.165581 -4.524548 -2.364023
 C 4.741854 -4.832451 -3.474658
 O -0.347713 -1.427159 -1.037993
 P -0.177291 0.230068 -0.880268
 N -0.749442 0.746571 -2.423955
 C -0.656451 2.258764 -2.699718
 C -0.472403 3.069217 -1.393982
 O -1.384789 0.598337 0.244973
 C -2.468224 2.377763 2.516435
 C -3.716029 6.749311 0.379995
 C -5.197189 2.499212 -1.842967
 Pd 1.954027 1.061073 -0.047365
 N 3.623309 2.144996 0.676881
 C 3.459247 1.680856 2.047442
 O 4.294734 1.935593 2.929252
 N 2.314057 0.994680 2.100582
 C 1.756491 0.530966 3.390651
 C 2.779159 -0.356584 4.139176

C 3.000786 0.816030 -2.005540
 C 3.810670 -0.196181 -1.441529
 C 4.948500 -0.048120 -0.635966
 C 5.505640 1.167170 -0.254450
 C 6.620187 1.230862 0.751033
 C 1.379770 1.740284 4.271884
 C 0.511011 -0.309203 3.099356
 C -1.123565 -0.252344 -3.541559
 C -1.595332 0.386395 -4.873360
 C 0.112122 -1.103633 -3.919907
 C -2.328524 -1.122272 -3.111848
 C -1.973117 2.809842 -3.313960
 C 0.536600 2.620987 -3.613093
 C 3.608642 3.655599 0.601547
 C 4.929278 4.247922 1.150643
 C 3.461467 4.103841 -0.862880
 C 2.433518 4.246061 1.415027
 H 4.880741 5.342241 1.089620
 H 5.086863 3.948832 2.186552
 H 5.789223 3.920724 0.557582
 H 3.469726 5.198978 -0.911684
 H 4.287307 3.746826 -1.488053
 H 2.521509 3.755481 -1.297687
 H 2.394991 5.332560 1.270533
 H 1.475992 3.822380 1.096117
 H 2.556095 4.049535 2.483102
 H 0.942271 1.407014 5.221395
 H 2.266981 2.340630 4.492653
 H 0.644955 2.373276 3.761462
 H 2.325194 -0.751884 5.057095
 H 3.075939 -1.207077 3.515108
 H 3.673286 0.212884 4.395960
 H 0.040230 -0.636728 4.033540
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 H 3.427892 1.800821 -2.161820
 H 3.462219 -1.216805 -1.581626
 H 5.375108 2.024627 -0.900565
 H 7.027085 0.232173 0.945229
 H 7.433757 1.882088 0.409110
 H 5.322512 -0.944791 -0.147042
 H 2.301943 0.502558 -2.773755
 H 6.245336 1.624735 1.703579
 H 1.072546 -4.946465 1.469899
 H 0.060205 -5.514632 3.622528
 H -3.419143 -3.378015 4.974446
 H -3.399297 -2.009701 2.945032
 H -1.712468 -5.165183 5.320803
 H -5.928007 0.936037 0.359310
 H -3.417955 -4.009212 0.375508
 H -7.386076 -1.018630 0.206789
 H -7.675477 -3.480666 0.149607
 H -5.668101 -4.962077 0.203534
 H 2.037893 -5.058066 -3.801909
 H 4.984933 -3.788925 -0.965475
 H -2.663507 5.009554 2.200573

H -4.893207 5.097969 -1.452074
 H 1.479773 2.544854 -3.072571
 H 0.607741 1.992679 -4.502320
 H 0.429187 3.659493 -3.949533
 H -0.175204 -1.875552 -4.643771
 H 0.871104 -0.473233 -4.397113
 H 0.565131 -1.603836 -3.066297
 H -2.636293 -1.754471 -3.953219
 H -2.120359 -1.767583 -2.264447
 H -3.175859 -0.479844 -2.849741
 H -2.105342 3.849736 -2.999370
 H -1.976176 2.806117 -4.403604
 H -2.836076 2.250635 -2.954672
 H -0.900516 1.108260 -5.300786
 H -1.676782 -0.436318 -5.591332
 H -2.583382 0.840638 -4.797987
 H -1.330153 2.983489 -0.726708
 H 0.434962 2.802773 -0.842851
 H -0.369422 4.122281 -1.676300
 H -3.006103 1.465231 2.792433
 H -1.442169 2.085785 2.271813
 H -2.429382 3.027340 3.396570
 H -6.252215 2.366045 -1.569111
 H -5.179259 3.137508 -2.732513
 H -4.816750 1.512823 -2.118401
 H -3.925368 7.139411 1.382787
 H -2.729187 7.131720 0.087164
 H -4.451925 7.176079 -0.309335
 H -0.659063 -5.131407 -1.595292
 H -0.764085 -3.617057 -2.488339
 H -0.204902 -5.080351 -3.306144
 H 3.007596 -3.543503 1.808244
 H 4.439511 -2.846380 1.049953
 H 2.936615 -1.917868 1.136452
 H 5.055120 -3.978440 -4.090285
 H 5.630619 -5.190376 -2.943482
 H 4.413547 -5.622659 -4.158406

(XVII-si-c)₁

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 E0+ZPE = -3188.928010
 E298 = -3188.856540
 H298 = -3188.855596
 G298 = -3189.031403
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 C 3.737595 2.448652 -0.194405
 C 3.052552 3.129248 -1.233713
 C 3.048680 4.527057 -1.254301
 C 3.706796 5.290597 -0.287341
 C 4.413549 4.607301 0.701842
 C 3.811524 0.950811 -0.184155
 C 5.062237 0.365800 -0.257498
 C 5.260063 -1.034328 -0.279094
 C 4.117040 -1.885145 -0.377799
 C 2.807776 -1.288760 -0.453756

C 2.670912 0.072078 -0.195154
 C 6.561188 -1.603636 -0.224872
 C 6.733854 -2.968396 -0.231150
 C 5.602992 -3.817048 -0.292474
 C 4.331418 -3.292035 -0.372423
 C 1.657296 -2.136633 -0.878773
 C 0.515511 -2.275236 -0.104566
 C -0.453217 -3.299249 -0.346636
 C -0.299663 -4.064362 -1.485504
 C 0.738972 -3.840480 -2.420488
 C 1.738331 -2.861832 -2.122552
 C 0.808092 -4.572722 -3.636393
 C 1.806184 -4.328414 -4.550422
 C 2.775050 -3.333318 -4.279667
 C 2.747348 -2.625223 -3.098003
 C -1.542208 -3.668662 0.614063
 C -2.898486 -3.459669 0.279429
 C -3.890413 -3.901639 1.163337
 C -3.583785 -4.551588 2.362477
 C -2.237395 -4.784299 2.652783
 C -1.211893 -4.367158 1.797009
 C -3.304002 -2.788921 -1.014282
 C 0.220658 -4.725046 2.127727
 C -4.675332 -4.984551 3.313369
 O 0.374945 -1.479760 1.030199
 P 0.122056 0.168915 0.935860
 N 0.476854 0.611978 2.567097
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 C 2.348222 2.406533 -2.358607
 C 3.652541 6.800154 -0.315296
 C 5.308621 2.596146 1.858771
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 C 0.828960 0.131490 5.110759
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 C 2.130128 -1.117511 3.410376
 C 2.132732 2.417582 3.173271
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 C -3.581559 3.670556 -0.652675
 C -2.366888 4.232927 -1.426647
 C -4.873795 4.266950 -1.262655

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 H -2.444450 4.017426 -2.495298
 H -4.819314 5.361398 -1.209275
 H -4.994126 3.958447 -2.300420
 H -5.759133 3.951240 -0.701461
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 H -2.278579 2.333082 -4.517137
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 H -3.020405 -1.227511 -3.530219
 H -3.648151 0.181904 -4.406720
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 H 0.264129 0.307345 -2.571871
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 H -7.420721 1.896649 -0.416655
 H -5.320280 -0.896016 0.243863
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 H 3.492504 -1.860234 -2.916487
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 H 3.477655 -3.958485 -0.412746
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 H 7.731132 -3.396325 -0.179271
 H 5.738165 -4.895093 -0.274357
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 H 4.957805 5.176879 1.453146
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 H 1.315642 2.162948 -2.089454
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 H 5.284727 3.226912 2.753882
 H 4.987083 1.591568 2.140680
 H 4.475518 7.241973 0.256312
 H 3.706639 7.183905 -1.340318
 H 2.714842 7.172917 0.118336
 H 0.680485 -5.307092 1.319855
 H 0.845632 -3.838169 2.277633
 H 0.268281 -5.324292 3.042372
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 H -2.961651 -3.352085 -1.889266
 H -4.393051 -2.707855 -1.082223
 H -5.569952 -5.314718 2.773821
 H -4.344298 -5.806855 3.956580
 H -4.980924 -4.159051 3.970283

XIV-re

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 C 4.457597 0.373305 1.777291
 C 4.463916 -0.162005 3.082002
 C 4.568437 0.659091 4.206979
 Si 4.482720 -0.793286 0.286618
 C 6.128567 -1.751741 0.335791
 C 7.012153 -1.726575 1.429253
 C 8.220167 -2.429857 1.406431
 C 8.574694 -3.176842 0.283248
 C 7.717696 -3.212273 -0.819860
 C 6.515754 -2.505468 -0.791819
 C 3.086718 -2.091431 0.333243
 C 3.433901 -3.413268 0.560183
 C 2.504140 -4.481494 0.468188
 C 1.179239 -4.209545 0.003504
 C 0.819592 -2.851319 -0.306628
 C 1.717708 -1.840245 -0.004020
 C 2.875187 -5.813685 0.792577
 C 1.970600 -6.845172 0.682404
 C 0.653536 -6.577198 0.240579
 C 0.268074 -5.297036 -0.095431
 C -0.489076 -2.555163 -0.958745
 C -1.447242 -1.773952 -0.328949
 C -2.823960 -1.774153 -0.719788

C -3.114661 -2.374343 -1.935845
 C -2.127559 -2.980632 -2.755724
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 C -2.445042 -3.503839 -4.037613
 C -1.485077 -4.126032 -4.802964
 C -0.165304 -4.250314 -4.307871
 C 0.169607 -3.765907 -3.061524
 Si -4.304571 -1.286752 0.391764
 C -3.979750 -1.560057 2.239010
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 C -4.238705 -2.915393 4.259501
 C -3.569604 -1.950663 5.012894
 C -3.105950 -0.790098 4.389066
 C -3.304443 -0.602878 3.020340
 O -1.078158 -1.042960 0.790538
 P 0.044982 0.209499 0.716589
 Pd -0.161148 2.314212 -0.341191
 C -1.238319 1.854285 -2.631173
 C -1.706020 3.134500 -2.967087
 C -0.902058 4.255436 -3.153510
 C -1.500512 5.618361 -3.361204
 O 1.306541 -0.524416 -0.147119
 N 0.415238 0.200697 2.343201
 C 0.548022 -1.009893 3.158081
 C 0.984111 1.397600 2.966755
 N -1.056126 3.968344 0.732555
 C -1.852091 4.294818 1.933533
 C -3.110055 5.110030 1.549480
 N 0.179480 4.258008 -1.120388
 C 1.580928 4.822266 -1.124162
 C 1.604856 6.216278 -1.795259
 C 0.092616 1.444431 -2.378395
 C -0.662455 4.910841 -0.131230
 O -0.911350 6.125649 -0.174436
 C 2.131084 4.953939 0.314528
 C 2.514013 3.889447 -1.912096
 C -2.323085 2.980570 2.567086
 C -0.998552 5.098358 2.937045
 C 4.506402 0.133992 -1.362778
 C 5.549146 1.048701 -1.617086
 C 5.673074 1.688931 -2.850650
 C 4.761764 1.415759 -3.873462
 C 3.730446 0.502447 -3.651124
 C 3.605042 -0.126930 -2.409650
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 C -7.028122 -1.952894 -0.304708
 C -8.093770 -2.801664 -0.615980
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 C -6.596993 -4.692963 -0.563373
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 C -5.545699 1.234361 1.051773
 C -6.113104 2.477069 0.759033
 C -6.041173 2.991390 -0.536626
 C -5.399003 2.257858 -1.537000
 C -4.830670 1.018536 -1.237789

H 3.529457 4.301877 -1.913875
H 2.557948 2.889915 -1.470091
H 2.207935 3.790430 -2.959265
H 0.954871 6.912771 -1.265891
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H 1.278462 6.157990 -2.838788
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H 1.539213 5.659359 0.903639
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H -8.708708 -4.836297 -0.987811
H -5.613727 0.850091 2.066204
H -4.342158 0.458362 -2.032023
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H -6.482826 3.957478 -0.766155
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H -2.927212 0.302560 2.558875
H -4.609152 -3.819808 4.735711
H -2.593365 -0.025724 4.968018

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 H 2.793624 -0.832347 -2.264257
 H 6.485853 2.391451 -3.016875
 H 3.021502 0.276196 -4.443594
 H 4.860265 1.905974 -4.838640
 H 6.763337 -1.144144 2.311622
 H 5.870865 -2.536446 -1.667391
 H 8.884550 -2.389356 2.266130
 H 7.988907 -3.785200 -1.703132
 H 9.514324 -3.723155 0.263313
 H 4.515875 2.225029 0.662717
 H 4.396637 -1.238919 3.225310
 H 4.688725 3.677279 2.643764
 H 4.579017 0.218814 5.200944
 H 4.741595 2.687473 4.925357

XIV-*re-b*

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 H298 = -4222.710748
 G298 = -4222.911390
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 C -3.880295 -0.883944 -3.078687
 C -3.953196 -0.301464 -4.346087
 Si -4.411100 -1.128026 -0.274699
 C -5.926015 -2.279656 -0.322508
 C -6.520282 -2.692559 -1.529137
 C -7.623798 -3.549472 -1.541592
 C -8.162710 -4.013783 -0.341077
 C -7.594381 -3.614018 0.870765
 C -6.493265 -2.756775 0.876529
 C -2.872936 -2.221884 0.008234
 C -3.093782 -3.585697 0.099167
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 C -1.329769 -6.805824 0.747480
 C -0.047847 -6.324793 1.100534
 C 0.213177 -4.971563 1.147406
 C 0.740306 -2.087862 1.354459
 C 1.627843 -1.423368 0.523776
 C 3.038446 -1.404495 0.752387
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 C 2.561298 -2.229415 3.018830
 C 1.181907 -2.414093 2.684471
 C 3.005850 -2.526746 4.334201
 C 2.125594 -2.975843 5.293353
 C 0.760557 -3.151684 4.966802

C 0.301153 -2.887303 3.693852
 Si 4.295226 -1.199976 -0.665722
 C 3.996049 -2.557440 -1.961622
 C 4.968060 -2.754119 -2.964336
 C 4.824568 -3.744034 -3.937372
 C 3.703839 -4.577486 -3.925325
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 H -0.821904 1.134048 -4.131905
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 H -5.448106 2.630932 -3.490427
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 C 5.502941 1.284872 -1.391622
 C 4.507486 0.295352 -1.257807
 C 3.702677 0.028691 -2.378710
 C 3.879360 0.719901 -3.580093
 Si 4.451787 -0.761556 0.306878
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 C 4.433454 1.682532 1.876398
 C 4.545577 2.423461 3.056696
 C 4.672039 1.772470 4.284859
 C 4.666855 0.375776 4.328768
 C 4.547073 -0.358425 3.146734
 C 3.035535 -2.040660 0.234216
 C 3.377277 -3.376213 0.374941
 C 2.447487 -4.434480 0.210089
 C 1.122605 -4.130310 -0.231827
 C 0.762868 -2.753154 -0.448600
 C 1.666889 -1.763224 -0.089735
 C 2.818738 -5.785190 0.446377
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 C 0.593897 -6.508536 -0.142169
 C 0.209066 -5.208973 -0.393640
 C -0.568464 -2.422809 -1.037431
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XIV-si-d

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G298 = -4222.909780
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C 4.023291 0.229341 -2.463452
C 4.213682 0.882356 -3.684265
Si 4.679526 -0.424820 0.285376
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C 4.375015 0.096631 3.084154
C 4.391332 0.863389 4.251478
C 4.542520 2.250128 4.173894
C 4.669310 2.859798 2.924766
C 4.661472 2.085204 1.760869
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C 3.707301 -3.069196 0.316975
C 2.839388 -4.168993 0.097721
C 1.522466 -3.922908 -0.399348
C 1.107973 -2.560571 -0.615416
C 1.943526 -1.532093 -0.207821
C 3.266634 -5.502650 0.335285
C 2.421139 -6.564950 0.110377
C 1.109418 -6.325547 -0.362115
C 0.671582 -5.042873 -0.615295
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C -2.217702 -3.230417 -4.290235
C -1.233405 -3.674535 -5.144035
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N 0.488677 0.413477 2.192640
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 C 0.825796 6.867992 -1.034665
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 H -8.004972 0.997543 1.714283
 H -5.754164 2.463510 -1.644116
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 H 8.847385 -2.155953 2.623662
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 H 4.774171 2.581784 0.801332
 H 4.284054 0.379932 5.219266
 H 4.780427 3.938813 2.854240
 H 4.556426 2.850258 5.079838
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 H 3.256882 -0.537248 -2.396137
 H 6.757088 2.953712 -2.789542
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XX-re

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 C 1.299983 4.220012 1.202942
 C 0.237359 5.097223 0.488102
 C -1.021164 4.384412 -0.077344
 P 0.220723 0.605967 -0.177469
 Pd -1.932490 -0.251441 -0.525194
 C -1.442331 -0.882421 -2.588915
 C -1.277855 -2.193294 -2.065746
 C -2.277033 -3.123019 -1.751268
 C -3.643604 -2.916742 -1.946085
 C -4.655028 -3.904534 -1.435249
 C 0.882291 3.778870 2.619170
 C 2.602358 5.037807 1.316448
 C -2.057857 4.049768 1.011500
 C -1.692243 5.321665 -1.101593
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 C 3.065292 1.220070 -2.415772
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 C 3.428136 -0.332035 -0.547827
 C 6.680282 1.333823 -1.516339
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 C 7.056645 -0.039615 0.431451
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 C 2.865928 -1.366366 0.364633
 C 1.778015 -1.060445 1.170351
 C 1.254744 -1.969683 2.116514
 C 1.797313 -3.225611 2.226697
 C 2.850162 -3.638741 1.368906
 C 3.382796 -2.710897 0.412087
 C 4.380814 -3.184160 -0.485935
 C 4.848942 -4.478078 -0.415871
 C 4.350382 -5.375840 0.557055
 C 3.367752 -4.960916 1.425718
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 C -4.072162 -1.216285 0.635144
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 H 2.958352 -5.644916 2.165256
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 H 0.090676 3.027566 2.604100
 H 2.959604 5.368562 0.333381
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(XX-re)₁

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G298 = -2529.511302

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C 6.742011 1.190829 -1.288820
C 7.570221 0.616140 -0.352476
C 4.487064 1.516455 -2.256461
C 3.136117 1.273678 -2.229096
C 2.606627 0.346247 -1.302257
C 3.412739 -0.388295 -0.443594
O 1.237428 0.141628 -1.329421
P 0.212159 0.610384 -0.073301
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C 4.157540 -5.514184 0.381166
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 H 4.507176 -6.542787 0.376435
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G298 = -2529.517526
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C 0.272003 5.206461 0.588776
C 1.613594 4.438240 0.728054
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C -2.190985 -3.122225 -1.568001
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 H -6.101404 -1.628985 -2.293585
 H -6.585536 -1.191960 -0.643989
 H -5.904351 1.886710 -1.034464
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 H -0.985382 0.130763 2.827980
 H -2.068439 1.532475 2.793208
 H -2.158799 -0.707306 -3.059975
 H -0.171303 -2.486193 -1.520707
 H -3.807591 -2.298839 -2.691966
 H -4.124408 -4.785885 -0.948268
 H -5.167647 -3.418261 -0.541552
 H -1.928704 -3.966016 -0.932420
 H -0.373334 -0.443146 -2.776822
 H -5.282468 -4.162696 -2.150356
 H 0.150991 -1.857023 2.628108
 H 0.902765 -4.227409 2.557979
 H 2.317168 -5.966050 1.576626
 H 5.155103 -4.966251 -1.495525
 H 4.547298 -2.600681 -1.321965
 H 4.071509 -6.667807 -0.026419
 H 5.125416 2.249150 -2.673935
 H 5.171912 -1.587443 1.357772
 H 7.304672 1.714732 -1.684734
 H 8.679072 0.452221 -0.054893
 H 7.584992 -1.178501 1.484711
 H 2.648209 1.980406 -2.681207
 H 0.461211 6.184415 0.124838
 H -0.090048 5.418904 1.605393
 H 2.249225 2.381857 1.080150
 H 1.030085 2.963225 2.213907
 H -1.771711 2.495528 -0.113930
 H -1.331671 3.136027 1.473895
 H -2.386751 5.302391 1.228556
 H -2.150200 6.270412 -0.236232
 H -3.055591 4.750761 -0.318651
 H -1.642200 4.111481 -2.161385
 H -0.452895 5.420811 -2.089515

H 0.069452 3.729270 -1.986554
H 2.600100 5.534202 -0.877804
H 3.441006 4.050199 -0.397970
H 1.987452 3.956091 -1.388711
H 2.665577 6.142484 1.602124
H 1.899553 5.092563 2.806484
H 3.393569 4.578521 1.999967

(XX-re)₃

E0 = -2530.3417983
E0+ZPE = -2529.430356
E298 = -2529.378853
H298 = -2529.377909
G298 = -2529.514071
NImag = 1, (-199.1044)
C 6.990005 -0.496910 0.705947
C 5.643000 -0.779145 0.636067
C 4.807301 -0.150567 -0.329027
C 5.405294 0.815574 -1.205684
C 6.800305 1.069865 -1.119074
C 7.582025 0.426547 -0.187031
C 4.586071 1.516571 -2.131057
C 3.228091 1.321093 -2.150084
C 2.638434 0.381080 -1.271504
C 3.394072 -0.416592 -0.423193
O 1.262546 0.236434 -1.344902
P 0.207545 0.648406 -0.095657
O 1.147441 0.129154 1.185987
C 1.627583 -1.175998 1.152359
C 0.980036 -2.126814 1.972237
C 1.420052 -3.426996 1.980708
C 2.486313 -3.837370 1.136855
C 3.137583 -2.868414 0.301074
C 2.725309 -1.488765 0.364301
C 2.899051 -5.196222 1.084756
C 3.890747 -5.604067 0.222948
C 4.505092 -4.660930 -0.633820
C 4.140825 -3.332724 -0.595563
Pd -1.906584 -0.257033 -0.482872
N -3.136664 -0.298868 1.273246
C -3.108498 -0.034394 2.726636
C -1.895819 0.850348 3.037105
N -3.881080 -0.972459 -0.739346
C -3.587215 -3.092326 -1.543038
C -2.240562 -3.284232 -1.230501
C -1.199549 -2.435164 -1.629342
C -1.294800 -1.229761 -2.374503
C -4.913119 -0.138637 -1.461286
C -5.154671 1.210027 -0.744815
C -4.435309 0.163094 -2.891880
C -6.256028 -0.902289 -1.538877
C -4.126439 -0.993766 0.699784
O -5.097827 -1.579730 1.199093
C -4.652709 -3.970420 -0.948004
C -4.389987 0.710296 3.162336
C -2.990561 -1.365245 3.501650

N 0.291556 2.290280 0.177286
 C 1.528065 2.980143 0.611393
 C 1.256669 4.355452 1.251712
 C 0.426422 5.250756 0.279623
 C -0.505121 4.497456 -0.721672
 C -0.887996 3.122762 -0.143588
 H -5.192141 0.762133 -3.411564
 H -3.498550 0.729696 -2.887021
 H -4.286194 -0.749205 -3.479743
 H -6.999595 -0.278664 -2.050509
 H -6.151004 -1.830940 -2.108906
 H -6.618359 -1.149048 -0.540170
 H -5.854487 1.816289 -1.332307
 H -5.585260 1.062742 0.248987
 H -4.221122 1.771492 -0.634501
 H -2.932246 -1.180103 4.581881
 H -3.856818 -1.998227 3.296268
 H -2.087598 -1.907408 3.196984
 H -4.362794 0.922266 4.238569
 H -4.474396 1.664958 2.629966
 H -5.275341 0.108462 2.945636
 H -1.858323 1.084838 4.107528
 H -0.958734 0.358864 2.761085
 H -1.958390 1.793278 2.482631
 H -2.154149 -1.082790 -3.018152
 H -0.210890 -2.678859 -1.241005
 H -3.832983 -2.577826 -2.462525
 H -4.207148 -4.834599 -0.442814
 H -5.229028 -3.413221 -0.200335
 H -1.998077 -4.046122 -0.492031
 H -0.368906 -0.804281 -2.746534
 H -5.347443 -4.332168 -1.715576
 H -0.174568 5.940720 0.885463
 H 1.110170 5.882695 -0.301401
 H 0.144975 -1.802404 2.582324
 H 0.936485 -4.164076 2.616549
 H 2.401608 -5.912788 1.734014
 H 5.268653 -4.987717 -1.334495
 H 4.615714 -2.628404 -1.268173
 H 4.192656 -6.647076 0.187412
 H 5.048185 2.228867 -2.809915
 H 5.204735 -1.482340 1.334643
 H 7.237336 1.796858 -1.799692
 H 8.646679 0.634169 -0.126094
 H 7.602409 -0.985683 1.458805
 H 2.581785 1.862618 -2.833457
 H 2.200218 3.113318 -0.246061
 H 2.045316 2.338420 1.329061
 H -1.513335 2.581232 -0.861733
 H -1.502309 3.266184 0.754809
 C 0.537285 4.184593 2.606671
 H 1.132147 3.559189 3.283077
 H 0.396728 5.159811 3.088455
 H -0.445941 3.716429 2.510717
 C 2.621250 5.022361 1.516274
 H 2.482950 6.022583 1.943714

H 3.220820 4.437144 2.224135
 H 3.200024 5.131117 0.591266
 C -1.801599 5.304311 -0.925267
 H -2.359018 5.408198 0.013314
 H -1.574554 6.312602 -1.291473
 H -2.460641 4.823395 -1.658768
 C 0.182580 4.325448 -2.091994
 H 1.126059 3.776139 -2.019681
 H -0.467465 3.780507 -2.787893
 H 0.401046 5.304453 -2.535312

XX-si-c

E0 = -2530.3361312
 E0+ZPE = -2529.425244
 E298 = -2529.373601
 H298 = -2529.372657
 G298 = -2529.509214
 NImag = 1, (-159.3266)
 C -4.572922 0.542710 -2.344087
 C -5.018381 0.453804 -0.865994
 C -6.476726 -0.060559 -0.819763
 C -4.978124 1.868855 -0.264387
 N -4.123919 -0.461221 -0.068087
 C -4.827245 -0.931796 2.121591
 C -5.839985 -2.037397 2.051251
 Pd -2.076045 -0.005175 0.115728
 C -3.580974 -1.126569 2.703799
 C -2.525350 -0.201873 2.677742
 C -2.468957 1.062510 2.043914
 N -2.568703 -1.686130 -1.121915
 C -1.951193 -2.769777 -1.917836
 C -2.003381 -4.088925 -1.115454
 C -2.695104 -2.934161 -3.261159
 C -0.490246 -2.407855 -2.197458
 H -5.200331 1.269788 -2.873495
 H -3.528978 0.862796 -2.424833
 H -4.672612 -0.422378 -2.847961
 H -7.113978 0.600846 -1.419814
 H -6.539606 -1.076260 -1.211788
 H -6.864607 -0.059377 0.204213
 H -5.640981 2.530627 -0.833898
 H -5.321608 1.882409 0.775964
 H -3.967113 2.287323 -0.301451
 H -2.232358 -3.729586 -3.858644
 H -3.744123 -3.187757 -3.091731
 H -2.645885 -2.003627 -3.838901
 H -1.523315 -4.898821 -1.679528
 H -1.471025 -3.972823 -0.164068
 H -3.038596 -4.368658 -0.906825
 H -0.022777 -3.185169 -2.813881
 H -0.416092 -1.453081 -2.727333
 H 0.079301 -2.321055 -1.267971
 H -3.391920 1.587865 1.825871
 H -1.596018 -0.539962 3.134837
 H -5.188474 0.079395 1.990604
 H -5.557748 -2.868070 2.707650

H -6.839682 -1.686867 2.334006
 H -3.348649 -2.124274 3.072179
 H -1.640517 1.707970 2.323138
 H -5.890790 -2.428928 1.027436
 P 0.163159 0.689174 0.150206
 C 1.640243 2.976963 0.734448
 C -0.735314 3.235038 -0.101424
 C 1.433294 4.377009 1.343995
 C -0.245333 4.571175 -0.692476
 C 0.675666 5.297694 0.336442
 N 0.367496 2.343441 0.322142
 O 1.167732 0.208315 1.398119
 O 1.075980 0.160942 -1.151488
 C 1.670387 -1.088220 1.399084
 C 1.128293 -1.989382 2.342133
 C 2.699364 -1.439339 0.537323
 C 1.591865 -3.279728 2.397750
 C 3.129067 -2.815403 0.527472
 C 2.578882 -3.733598 1.483742
 C 3.009497 -5.087643 1.483339
 H 0.356774 -1.633264 3.015404
 H 1.187238 -3.976986 3.126713
 C 3.922241 -5.541134 0.559613
 C 4.051685 -3.327383 -0.427774
 C 4.434911 -4.650656 -0.412490
 H 2.587533 -5.764700 2.222195
 H 5.133440 -5.015093 -1.160809
 H 4.446496 -2.665751 -1.189447
 H 4.237535 -6.580755 0.563609
 C 2.451804 0.309207 -1.215890
 C 3.283905 -0.418523 -0.376849
 C 4.696919 -0.139267 -0.423135
 C 2.954759 1.176364 -2.214574
 C 4.307461 1.379305 -2.325106
 H 4.703061 2.034889 -3.096806
 C 5.208700 0.759552 -1.418276
 C 5.617977 -0.688875 0.511930
 H 5.248215 -1.339886 1.295559
 C 6.603164 1.026601 -1.468849
 H 6.973479 1.700680 -2.237742
 C 7.467553 0.460390 -0.560116
 H 8.531199 0.676957 -0.605396
 C 6.962810 -0.395643 0.446458
 H 7.641621 -0.823595 1.179168
 H 2.247714 1.654706 -2.884137
 C -3.858736 -1.707350 -0.774623
 O -4.737159 -2.563849 -0.954542
 H 1.402296 5.899939 -0.223754
 H 0.078089 6.014404 0.914251
 H -1.349039 2.713950 -0.844024
 H -1.393954 3.448101 0.751212
 H 2.322347 3.055943 -0.121784
 H 2.122197 2.327742 1.468407
 C 0.493601 4.332602 -2.025494
 H 1.403789 3.740671 -1.898567
 H -0.151639 3.804012 -2.738336

H 0.779260 5.289252 -2.479414
 C -1.484302 5.442431 -0.976156
 H -2.077118 5.603400 -0.067673
 H -1.183568 6.425806 -1.356906
 H -2.135226 4.979031 -1.727939
 C 2.824568 4.972021 1.635547
 H 2.731783 5.989935 2.032716
 H 3.367594 4.372681 2.376571
 H 3.436632 5.022098 0.727157
 C 0.666317 4.268735 2.679311
 H 1.194153 3.607027 3.376726
 H 0.581505 5.254645 3.152093
 H -0.346715 3.874939 2.553827

(XX-si-c)₁

E0 = -2530.3379707
 E0+ZPE = -2529.426722
 E298 = -2529.375223
 H298 = -2529.374279
 G298 = -2529.509977
 NImag = 1, (-177.5270)
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 C -5.753857 -0.293428 -0.206727
 C -4.694713 0.144714 0.637061
 C -4.999443 1.127171 1.638647
 C -6.337592 1.580594 1.789688
 C -7.340594 1.117100 0.969871
 C -3.952949 1.647196 2.447082
 C -2.651193 1.263826 2.240076
 C -2.355565 0.304889 1.243839
 C -3.338266 -0.321526 0.493028
 O -1.022676 -0.035266 1.067488
 P -0.153506 0.443108 -0.282123
 O -1.266952 -0.010915 -1.457611
 C -1.971160 -1.204908 -1.399947
 C -1.691208 -2.156470 -2.409096
 C -2.352310 -3.358943 -2.424527
 C -3.286944 -3.683291 -1.406565
 C -3.586215 -2.710532 -0.395384
 C -2.962572 -1.411397 -0.448979
 C -3.912205 -4.958272 -1.360825
 C -4.777268 -5.286938 -0.342811
 C -5.043263 -4.346986 0.680137
 C -4.467489 -3.095489 0.654065
 Pd 2.049130 -0.371131 -0.210346
 N 2.949120 -0.227837 1.730167
 C 4.017457 -0.957776 1.391778
 O 4.852616 -1.555396 2.084253
 N 4.068887 -0.966928 -0.069321
 C 5.175759 -0.078270 -0.584699
 C 4.978329 0.191228 -2.086139
 C 5.215482 1.284778 0.144276
 C 6.540561 -0.778317 -0.380376
 C 1.883629 -1.398226 -2.159330
 C 1.721455 -2.610595 -1.437460
 C 2.712941 -3.395625 -0.834051

C 4.079629 -3.128863 -0.882925
 C 5.054923 -3.931660 -0.069930
 C 2.593749 0.057743 3.136791
 C 1.481792 1.115073 3.151412
 C 2.096801 -1.234707 3.817483
 C 3.811875 0.625303 3.900518
 N -0.280117 2.092771 -0.512843
 C -1.504946 2.744713 -1.041072
 C -1.495105 4.278309 -0.883054
 C -0.207476 4.883138 -1.521044
 C 1.053800 3.962859 -1.518036
 C 0.935159 2.922915 -0.389132
 C -2.732479 4.824904 -1.623556
 C -1.623020 4.671250 0.604895
 C 2.312943 4.810846 -1.258459
 C 1.212932 3.245645 -2.875227
 H 5.984183 1.919410 -0.312888
 H 4.253007 1.800520 0.072654
 H 5.459006 1.166331 1.203289
 H 7.344809 -0.112643 -0.717138
 H 6.694038 -1.023126 0.671762
 H 6.604815 -1.701637 -0.964647
 H 5.801865 0.811029 -2.459210
 H 4.977563 -0.732632 -2.674594
 H 4.040612 0.724536 -2.274787
 H 3.531088 0.855785 4.935817
 H 4.635360 -0.090614 3.906256
 H 4.158270 1.553486 3.430150
 H 1.806066 -1.040730 4.858080
 H 1.225934 -1.633639 3.284992
 H 2.887284 -1.990543 3.812029
 H 1.221763 1.375326 4.184786
 H 1.813761 2.028122 2.642477
 H 0.584417 0.742757 2.652819
 H 2.840347 -1.187885 -2.622513
 H 0.694416 -2.922052 -1.251039
 H 4.471327 -2.594203 -1.737943
 H 4.584312 -4.845377 0.309974
 H 5.938961 -4.207559 -0.656602
 H 2.375026 -4.170632 -0.148383
 H 1.031262 -1.033828 -2.724598
 H 5.385612 -3.346273 0.796733
 H -0.419084 5.167144 -2.559740
 H 0.022515 5.819595 -0.996991
 H -0.957752 -1.905829 -3.167397
 H -2.146508 -4.086916 -3.205024
 H -3.679680 -5.677139 -2.142947
 H -5.703424 -4.616452 1.500029
 H -4.674003 -2.395099 1.454649
 H -5.243578 -6.267717 -0.313454
 H -4.194864 2.373085 3.219294
 H -5.539672 -1.003070 -0.996991
 H -6.550836 2.315249 2.562638
 H -8.358764 1.476201 1.090949
 H -7.824319 -0.165290 -0.711037
 H -1.834517 1.669698 2.827335

H -2.378837 2.338519 -0.526570
 H -1.618528 2.492946 -2.102958
 H 0.952534 3.432236 0.583117
 H 1.804822 2.256418 -0.405256
 H -2.759415 5.919774 -1.568343
 H -2.721250 4.543738 -2.683345
 H -3.662146 4.445526 -1.182000
 H -1.676377 5.761948 0.706356
 H -2.536599 4.246943 1.037268
 H -0.781971 4.322860 1.210481
 H 2.409969 5.599592 -2.014169
 H 2.272269 5.294545 -0.274964
 H 3.222331 4.198532 -1.296294
 H 2.093315 2.591263 -2.868218
 H 0.345323 2.626600 -3.124086
 H 1.344399 3.977017 -3.681766

(XX-si-c)₂

E0+ZPE = -2529.428130
 E298 = -2529.376482
 H298 = -2529.375538
 G298 = -2529.512197
 NImag = 1, (-155.8954)
 C -6.893095 -0.732049 -0.486367
 C -5.531605 -0.932219 -0.555814
 C -4.646810 -0.311237 0.369753
 C -5.215495 0.557456 1.360756
 C -6.625184 0.726862 1.416522
 C -7.451779 0.094916 0.516320
 C -4.355762 1.244495 2.258271
 C -2.992647 1.141476 2.136538
 C -2.435146 0.305379 1.142074
 C -3.218295 -0.495008 0.321152
 O -1.051852 0.245166 1.082972
 P -0.155187 0.734612 -0.235490
 O -1.129396 0.183044 -1.472300
 C -1.566447 -1.138764 -1.433953
 C -0.979007 -2.039226 -2.349138
 C -1.376478 -3.352519 -2.362802
 C -2.337205 -3.826550 -1.431263
 C -2.932827 -2.907712 -0.503128
 C -2.576677 -1.511148 -0.560137
 C -2.696006 -5.200641 -1.385809
 C -3.580515 -5.671467 -0.443582
 C -4.135551 -4.778374 0.502386
 C -3.823266 -3.436804 0.473059
 Pd 2.097170 0.073682 -0.139419
 N 2.592525 -1.578208 1.136843
 C 3.886942 -1.590909 0.805994
 O 4.772388 -2.433968 1.012948
 N 4.146801 -0.356547 0.078010
 C 5.020856 0.585801 0.866232
 C 4.975391 1.985452 0.229810
 C 4.553412 0.704594 2.335266
 C 6.484781 0.085350 0.852026
 C 2.505801 1.096340 -2.094136

C 2.586786 -0.180687 -2.697723
 C 3.653633 -1.093222 -2.688317
 C 4.889592 -0.869635 -2.096254
 C 5.915157 -1.959800 -1.986937
 C 1.978096 -2.653085 1.946856
 C 0.512258 -2.298677 2.209998
 C 2.047067 -3.984417 1.166130
 C 2.712927 -2.789270 3.298263
 N -0.407778 2.390525 -0.474205
 C -1.284004 2.972353 -1.509564
 C -1.923729 4.318651 -1.090768
 C -0.835287 5.248255 -0.489646
 C 0.165047 4.620342 0.517359
 C 0.684764 3.299959 -0.088887
 C -2.476650 4.985114 -2.368170
 C -3.108090 4.090015 -0.133565
 C -0.439783 4.372185 1.911608
 C 1.361922 5.579333 0.675127
 H 5.165293 1.450582 2.856430
 H 3.505049 1.015011 2.393528
 H 4.656166 -0.247627 2.862485
 H 7.107054 0.767026 1.445040
 H 6.552238 -0.920270 1.268439
 H 6.886860 0.066592 -0.166323
 H 5.622479 2.667921 0.792934
 H 5.334673 1.977190 -0.805278
 H 3.959850 2.394283 0.241056
 H 2.251381 -3.578143 3.905287
 H 3.765138 -3.037317 3.141286
 H 2.651831 -1.849635 3.859929
 H 1.570475 -4.789671 1.739742
 H 1.520076 -3.888171 0.209520
 H 3.086198 -4.258138 0.968907
 H 0.047330 -3.068714 2.837345
 H 0.426931 -1.334932 2.721716
 H -0.050852 -2.234460 1.274921
 H 3.418054 1.638820 -1.873172
 H 1.668449 -0.540255 -3.160263
 H 5.235185 0.148786 -1.980245
 H 5.655750 -2.806658 -2.632013
 H 6.915073 -1.601305 -2.258498
 H 3.437921 -2.101640 -3.037040
 H 1.677811 1.727590 -2.406701
 H 5.952541 -2.330732 -0.954807
 H -0.237413 5.634160 -1.328350
 H -1.316743 6.124522 -0.033733
 H -0.227363 -1.665816 -3.035063
 H -0.937873 -4.051042 -3.070519
 H -2.240837 -5.877927 -2.104430
 H -4.810449 -5.154848 1.266234
 H -4.249334 -2.773391 1.215858
 H -3.840576 -6.725797 -0.412682
 H -4.791916 1.876062 3.027971
 H -5.120943 -1.562878 -1.335832
 H -7.037918 1.380208 2.181629
 H -8.527687 0.237553 0.564849

H -7.543780 -1.211666 -1.212555
 H -2.317752 1.675152 2.797303
 H -2.061382 2.252732 -1.766117
 H -0.679041 3.138893 -2.417537
 H 1.342421 2.791110 0.624176
 H 1.293534 3.534868 -0.977589
 H -2.944000 5.948165 -2.130013
 H -1.684470 5.170368 -3.103740
 H -3.238743 4.355366 -2.843707
 H -3.917860 3.559088 -0.649001
 H -2.838355 3.495207 0.738720
 H -3.510535 5.047823 0.218733
 H 0.347871 4.093415 2.622997
 H -0.928918 5.275816 2.294431
 H -1.174044 3.565001 1.903752
 H 1.849389 5.779768 -0.286883
 H 1.035783 6.540558 1.090431
 H 2.115436 5.163067 1.355332

XX-si

E0 = -2530.344844
 E0+ZPE = -2529.433516
 E298 = -2529.382172
 H298 = -2529.381228
 G298 = -2529.516386
 NImag = 1, (-187.4940)
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 C 5.560368 -1.121300 0.739063
 C 4.797174 -0.379519 -0.206054
 C 5.493717 0.558766 -1.038776
 C 6.905418 0.678278 -0.931138
 C 7.612877 -0.070580 -0.019161
 C 4.753267 1.365189 -1.943226
 C 3.382818 1.303184 -1.972885
 C 2.695974 0.396591 -1.132267
 C 3.366199 -0.511417 -0.321782
 O 1.312830 0.393074 -1.232662
 P 0.244720 0.728339 0.015593
 O 1.146246 0.118598 1.281880
 C 1.527575 -1.218011 1.194154
 C 0.802272 -2.158145 1.959129
 C 1.146725 -3.485829 1.903614
 C 2.187285 -3.930246 1.045317
 C 2.915977 -2.971198 0.264279
 C 2.606993 -1.569535 0.399152
 C 2.498013 -5.311686 0.924992
 C 3.463731 -5.747990 0.047703
 C 4.153016 -4.810859 -0.756815
 C 3.888287 -3.462805 -0.651409
 Pd -1.806107 -0.294052 -0.420279
 N -3.149101 -0.300437 1.263534
 C -4.171834 -0.809375 0.566645
 O -5.384447 -0.854728 0.818764
 N -3.612866 -1.350294 -0.669662
 C -3.615867 -2.861806 -0.660102
 C -2.704238 -3.397281 -1.777477

C -3.102798 -3.428691 0.683463
 C -5.052890 -3.383643 -0.897537
 C -2.444948 0.838626 -2.671470
 C -1.522023 -0.237387 -2.616551
 C -3.844135 0.787317 -2.606018
 C -4.596670 -0.382694 -2.520382
 C -6.080468 -0.334088 -2.289085
 C -3.336637 0.297502 2.602437
 C -1.960466 0.624674 3.195919
 C -4.177043 1.587223 2.482846
 C -4.043582 -0.699700 3.548687
 N 0.335637 2.367130 0.365251
 C 1.455755 2.988208 1.100748
 C 1.749387 4.440394 0.648531
 C 0.421972 5.241558 0.590628
 C -0.793776 4.558865 -0.090622
 C -0.919288 3.133753 0.484501
 C 2.661017 5.083998 1.714083
 C 2.506300 4.464230 -0.692375
 C -2.064232 5.344693 0.292063
 C -0.700957 4.517787 -1.628525
 H -3.064757 -4.523007 0.623048
 H -2.097081 -3.060575 0.907533
 H -3.763686 -3.158154 1.511236
 H -5.052978 -4.479768 -0.853760
 H -5.736257 -2.994218 -0.141559
 H -5.424469 -3.090165 -1.884549
 H -2.733180 -4.493083 -1.778162
 H -3.027769 -3.066056 -2.770273
 H -1.665050 -3.088003 -1.626695
 H -4.144070 -0.265356 4.551318
 H -5.035846 -0.952886 3.170813
 H -3.456669 -1.621675 3.636012
 H -4.319915 2.052496 3.466690
 H -3.678061 2.312535 1.829916
 H -5.157232 1.355342 2.058434
 H -2.073474 1.113506 4.170745
 H -1.371574 -0.286892 3.341913
 H -1.389227 1.290402 2.543440
 H -1.854613 -1.226739 -2.907515
 H -2.010191 1.838456 -2.671398
 H -4.194453 -1.287425 -2.955408
 H -6.464099 0.681732 -2.436070
 H -6.615341 -1.013656 -2.962985
 H -4.364676 1.731078 -2.451374
 H -0.486269 -0.023044 -2.860050
 H -6.306601 -0.626703 -1.256584
 H 0.124504 5.454084 1.627916
 H 0.607456 6.218354 0.122909
 H -0.015562 -1.805684 2.576642
 H 0.604203 -4.217096 2.497134
 H 1.942663 -6.021283 1.533682
 H 4.895224 -5.157404 -1.470835
 H 4.419077 -2.762958 -1.285629
 H 3.687448 -6.807486 -0.040308
 H 5.285151 2.052380 -2.596372

H 5.051756 -1.807548 1.406055
 H 7.415655 1.387097 -1.579147
 H 8.691394 0.034355 0.058912
 H 7.481686 -1.541684 1.569169
 H 2.798783 1.929885 -2.637708
 H 2.348818 2.370493 0.987051
 H 1.201008 2.991974 2.172513
 H -1.721968 2.581904 -0.014269
 H -1.191716 3.209044 1.548987
 H 2.901931 6.118747 1.442335
 H 2.181049 5.099623 2.699940
 H 3.607072 4.536506 1.807560
 H 2.648794 5.496450 -1.035057
 H 3.496420 4.007428 -0.582874
 H 1.981652 3.919395 -1.478565
 H -2.193297 5.399176 1.379521
 H -2.013429 6.371356 -0.090354
 H -2.961968 4.876571 -0.130087
 H -1.672799 4.242244 -2.057275
 H -0.429661 5.499241 -2.035185
 H 0.031977 3.789251 -1.982809

(XX-si)₁

E0 = -2530.3450884
 E0+ZPE = -2529.434210
 E298 = -2529.382654
 H298 = -2529.381710
 G298 = -2529.517456
 NImag = 1, (-177.4689)
 C 1.788053 2.975529 0.298256
 N 0.468602 2.383748 -0.008272
 C -0.366848 3.259971 -0.851441
 C -0.627686 4.649756 -0.221911
 C 0.715947 5.243028 0.278621
 C 1.658590 4.302574 1.074566
 P 0.242064 0.724133 -0.187146
 Pd -1.847632 -0.276060 -0.503318
 C -1.651911 -0.346903 -2.724800
 C -2.634674 0.668726 -2.809881
 C -4.027773 0.550759 -2.685119
 C -4.714467 -0.645270 -2.500262
 C -6.188754 -0.660924 -2.214673
 C -1.181122 5.568169 -1.331335
 C -1.690479 4.563363 0.888834
 C 3.053949 4.956611 1.133387
 C 1.192771 4.036164 2.519404
 O 1.239269 0.156766 -1.424767
 C 2.622646 0.224169 -1.375798
 C 3.254292 1.059984 -2.326709
 C 4.621131 1.178191 -2.332741
 C 5.409469 0.503542 -1.362255
 C 4.767540 -0.357359 -0.409843
 C 3.340474 -0.548361 -0.473147
 C 6.817515 0.683450 -1.305160
 C 7.572369 0.068691 -0.332732
 C 6.939398 -0.749725 0.631867

C 5.577838 -0.958500 0.593702
 C 2.621985 -1.518298 0.400081
 C 1.555874 -1.088511 1.176129
 C 0.873151 -1.936608 2.075426
 C 1.244409 -3.254152 2.178697
 C 2.272161 -3.784273 1.354866
 C 2.958631 -2.919224 0.437598
 C 3.919781 -3.504520 -0.434011
 C 4.212865 -4.849405 -0.373664
 C 3.565000 -5.689122 0.562370
 C 2.611670 -5.163354 1.403225
 O 1.148980 0.243128 1.121637
 N -3.152338 -0.194733 1.197420
 C -3.323441 0.504476 2.487217
 C -3.858203 -0.467048 3.562656
 N -3.605415 -1.434006 -0.616014
 C -3.517160 -2.937772 -0.497975
 C -4.926482 -3.557270 -0.651452
 C -4.158414 -0.835707 0.593944
 O -5.351895 -0.952530 0.906370
 C -2.608037 -3.498735 -1.604906
 C -2.933319 -3.371840 0.866321
 C -1.958423 1.035976 2.938823
 C -4.305506 1.682918 2.309713
 H -2.827819 -4.463252 0.885603
 H -1.946980 -2.928158 1.032670
 H -3.587904 -3.080047 1.692117
 H -4.857135 -4.646154 -0.538507
 H -5.607662 -3.159645 0.101948
 H -5.344929 -3.350443 -1.641786
 H -2.563655 -4.590853 -1.522384
 H -2.986398 -3.266512 -2.606724
 H -1.587347 -3.112515 -1.517759
 H -3.959827 0.048392 4.525971
 H -4.832774 -0.863680 3.270177
 H -3.164867 -1.305714 3.697671
 H -4.428250 2.231335 3.252535
 H -3.928956 2.380454 1.553102
 H -5.282095 1.313579 1.987333
 H -2.059211 1.601020 3.873066
 H -1.255557 0.214864 3.112387
 H -1.522928 1.693490 2.181304
 H -1.937047 -1.372184 -2.928853
 H -2.259388 1.689112 -2.894246
 H -4.275175 -1.558605 -2.877707
 H -6.629451 0.327890 -2.383485
 H -6.711600 -1.392111 -2.842867
 H -4.590036 1.475902 -2.569410
 H -0.638903 -0.095762 -3.022193
 H -6.363292 -0.925136 -1.164568
 H 1.274562 5.575158 -0.609065
 H 0.516415 6.149568 0.866669
 H 0.067435 -1.521738 2.669725
 H 0.734096 -3.913705 2.875653
 H 2.088370 -5.800001 2.112648
 H 4.945319 -5.270091 -1.057265

H 4.418450 -2.880851 -1.166314
 H 3.810809 -6.746569 0.603970
 H 5.114936 1.810123 -3.066599
 H 5.108696 -1.581515 1.346186
 H 7.287008 1.330665 -2.042300
 H 8.647692 0.218942 -0.295512
 H 7.531919 -1.215183 1.414806
 H 2.632134 1.588242 -3.042545
 H -1.321621 2.756001 -1.035327
 H 0.128655 3.403700 -1.827227
 H 2.368701 2.255519 0.876870
 H 2.327984 3.162850 -0.643217
 H -1.386431 6.569814 -0.935420
 H -0.471054 5.675199 -2.160411
 H -2.121115 5.175409 -1.739200
 H -1.817005 5.537042 1.377502
 H -2.661021 4.275772 0.466651
 H -1.440852 3.832075 1.657533
 H 3.447521 5.162114 0.130463
 H 3.011606 5.907945 1.677519
 H 3.771675 4.308959 1.651652
 H 1.992784 3.546983 3.088498
 H 0.945914 4.973764 3.031857
 H 0.320064 3.382358 2.563418

XXI-*re*

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 E298 = -2491.237561
 H298 = -2491.236616
 G298 = -2491.370270
 NImag = 1, (-210.3716)
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 C -2.823461 2.676746 0.300521
 C -2.074877 3.579177 1.129495
 C -2.343807 4.973421 1.066275
 C -3.286962 5.475074 0.199773
 C -3.995549 4.594531 -0.651185
 C -1.059366 3.066316 1.979224
 C -0.757016 1.727365 1.980042
 C -1.498558 0.844358 1.165613
 C -2.561582 1.261002 0.376423
 C -3.355192 0.260931 -0.392436
 C -4.787373 0.156121 -0.277749
 C -5.498762 -0.761171 -1.122525
 C -4.772961 -1.573707 -2.033857
 C -3.401645 -1.529716 -2.071571
 C -2.701836 -0.633338 -1.230683
 C -6.912358 -0.857897 -1.017069
 C -7.608285 -0.108745 -0.096551
 C -6.907892 0.766710 0.766016
 C -5.539118 0.896998 0.677396
 O -1.323691 -0.631288 -1.318272
 P -0.299007 -1.122612 -0.063617
 N -0.532867 -2.806924 0.142190
 C 0.340915 -3.680202 -0.775201
 C -0.471923 -4.834675 -1.427635

O -1.161064 -0.508713 1.221391
 Pd 1.826921 -0.042740 -0.456692
 C 1.109970 0.944467 -2.297042
 C 0.973408 2.142420 -1.545704
 C 1.984130 3.039274 -1.183713
 C 3.326043 2.907676 -1.550694
 C 4.370919 3.835526 -0.994428
 N 3.158854 0.093016 1.257014
 C 4.066311 0.840945 0.625292
 O 5.038459 1.476461 1.062711
 N 3.736043 0.813678 -0.797588
 C 4.783852 0.052910 -1.582560
 C 4.272295 -0.252415 -3.001291
 C -1.357052 -3.407896 1.313486
 C -0.710743 -3.050923 2.668980
 C -2.821623 -2.920365 1.261949
 C -1.469404 -4.950938 1.301169
 C 0.875684 -2.885270 -1.996635
 C 1.571408 -4.210620 -0.012141
 C 3.277067 -0.180577 2.704358
 C 4.620046 -0.874907 3.022031
 C 3.169025 1.135832 3.505850
 C 2.132629 -1.114286 3.099419
 C 6.079654 0.889917 -1.705763
 C 5.131663 -1.290669 -0.901500
 H 5.048343 -0.791232 -3.557193
 H 3.376456 -0.880066 -2.980678
 H 4.046602 0.658278 -3.566461
 H 6.829254 0.312173 -2.260493
 H 5.901357 1.818739 -2.256593
 H 6.473427 1.141449 -0.720783
 H 5.841020 -1.844577 -1.528081
 H 5.592718 -1.134605 0.076899
 H 4.237953 -1.908116 -0.766081
 H 3.205191 0.935290 4.584420
 H 3.988516 1.807349 3.241230
 H 2.222628 1.643063 3.283672
 H 4.691588 -1.097953 4.094084
 H 4.699166 -1.820572 2.472836
 H 5.458933 -0.234169 2.741217
 H 2.170374 -1.348893 4.169883
 H 1.165545 -0.653164 2.881058
 H 2.191565 -2.052483 2.538168
 H 1.955543 0.851418 -2.967901
 H -0.013116 2.338792 -1.129081
 H 3.553582 2.424655 -2.491753
 H 3.903195 4.674876 -0.467668
 H 5.002763 3.304626 -0.273098
 H 1.735617 3.789020 -0.435010
 H 0.197991 0.475845 -2.649594
 H 5.015240 4.234010 -1.787320
 H 0.039925 1.324541 2.593430
 H -0.502361 3.752849 2.611374
 H -1.775003 5.639310 1.710815
 H -4.719883 4.993968 -1.355767
 H -4.317226 2.579186 -1.269210

H -3.478643 6.543524 0.155773
 H -5.318670 -2.252003 -2.685021
 H -5.020227 1.565739 1.354176
 H -7.433934 -1.550094 -1.673937
 H -8.688489 -0.196374 -0.020814
 H -7.453982 1.339138 1.510917
 H -2.829218 -2.162320 -2.742152
 H 0.026155 -5.137038 -2.354209
 H -0.547321 -5.727995 -0.811971
 H -1.480320 -4.498598 -1.688708
 H 2.170401 -4.856856 -0.665452
 H 2.202638 -3.376259 0.312244
 H 1.302951 -4.792019 0.872367
 H 1.434286 -3.585586 -2.625820
 H 0.067071 -2.462329 -2.600014
 H 1.566910 -2.081836 -1.729545
 H -1.319464 -3.465352 3.481275
 H 0.291635 -3.482556 2.748549
 H -0.638886 -1.977197 2.823662
 H -3.393864 -3.439590 2.039658
 H -2.921428 -1.852486 1.435749
 H -3.273459 -3.162046 0.295451
 H -1.966951 -5.227970 2.235886
 H -2.093502 -5.322694 0.487868
 H -0.510835 -5.470260 1.290785

(XXI-re)₁

E0+ZPE = -2491.287957
 E298 = -2491.236752
 H298 = -2491.235808
 G298 = -2491.368680
 NImag = 1, (-204.7490)
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 C -2.914181 2.685616 0.230668
 C -2.168541 3.646005 0.994589
 C -2.507883 5.023473 0.909875
 C -3.518352 5.455499 0.082553
 C -4.226297 4.518388 -0.706003
 C -1.085774 3.205880 1.801204
 C -0.717326 1.883859 1.819732
 C -1.455836 0.943228 1.068786
 C -2.579219 1.286746 0.330608
 C -3.357652 0.227828 -0.370061
 C -4.778173 0.064240 -0.194177
 C -5.484698 -0.891049 -0.999627
 C -4.763110 -1.682663 -1.932085
 C -3.396721 -1.584822 -2.023937
 C -2.699578 -0.651603 -1.221008
 C -6.887952 -1.043021 -0.836121
 C -7.575930 -0.310637 0.103618
 C -6.877664 0.602927 0.927764
 C -5.519976 0.786812 0.782452
 O -1.325833 -0.592212 -1.364268
 P -0.260809 -1.061859 -0.133753
 N -0.448067 -2.743560 0.101759
 C 0.510032 -3.549122 -0.823421

C 1.905339 -3.666630 -0.176562
 O -1.057036 -0.387522 1.150905
 Pd 1.850218 -0.023499 -0.496147
 C 1.189676 1.002275 -2.340050
 C 1.002249 2.172676 -1.557200
 C 1.972029 3.074082 -1.102108
 C 3.336731 2.987385 -1.382473
 C 4.319936 3.907050 -0.712437
 N 3.060098 0.049499 1.294049
 C 4.009978 0.819805 0.751680
 O 4.958963 1.421293 1.277626
 N 3.762356 0.863927 -0.686632
 C 4.868163 0.168966 -1.452077
 C 4.419837 -0.107695 -2.897283
 C -1.327453 -3.489541 1.129725
 C -0.461591 -4.425021 2.007173
 C -2.043736 -2.574448 2.153461
 C -2.475141 -4.268019 0.435185
 C 0.002681 -4.963298 -1.190289
 C 0.663355 -2.867227 -2.211166
 C 3.097407 -0.324354 2.724322
 C 4.401111 -1.086846 3.048818
 C 3.004217 0.937688 3.611135
 C 1.902037 -1.238988 3.017859
 C 6.135360 1.056559 -1.493961
 C 5.242451 -1.183719 -0.804623
 H 5.233013 -0.601774 -3.441696
 H 3.545825 -0.765905 -2.925341
 H 4.180475 0.812004 -3.441880
 H 6.933647 0.520000 -2.021441
 H 5.951282 1.990754 -2.033913
 H 6.469189 1.297042 -0.484239
 H 6.002618 -1.683784 -1.416676
 H 5.652646 -1.045666 0.198781
 H 4.371566 -1.842213 -0.735969
 H 2.996326 0.660175 4.672960
 H 3.853218 1.596958 3.420409
 H 2.082955 1.492577 3.398647
 H 4.418363 -1.387262 4.104099
 H 4.476244 -1.992493 2.435766
 H 5.271420 -0.456294 2.851634
 H 1.892600 -1.526682 4.076052
 H 0.957556 -0.737355 2.788580
 H 1.955673 -2.151501 2.415405
 H 2.061897 0.937411 -2.979893
 H -0.007755 2.337938 -1.186200
 H 3.641665 2.543252 -2.320503
 H 3.798680 4.707147 -0.175095
 H 4.918416 3.352725 0.019837
 H 1.658981 3.785822 -0.340459
 H 0.295979 0.535241 -2.741258
 H 5.004712 4.360653 -1.439142
 H 0.130910 1.537334 2.397221
 H -0.531833 3.935445 2.386241
 H -1.938996 5.733410 1.505484
 H -5.004898 4.862609 -1.381269

H -4.480782 2.474233 -1.254875
 H -3.763887 6.512002 0.021216
 H -5.305798 -2.388164 -2.556250
 H -5.001238 1.483941 1.430159
 H -7.407000 -1.763525 -1.463868
 H -8.647835 -0.440255 0.223882
 H -7.416398 1.162210 1.687816
 H -2.827630 -2.200179 -2.712750
 H 2.595694 -4.166144 -0.867261
 H 2.312249 -2.676844 0.050220
 H 1.882823 -4.245372 0.749484
 H 1.247072 -3.533116 -2.855823
 H -0.307876 -2.702213 -2.685272
 H 1.198469 -1.915580 -2.174719
 H 0.772342 -5.421304 -1.820267
 H -0.146951 -5.632142 -0.345243
 H -0.917752 -4.922092 -1.778283
 H -1.115719 -4.935193 2.723018
 H 0.073598 -5.197844 1.458155
 H 0.268587 -3.843047 2.577560
 H -2.584525 -3.240134 2.834297
 H -1.350208 -1.982110 2.749053
 H -2.775093 -1.910207 1.692987
 H -3.185165 -4.605190 1.198725
 H -3.014903 -3.612310 -0.253313
 H -2.153524 -5.152616 -0.109335

(XXI-re)₂

E0 = -2492.1914878
 E0+ZPE = -2491.288222
 E298 = -2491.236619
 H298 = -2491.235675
 G298 = -2491.369625
 NImag = 1, (-209.3265)
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 C -4.778238 0.207614 -0.247152
 C -5.527281 -0.664766 -1.105739
 C -6.942891 -0.711210 -0.996725
 C -7.607445 0.045561 -0.059351
 C -6.871456 0.877741 0.816088
 C -4.834056 -1.481123 -2.037962
 C -3.463016 -1.492433 -2.072254
 C -2.720537 -0.653479 -1.206600
 C -3.341819 0.261371 -0.362885
 C -2.525113 1.240206 0.406543
 C -2.753752 2.662598 0.341136
 C -1.983303 3.539061 1.178312
 C -0.980508 2.995231 2.024514
 C -0.709547 1.649593 2.014143
 C -1.473493 0.794110 1.191724
 C -2.217295 4.940104 1.125939
 C -3.146283 5.472115 0.262274
 C -3.875553 4.616643 -0.596703
 C -3.686732 3.252533 -0.557850
 O -1.177232 -0.568986 1.227716
 P -0.278128 -1.154985 -0.040427

Pd 1.805286 -0.016486 -0.454474
C 0.908526 2.193935 -1.450494
C 1.916396 3.089300 -1.075301
C 3.253280 2.986132 -1.465817
C 4.296237 3.904407 -0.889811
O -1.345587 -0.728082 -1.300420
N -0.367585 -2.841822 0.232592
C -1.259889 -3.492869 1.323705
C -1.036073 -5.016892 1.497505
C 0.257357 -3.691400 -0.887183
C 1.328165 -4.666184 -0.335254
C -0.830203 -4.425253 -1.706431
C 1.018549 -2.835765 -1.933592
N 3.161834 0.048502 1.232080
C 3.303159 -0.317340 2.655359
C 3.187403 0.941502 3.543172
N 3.699195 0.871293 -0.791676
C 4.741265 0.153357 -1.623809
C 6.012031 1.025750 -1.760793
C 1.037254 1.023852 -2.245196
C 4.052429 0.837663 0.625971
O 5.024217 1.461618 1.079322
C 5.144772 -1.197061 -0.988166
C 4.192972 -0.129391 -3.033265
C -0.919398 -2.940800 2.729732
C -2.753351 -3.269811 1.012794
C 2.178235 -1.295742 2.999334
C 4.660507 -1.009274 2.911110
H 4.961615 -0.638467 -3.626356
H 3.310226 -0.774968 -2.997533
H 3.930480 0.789685 -3.568205
H 6.765662 0.476159 -2.338290
H 5.799669 1.957689 -2.294017
H 6.418555 1.271575 -0.779293
H 5.838967 -1.721420 -1.655734
H 5.643360 -1.051661 -0.026702
H 4.271356 -1.836976 -0.828584
H 3.240703 0.671476 4.605722
H 3.994653 1.640144 3.312569
H 2.231996 1.449503 3.366363
H 4.749751 -1.298512 3.965848
H 4.746738 -1.916517 2.301626
H 5.485779 -0.338614 2.661411
H 2.243640 -1.612919 4.047087
H 1.198374 -0.836446 2.840160
H 2.239650 -2.185190 2.362236
H 1.867401 0.958569 -2.938422
H -0.070436 2.366122 -1.007037
H 3.473206 2.537131 -2.425472
H 3.826465 4.723065 -0.333101
H 4.938594 3.356326 -0.190989
H 1.671405 3.809016 -0.296483
H 0.119193 0.562717 -2.593975
H 4.930963 4.333033 -1.674624
H 0.078214 1.222135 2.622923
H -0.407858 3.663518 2.662146

H -1.632849 5.586491 1.776288
 H -4.588344 5.039876 -1.299142
 H -4.247247 2.614782 -1.230857
 H -3.310771 6.545387 0.226421
 H -5.405036 -2.118092 -2.708827
 H -4.953629 1.593738 1.412060
 H -7.491810 -1.370819 -1.664738
 H -8.689864 -0.003308 0.019546
 H -7.392717 1.455921 1.574234
 H -2.920024 -2.125646 -2.765367
 H 1.362064 -3.520097 -2.717266
 H 0.394692 -2.081942 -2.419012
 H 1.901250 -2.346416 -1.512418
 H -0.347709 -5.069639 -2.450778
 H -1.493422 -5.051596 -1.112558
 H -1.449645 -3.700687 -2.242368
 H 1.962333 -5.005868 -1.161430
 H 1.967525 -4.147750 0.386058
 H 0.921319 -5.558114 0.136216
 H -3.365813 -3.764287 1.776117
 H -3.012243 -2.210995 1.017608
 H -3.027875 -3.687226 0.039789
 H -1.764496 -5.351887 2.242675
 H -1.201831 -5.620372 0.607434
 H -0.045515 -5.239258 1.899197
 H -1.500789 -3.503183 3.469178
 H 0.139460 -3.093672 2.952226
 H -1.155910 -1.889048 2.854624

XXI-*si*

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 E298 = -2491.235168
 H298 = -2491.234224
 G298 = -2491.368055
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 C -1.923820 -3.476555 -1.332568
 C -2.137085 -4.881541 -1.321858
 C -3.038181 -5.455623 -0.455332
 C -3.760099 -4.639635 0.446939
 C -0.948466 -2.891417 -2.183275
 C -0.689208 -1.544521 -2.126305
 C -1.445955 -0.729455 -1.257268
 C -2.483073 -1.212478 -0.475834
 C -3.323932 -0.267313 0.311560
 C -4.762096 -0.254753 0.187888
 C -5.543657 0.578353 1.056352
 C -4.882147 1.402025 2.004407
 C -3.512737 1.457909 2.044286
 C -2.737501 0.657007 1.170662
 C -6.959550 0.580676 0.942199
 C -7.595621 -0.180210 -0.011330
 C -6.828839 -0.970781 -0.898546
 C -5.454814 -1.009179 -0.800877
 O -1.366631 0.778227 1.283482

P -0.280848 1.196049 0.037998
 N -0.365176 2.889773 -0.234204
 C 0.191539 3.741702 0.918321
 C -0.948689 4.366680 1.752729
 O -1.163858 0.634576 -1.250574
 Pd 1.691087 -0.184977 0.330149
 N 3.453834 0.467960 -0.743824
 C 4.249491 -0.445739 -0.184212
 O 5.485076 -0.516474 -0.110714
 C 0.844407 -1.274819 2.056141
 C 1.697858 -0.531428 2.911950
 C 3.062376 -0.725978 3.154866
 C 3.825067 -1.761878 2.613856
 C 5.315435 -1.801631 2.806417
 N 3.377337 -1.465382 0.400302
 C 3.420040 -2.740966 -0.414085
 C 3.311651 -2.455768 -1.929530
 C -1.226659 3.519925 -1.359364
 C -0.765854 3.006308 -2.746480
 C -2.726320 3.232086 -1.136400
 C -1.075996 5.055665 -1.484695
 C 1.005700 2.879724 1.914731
 C 1.179958 4.836025 0.435176
 C 4.750244 -3.488485 -0.156567
 C 2.254537 -3.662260 -0.016640
 C 3.992008 1.592219 -1.535508
 C 4.716247 2.587564 -0.603894
 C 4.969501 1.092988 -2.623307
 C 2.810702 2.279568 -2.227028
 H 3.255731 -3.405922 -2.474462
 H 2.416475 -1.870108 -2.155309
 H 4.182227 -1.906000 -2.296300
 H 4.785302 -4.386674 -0.785324
 H 5.604506 -2.852532 -0.391886
 H 4.832059 -3.809879 0.886334
 H 2.313768 -4.591832 -0.595184
 H 2.290235 -3.942110 1.041710
 H 1.286796 -3.196773 -0.223520
 H 5.324249 1.938625 -3.225931
 H 5.829266 0.591928 -2.174960
 H 4.464416 0.388427 -3.294439
 H 5.107586 3.441488 -1.172091
 H 4.029715 2.971073 0.159900
 H 5.550207 2.090177 -0.101293
 H 3.151212 3.145348 -2.808478
 H 2.307095 1.583894 -2.908303
 H 2.075510 2.616516 -1.492878
 H 1.105807 -2.299946 1.823626
 H 1.260654 0.354945 3.369014
 H 3.332917 -2.700268 2.396108
 H 5.628792 -1.071383 3.560901
 H 5.654361 -2.796861 3.117799
 H 3.592503 0.072842 3.670920
 H -0.219997 -1.086809 2.137917
 H 5.820295 -1.543532 1.868272
 H 0.076618 -1.081249 -2.738615

H -0.385205 -3.530382 -2.858025
 H -1.558397 -5.497644 -2.005895
 H -4.450770 -5.096030 1.150735
 H -4.147142 -2.664183 1.152676
 H -3.186309 -6.531879 -0.451142
 H -5.476278 2.008389 2.683437
 H -4.887355 -1.612727 -1.499123
 H -7.531859 1.210326 1.619449
 H -8.678751 -0.165404 -0.094141
 H -7.327376 -1.550718 -1.670515
 H -2.995063 2.095871 2.751791
 H -1.360649 5.617421 -0.595826
 H -0.070327 5.348995 -1.789552
 H -1.756318 5.367553 -2.283541
 H -0.895736 1.936572 -2.878173
 H -1.355269 3.512847 -3.519413
 H 0.285845 3.255233 -2.911169
 H -3.314369 3.723534 -1.920538
 H -2.949244 2.166817 -1.174551
 H -3.065138 3.620339 -0.170922
 H 1.824714 4.460508 -0.362698
 H 0.691771 5.746316 0.092208
 H 1.824373 5.123433 1.272729
 H -0.517555 4.994227 2.542202
 H -1.625522 4.991536 1.170064
 H -1.543087 3.584862 2.231705
 H 0.400070 2.106424 2.392249
 H 1.885162 2.418124 1.458378
 H 1.352150 3.543949 2.713738

(XXI-si)₁

E0 = -2492.1884798
 E0+ZPE = -2491.284761
 E298 = -2491.233403
 H298 = -2491.232459
 G298 = -2491.365503
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 C 2.593343 2.729768 -0.411532
 C 1.809774 3.555793 -1.286069
 C 2.000232 4.964038 -1.275495
 C 2.899094 5.551852 -0.416010
 C 3.641315 4.746289 0.479162
 C 0.838422 2.954872 -2.129415
 C 0.602959 1.604061 -2.070822
 C 1.375218 0.797001 -1.207022
 C 2.414103 1.298736 -0.435196
 C 3.284892 0.378204 0.351611
 C 4.720792 0.380199 0.217818
 C 5.513814 -0.452185 1.078119
 C 4.867613 -1.291688 2.023985
 C 3.498167 -1.356041 2.078117
 C 2.717816 -0.545365 1.220313
 C 6.929194 -0.440684 0.955385
 C 7.552901 0.331082 0.002498
 C 6.774564 1.119891 -0.876433

C 5.400927 1.145669 -0.771031
 O 1.347922 -0.661804 1.331639
 P 0.318452 -1.207793 0.103344
 N 0.635809 -2.874812 -0.145092
 C -0.104261 -3.825856 0.803438
 C -1.161083 -4.675252 0.064007
 O 1.100034 -0.568052 -1.214963
 Pd -1.748641 0.053289 0.426182
 N -3.345657 -0.387380 -0.966563
 C -4.215360 0.436725 -0.378695
 O -5.449013 0.522705 -0.467821
 C -1.152683 0.828368 2.417053
 C -2.115881 -0.012484 3.029893
 C -3.501578 0.167616 3.111569
 C -4.188529 1.284369 2.637213
 C -5.691336 1.315048 2.625890
 N -3.436444 1.328496 0.480709
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 C -3.123228 2.691995 -1.634738
 C 1.538157 -3.415347 -1.290681
 C 2.931427 -2.741152 -1.312330
 C 1.882887 -4.922934 -1.186487
 C 0.821066 -3.214302 -2.641805
 C 0.887127 -4.715943 1.603514
 C -0.888997 -3.051564 1.889850
 C -4.718050 3.455495 0.135440
 C -2.245379 3.528122 0.548528
 C -3.766214 -1.363734 -1.991081
 C -4.630833 -2.463879 -1.338576
 C -4.565284 -0.675391 -3.120540
 C -2.501977 -1.977577 -2.598587
 H -2.998915 3.718127 -2.001412
 H -2.218563 2.126794 -1.869345
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 H -4.680785 4.441348 -0.344150
 H -5.550659 2.886824 -0.280920
 H -4.900847 3.613649 1.202691
 H -2.226126 4.540098 0.127369
 H -2.388378 3.633584 1.629431
 H -1.269804 3.067880 0.367254
 H -4.840530 -1.409300 -3.888338
 H -5.474104 -0.215951 -2.727724
 H -3.957561 0.102048 -3.598277
 H -4.920695 -3.223706 -2.075795
 H -4.077262 -2.960231 -0.532721
 H -5.536730 -2.024578 -0.912436
 H -2.759724 -2.726307 -3.357299
 H -1.887992 -1.203529 -3.073557
 H -1.894990 -2.460219 -1.829779
 H -1.375504 1.882932 2.307891
 H -1.746491 -0.964224 3.407728
 H -3.675527 2.236645 2.629685
 H -6.100307 0.486593 3.215108
 H -6.078454 2.258417 3.028767
 H -4.093410 -0.690764 3.425621
 H -0.108152 0.605998 2.605036

H -6.059303 1.203073 1.599125
 H -0.159134 1.128404 -2.678209
 H 0.258159 3.583808 -2.799113
 H 1.405958 5.571172 -1.954190
 H 4.330262 5.212687 1.178116
 H 4.064671 2.777160 1.180423
 H 3.029968 6.630354 -0.411665
 H 5.473956 -1.902847 2.687795
 H 4.823306 1.748761 -1.461385
 H 7.511408 -1.068703 1.625696
 H 8.635669 0.326467 -0.086130
 H 7.264094 1.708716 -1.647435
 H 2.984282 -2.010195 2.775024
 H -0.091535 -3.815733 -2.694402
 H 0.556989 -2.170517 -2.809056
 H 1.480568 -3.530763 -3.458858
 H 3.408202 -2.806855 -0.330566
 H 3.564006 -3.283171 -2.024595
 H 2.906149 -1.701086 -1.622023
 H 2.384480 -5.186912 -2.123060
 H 2.588254 -5.129416 -0.379391
 H 1.027528 -5.589128 -1.092751
 H -1.689690 -2.431348 1.482925
 H -1.356571 -3.791979 2.547386
 H -0.232399 -2.431998 2.509068
 H -1.597832 -5.400658 0.761115
 H -1.970049 -4.039611 -0.305692
 H -0.765505 -5.233216 -0.784166
 H 1.218880 -5.601802 1.066211
 H 1.767687 -4.136847 1.899409
 H 0.396160 -5.068535 2.516951

(XXI-si)₂

E0 = -2492.1848684
 E0+ZPE = -2491.281057
 E298 = -2491.229741
 H298 = -2491.228797
 G298 = -2491.361812
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 C -5.488770 -0.620869 -1.009830
 C -6.898263 -0.685534 -0.842804
 C -7.539302 0.100439 0.086608
 C -6.785387 0.981855 0.896490
 C -4.819192 -1.469375 -1.930695
 C -3.449832 -1.456131 -2.025184
 C -2.695141 -0.556812 -1.235797
 C -3.294796 0.374874 -0.398670
 C -2.453784 1.389052 0.295959
 C -2.715145 2.803175 0.194110
 C -1.943216 3.723052 0.980265
 C -0.906836 3.226802 1.813821
 C -0.599625 1.889121 1.827725
 C -1.357242 0.989145 1.046459
 C -2.212071 5.115740 0.893222

C -3.179402 5.599633 0.043140
 C -3.913518 4.700802 -0.765670
 C -3.689961 3.343299 -0.691369
 O -1.015885 -0.354222 1.138780
 P -0.300655 -1.125597 -0.135195
 Pd 1.833251 -0.041507 -0.485713
 C 1.668467 0.154392 -2.688397
 C 2.703379 -0.801695 -2.847702
 C 4.086781 -0.630682 -2.703120
 C 4.719793 0.575651 -2.422050
 C 6.188397 0.624883 -2.111524
 O -1.319289 -0.589274 -1.373957
 N -0.662742 -2.773657 0.186571
 C -1.590305 -3.381661 1.262638
 C -0.760758 -4.226586 2.257631
 C 0.188560 -3.701594 -0.724221
 C 0.116564 -3.202916 -2.188091
 C 1.652444 -3.723523 -0.234273
 C -0.282695 -5.171679 -0.843743
 N 3.550191 1.190826 -0.520119
 C 3.440816 2.690847 -0.344908
 C 4.829264 3.345402 -0.545495
 N 3.109895 -0.115607 1.254701
 C 3.292556 -0.824511 2.538663
 C 3.811807 0.141582 3.626827
 C 4.104733 0.563512 0.676017
 O 5.293697 0.702420 0.999439
 C 1.933316 -1.376722 2.984644
 C 4.291105 -1.988925 2.357072
 C -2.329627 -2.353176 2.152548
 C -2.729223 -4.213241 0.612097
 C 2.463333 3.269461 -1.381604
 C 2.934025 3.074873 1.062757
 H 2.808495 4.162976 1.118969
 H 1.970551 2.606409 1.270765
 H 3.645190 2.775933 1.837342
 H 4.745441 4.424086 -0.364946
 H 5.556780 2.922580 0.148916
 H 5.198096 3.209051 -1.566691
 H 2.393622 4.355671 -1.251614
 H 2.797580 3.089239 -2.409334
 H 1.459866 2.848709 -1.261474
 H 3.913147 -0.383789 4.584848
 H 4.783697 0.551512 3.344701
 H 3.109313 0.971536 3.768034
 H 4.425490 -2.534730 3.299951
 H 3.926183 -2.694394 1.602137
 H 5.261200 -1.604119 2.032911
 H 2.040355 -1.942150 3.918306
 H 1.215465 -0.567428 3.156157
 H 1.514891 -2.042139 2.225191
 H 1.901812 1.203774 -2.822644
 H 2.387457 -1.830101 -3.012265
 H 4.250410 1.494072 -2.747254
 H 6.671722 -0.325202 -2.365184
 H 6.690043 1.432895 -2.656925

H 4.688219 -1.536938 -2.651871
 H 0.669829 -0.120636 -3.016757
 H 6.335197 0.794534 -1.037837
 H 0.211852 1.493740 2.427815
 H -0.335623 3.925315 2.419434
 H -1.623671 5.795020 1.505471
 H -4.657509 5.084857 -1.458315
 H -4.254380 2.672800 -1.328478
 H -3.370783 6.667211 -0.020102
 H -5.405586 -2.148671 -2.544306
 H -4.858728 1.755571 1.383757
 H -7.460775 -1.382708 -1.459363
 H -8.616858 0.037507 0.209859
 H -7.287648 1.583605 1.649067
 H -2.921480 -2.110799 -2.709565
 H -1.654685 -1.738195 2.744214
 H -2.999547 -1.705135 1.585474
 H -2.943248 -2.936482 2.847338
 H -2.422624 -5.197140 0.266006
 H -3.519451 -4.374999 1.352965
 H -3.169359 -3.664465 -0.225622
 H -1.439499 -4.709794 2.970248
 H -0.165439 -5.012056 1.794727
 H -0.082227 -3.583024 2.824511
 H 1.719992 -4.132014 0.778055
 H 2.260766 -4.354547 -0.893444
 H 2.095987 -2.724098 -0.226258
 H 0.459083 -5.679165 -1.469606
 H -0.328936 -5.722983 0.093282
 H -1.242526 -5.256707 -1.356402
 H -0.912240 -3.249753 -2.555999
 H 0.472856 -2.184682 -2.323861
 H 0.733591 -3.853297 -2.818438

XXII-*re*

E0 = -2525.5233177
 E0+ZPE = -2524.701142
 E298 = -2524.653034
 H298 = -2524.652090
 G298 = -2524.782435
 NImag = 1, (-197.1867)
 C -2.566850 3.772888 -1.827126
 C -1.488980 2.983721 -1.432904
 C -0.779022 3.274148 -0.255197
 C -1.117365 4.416447 0.499295
 C -2.193912 5.202618 0.069753
 C -2.928344 4.888948 -1.071152
 C -0.320656 4.847509 1.718980
 C 0.720545 3.813226 2.166013
 C 1.355992 3.142141 0.948563
 N 0.308862 2.448296 0.164395
 P 0.284635 0.780376 -0.114509
 Pd -1.724139 -0.347555 -0.465436
 C -0.995354 -1.345769 -2.304743
 C -0.746946 -2.493675 -1.506407
 C -1.668665 -3.445999 -1.052179

C -3.031749 -3.442019 -1.349379
C -3.969844 -4.411247 -0.685057
O 1.369080 0.477482 -1.360310
C 2.699649 0.860136 -1.251442
C 3.125740 1.949956 -2.043600
C 4.429771 2.372990 -1.970047
C 5.342848 1.755890 -1.073952
C 4.905859 0.647029 -0.272888
C 3.559181 0.158772 -0.416833
C 6.674127 2.234002 -0.937888
C 7.541104 1.670749 -0.030306
C 7.102525 0.603813 0.788892
C 5.823478 0.105596 0.670819
C 3.043518 -1.029601 0.320658
C 1.899849 -0.902720 1.095582
C 1.368986 -1.963798 1.860733
C 1.986014 -3.190245 1.832868
C 3.119980 -3.413948 1.007278
C 3.647670 -2.332921 0.222662
C 4.729334 -2.616036 -0.658161
C 5.280936 -3.876492 -0.727950
C 4.785209 -4.928093 0.078363
C 3.723796 -4.697726 0.922527
O 1.249334 0.327378 1.170239
N -2.927835 -0.457967 1.301664
C -3.826375 -1.299715 0.778986
O -4.720437 -1.966882 1.318816
N -3.584561 -1.333464 -0.661369
C -4.720571 -0.688189 -1.422900
C -5.944488 -1.634231 -1.455113
C -2.955958 -0.064723 2.724924
C -2.687185 -1.297619 3.615432
C -1.863259 0.985487 2.957197
C -4.324275 0.554104 3.087240
C -5.148014 0.649851 -0.777765
C -4.285804 -0.399762 -2.870001
H -5.120992 0.051661 -3.418143
H -3.443705 0.299012 -2.900181
H -4.002439 -1.311153 -3.407838
H -6.770548 -1.138755 -1.980048
H -5.718446 -2.561477 -1.991707
H -6.261531 -1.886999 -0.442718
H -5.925344 1.118440 -1.393318
H -5.557704 0.495985 0.223785
H -4.303592 1.341859 -0.704954
H -2.667676 -1.012632 4.675181
H -3.464454 -2.050269 3.464536
H -1.718214 -1.745578 3.364191
H -4.340709 0.854360 4.142483
H -4.513223 1.444792 2.476886
H -5.127878 -0.165870 2.916208
H -1.883012 1.331022 3.997975
H -0.869871 0.573268 2.754018
H -2.019726 1.849753 2.302240
H -1.869775 -1.334695 -2.944508
H 0.267503 -2.596398 -1.121979

H -3.352377 -3.014658 -2.290036
 H -3.411506 -5.184801 -0.146145
 H -4.597373 -3.887769 0.045524
 H -1.323404 -4.134325 -0.282725
 H -0.128989 -0.832626 -2.709365
 H -4.628056 -4.897291 -1.415179
 H 0.480430 -1.781582 2.454952
 H 1.595356 -4.012727 2.426337
 H 3.318144 -5.501330 1.532476
 H 6.101747 -4.065914 -1.414280
 H 5.115410 -1.826074 -1.291574
 H 5.234085 -5.915564 0.018051
 H 4.772424 3.203694 -2.581713
 H 5.501841 -0.705674 1.313433
 H 6.991047 3.066968 -1.560998
 H 8.554627 2.049234 0.068482
 H 7.779697 0.175626 1.522916
 H 2.405270 2.425398 -2.701196
 H -1.188928 2.142128 -2.049154
 H -3.762187 5.515278 -1.374788
 H -2.457207 6.082134 0.654132
 H -3.106533 3.524515 -2.736657
 H -1.004185 5.080355 2.544827
 H 0.189156 5.791669 1.477103
 H 1.496941 4.293490 2.773475
 H 0.255972 3.037683 2.784364
 H 2.109307 2.417389 1.248762
 H 1.837438 3.885503 0.299116

(XXII-re)₁

E0 = -2525.5208528
 E0+ZPE = -2524.698378
 E298 = -2524.650547
 H298 = -2524.649603
 G298 = -2524.778584
 NImag = 1, (-200.0198)
 C -3.778033 -3.382710 1.583090
 C -2.575353 -2.702632 1.419746
 C -1.599561 -3.182031 0.530369
 C -1.816707 -4.391857 -0.162951
 C -3.031241 -5.062488 0.032346
 C -4.014906 -4.567760 0.883684
 C -0.763905 -5.022316 -1.060808
 C 0.467473 -4.133562 -1.282360
 C 0.780507 -3.358802 -0.003466
 N -0.355704 -2.482277 0.357012
 P -0.170237 -0.840471 -0.000056
 Pd 2.010913 -0.128424 -0.424286
 C 1.448098 0.933802 -2.284866
 C 1.488057 2.132966 -1.525450
 C 2.612778 2.869827 -1.130418
 C 3.931572 2.560127 -1.465208
 C 5.080347 3.319006 -0.861647
 O -1.209660 -0.444764 -1.250555
 C -2.591459 -0.357986 -1.134994
 C -3.345675 -1.276350 -1.899840

C -4.715192 -1.243531 -1.846218
 C -5.384919 -0.323738 -0.995822
 C -4.615998 0.614323 -0.228867
 C -3.180870 0.633161 -0.363133
 C -6.800004 -0.335779 -0.872209
 C -7.444528 0.517088 -0.005874
 C -6.688349 1.415489 0.782375
 C -5.315413 1.464099 0.673294
 C -2.328576 1.639730 0.328228
 C -1.288282 1.213948 1.141187
 C -0.489681 2.102124 1.894422
 C -0.712950 3.453876 1.804821
 C -1.702523 3.968622 0.925227
 C -2.509886 3.059710 0.160881
 C -3.431780 3.612352 -0.772367
 C -3.574708 4.975428 -0.911955
 C -2.807313 5.866804 -0.125757
 C -1.888607 5.368995 0.768950
 O -1.020119 -0.150411 1.261488
 N 3.278374 -0.261242 1.294266
 C 4.317934 0.353670 0.716374
 O 5.351979 0.829182 1.206154
 N 4.038235 0.399548 -0.715780
 C 4.971111 -0.505892 -1.486427
 C 6.370884 0.144080 -1.594855
 C 3.252707 -0.566161 2.740931
 C 3.283086 0.746913 3.553643
 C 1.965586 -1.336225 3.059972
 C 4.464350 -1.444439 3.124615
 C 5.125093 -1.884685 -0.803881
 C 4.422322 -0.738129 -2.904117
 H 5.108709 -1.386703 -3.460718
 H 3.442627 -1.225912 -2.873960
 H 4.328781 0.194864 -3.470391
 H 7.042510 -0.529765 -2.141119
 H 6.328929 1.089952 -2.144331
 H 6.783304 0.337954 -0.603905
 H 5.756220 -2.531133 -1.425229
 H 5.595623 -1.795193 0.178576
 H 4.154133 -2.374343 -0.677116
 H 3.231562 0.536784 4.629564
 H 4.201122 1.300712 3.344122
 H 2.429117 1.381083 3.287695
 H 4.439471 -1.683331 4.195144
 H 4.443753 -2.387472 2.565801
 H 5.399941 -0.926063 2.902988
 H 1.925307 -1.579470 4.128274
 H 1.076069 -0.750567 2.810765
 H 1.923763 -2.274955 2.497108
 H 2.272774 0.707923 -2.950485
 H 0.536053 2.468587 -1.115291
 H 4.120124 2.044659 -2.397427
 H 4.721747 4.199558 -0.317309
 H 5.617120 2.685187 -0.146246
 H 2.453007 3.637398 -0.375449
 H 0.476274 0.604913 -2.638290

H 5.791599 3.645895 -1.629850
 H 0.284949 1.692199 2.532267
 H -0.113479 4.147333 2.388847
 H -1.276510 6.041816 1.364828
 H -4.280507 5.369553 -1.638007
 H -4.020995 2.945200 -1.390245
 H -2.935339 6.939476 -0.240946
 H -5.303962 -1.943645 -2.433082
 H -4.753797 2.152524 1.293826
 H -7.365104 -1.047035 -1.470028
 H -8.526949 0.493924 0.084474
 H -7.193914 2.071292 1.486051
 H -2.814830 -1.996687 -2.512732
 H -2.380468 -1.797844 1.979155
 H -4.949341 -5.107176 1.011108
 H -3.199098 -5.996252 -0.501210
 H -4.523577 -2.990553 2.269063
 H -1.213287 -5.300200 -2.022640
 H -0.445654 -5.967525 -0.597760
 H 1.329395 -4.743142 -1.578626
 H 0.289054 -3.412473 -2.089909
 H 1.675500 -2.740272 -0.114328
 H 0.953007 -4.045159 0.835812

(XXII-re)₂

E0 = -2525.5177011
 E0+ZPE = -2524.695425
 E298 = -2524.647469
 H298 = -2524.646525
 G298 = -2524.775887
 NImag = 1, (-193.2172)
 C 3.188521 3.874579 1.417277
 C 2.441611 2.976572 0.661978
 C 1.135233 3.291921 0.252924
 C 0.595369 4.555745 0.577212
 C 1.375198 5.444874 1.328411
 C 2.656491 5.118359 1.760520
 C -0.771546 5.017356 0.098318
 C -1.585755 3.920030 -0.595639
 C -0.658016 3.018207 -1.403978
 N 0.347093 2.379734 -0.524420
 P 0.193184 0.695875 -0.404220
 Pd -1.970546 -0.154331 -0.584094
 C -1.482417 -1.426097 -2.323084
 C -1.420003 -2.513592 -1.410699
 C -2.486192 -3.237374 -0.861094
 C -3.831913 -3.023075 -1.161872
 C -4.916463 -3.738976 -0.406534
 O 1.178562 0.009416 -1.576042
 C 2.556505 0.168955 -1.557150
 C 3.127859 0.972113 -2.569163
 C 4.486675 1.161993 -2.597869
 C 5.319362 0.597059 -1.595452
 C 4.734435 -0.218869 -0.568695
 C 3.317664 -0.479179 -0.594288
 C 6.717995 0.847459 -1.577309

C 7.515876 0.344764 -0.575682
 C 6.937606 -0.426061 0.460072
 C 5.587418 -0.700375 0.464060
 C 2.643728 -1.369301 0.393629
 C 1.580030 -0.885196 1.142300
 C 0.949666 -1.641362 2.154330
 C 1.363860 -2.927896 2.395341
 C 2.384940 -3.521091 1.606974
 C 3.024095 -2.746041 0.581200
 C 3.984902 -3.396616 -0.243125
 C 4.319547 -4.717771 -0.041765
 C 3.716818 -5.465736 0.997002
 C 2.767108 -4.876366 1.798871
 O 1.120743 0.417785 0.940004
 N -3.145391 0.139942 1.190428
 C -4.183022 -0.582901 0.750974
 O -5.160699 -1.046009 1.356471
 N -3.988078 -0.784984 -0.680641
 C -5.002779 -0.014167 -1.491467
 C -6.379638 -0.716373 -1.423778
 C -3.050802 0.580799 2.599640
 C -2.949011 -0.650760 3.526906
 C -1.799735 1.451621 2.765296
 C -4.289434 1.420261 2.985026
 C -5.163264 1.433532 -0.973551
 C -4.558734 0.053105 -2.962812
 H -5.310524 0.596111 -3.547173
 H -3.603920 0.578644 -3.067691
 H -4.459285 -0.941738 -3.410350
 H -7.114675 -0.129120 -1.987960
 H -6.337733 -1.715128 -1.870238
 H -6.712713 -0.812767 -0.389734
 H -5.848965 1.982887 -1.629681
 H -5.575156 1.452098 0.038848
 H -4.202296 1.957727 -0.963275
 H -2.841587 -0.338844 4.573596
 H -3.844057 -1.269796 3.432110
 H -2.078970 -1.261660 3.259162
 H -4.207459 1.766212 4.023009
 H -4.367662 2.302426 2.338657
 H -5.201816 0.828828 2.882538
 H -1.695820 1.771734 3.808684
 H -0.891874 0.912199 2.482610
 H -1.863867 2.351208 2.144012
 H -2.357078 -1.326822 -2.954948
 H -0.430616 -2.751203 -1.020103
 H -4.086338 -2.636841 -2.139898
 H -4.499340 -4.560728 0.186180
 H -5.409339 -3.047732 0.287592
 H -2.255694 -3.894548 -0.024502
 H -0.549861 -1.116314 -2.782820
 H -5.677395 -4.144575 -1.083693
 H 0.151131 -1.183335 2.726052
 H 0.893091 -3.515893 3.178814
 H 2.280300 -5.444288 2.588071
 H 5.050214 -5.191436 -0.691710

H 4.449060 -2.842735 -1.050597
 H 3.995307 -6.504751 1.149043
 H 4.938939 1.771563 -3.375868
 H 5.161592 -1.283401 1.272171
 H 7.144272 1.458661 -2.369228
 H 8.583035 0.548086 -0.569662
 H 7.563506 -0.801419 1.265072
 H 2.471524 1.419192 -3.308426
 H 2.875295 2.026088 0.387811
 H 3.234879 5.826515 2.347190
 H 0.953461 6.417376 1.575432
 H 4.194086 3.600743 1.724481
 H -0.623070 5.853165 -0.600890
 H -1.337200 5.432395 0.941760
 H -2.114506 3.297999 0.134290
 H -2.344068 4.363808 -1.251894
 H -0.124447 3.590977 -2.175012
 H -1.227962 2.232372 -1.910786

(XXII-re)₃

E0 = -2525.5221786
 E0+ZPE = -2524.699716
 E298 = -2524.651705
 H298 = -2524.650761
 G298 = -2524.780574
 NImag = 1, (-195.3208)
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 C -1.154796 2.973610 -1.532216
 C -0.663160 3.224013 -0.240724
 C -1.131604 4.346469 0.473972
 C -2.107987 5.159286 -0.103975
 C -2.642634 4.874410 -1.361788
 C -0.476727 4.673108 1.792466
 C 1.025608 4.394016 1.649534
 C 1.262934 2.910195 1.369790
 N 0.309383 2.367893 0.353842
 P 0.276296 0.714485 -0.031922
 Pd -1.749485 -0.349944 -0.425536
 C -1.043530 -1.350407 -2.272263
 C -0.852438 -2.520521 -1.490793
 C -1.818213 -3.440028 -1.060194
 C -3.177328 -3.372157 -1.367341
 C -4.161526 -4.311884 -0.727990
 O 1.348260 0.484597 -1.303845
 C 2.676513 0.873787 -1.177240
 C 3.088416 2.014155 -1.902561
 C 4.388133 2.445727 -1.805919
 C 5.310425 1.784284 -0.951752
 C 4.887003 0.624943 -0.217613
 C 3.544343 0.133422 -0.385956
 C 6.637473 2.266710 -0.791182
 C 7.513274 1.658407 0.077986
 C 7.088052 0.539830 0.832789
 C 5.813411 0.037139 0.689174
 C 3.040858 -1.096193 0.290209
 C 1.902660 -1.017959 1.079782

C 1.387084 -2.119561 1.796610
 C 2.013501 -3.338045 1.702603
 C 3.141667 -3.510987 0.857064
 C 3.654015 -2.387910 0.123028
 C 4.731310 -2.617239 -0.778530
 C 5.293155 -3.867674 -0.914731
 C 4.812431 -4.962308 -0.158131
 C 3.755594 -4.783587 0.704145
 O 1.244432 0.201225 1.221347
 N -2.960716 -0.434032 1.335713
 C -3.889689 -1.233508 0.799126
 O -4.807185 -1.876741 1.328438
 N -3.647478 -1.253075 -0.641362
 C -4.748324 -0.542658 -1.395099
 C -6.017131 -1.426481 -1.440860
 C -2.955121 -0.086073 2.770424
 C -2.718931 -1.355457 3.617922
 C -1.821110 0.915490 3.021483
 C -4.295389 0.570137 3.169916
 C -5.109039 0.806704 -0.732682
 C -4.295043 -0.255820 -2.836816
 H -5.103654 0.246971 -3.380056
 H -3.417820 0.398749 -2.853593
 H -4.058149 -1.172736 -3.387701
 H -6.816705 -0.884812 -1.961005
 H -5.834821 -2.356977 -1.988281
 H -6.348978 -1.676082 -0.432303
 H -5.863801 1.320231 -1.340367
 H -5.523094 0.661185 0.268443
 H -4.231416 1.455552 -0.654595
 H -2.677865 -1.105887 4.685925
 H -3.523096 -2.076202 3.452569
 H -1.768535 -1.827240 3.340109
 H -4.289344 0.836631 4.234338
 H -4.458149 1.486220 2.590339
 H -5.126598 -0.114097 2.984891
 H -1.818735 1.231968 4.071521
 H -0.845972 0.471223 2.797931
 H -1.949928 1.802296 2.391119
 H -1.909696 -1.292057 -2.921195
 H 0.152939 -2.672386 -1.098450
 H -3.471720 -2.912231 -2.301207
 H -3.641443 -5.128477 -0.214697
 H -4.759400 -3.778961 0.020667
 H -1.509550 -4.156224 -0.300615
 H -0.152372 -0.866296 -2.659000
 H -4.846041 -4.742119 -1.468688
 H 0.503652 -1.973271 2.408557
 H 1.635099 -4.192082 2.258220
 H 3.361736 -5.620061 1.276466
 H 6.110469 -4.015531 -1.615296
 H 5.105990 -1.793155 -1.374308
 H 5.269269 -5.941524 -0.270608
 H 4.720016 3.316452 -2.365676
 H 5.502235 -0.814497 1.282691
 H 6.943800 3.138896 -1.363927

H 8.523431 2.040303 0.196212
 H 7.772067 0.074999 1.537584
 H 2.360873 2.523076 -2.526338
 H -0.747144 2.159003 -2.121719
 H -3.411578 5.512921 -1.786819
 H -2.453649 6.030514 0.448140
 H -2.533256 3.561561 -3.070795
 H 1.574095 4.656137 2.561787
 H 1.430759 5.009139 0.836855
 H 2.287693 2.746878 1.023493
 H 1.134584 2.343487 2.295382
 H -0.663031 5.718439 2.062411
 H -0.886215 4.053838 2.603835

XXII-si

E0 = -2525.519444
 E0+ZPE = -2524.697433
 E298 = -2524.649226
 H298 = -2524.648282
 G298 = -2524.779754
 NImag = 1, (-184.5031)
 C 4.581471 -2.747287 -0.600673
 C 3.518660 -2.408884 0.283209
 C 2.955497 -3.456069 1.088499
 C 3.506496 -4.764093 1.017442
 C 4.550012 -5.049331 0.167615
 C 5.081124 -4.029945 -0.657215
 C 2.967619 -1.081181 0.365324
 C 1.831981 -0.900092 1.140712
 C 1.273092 -1.924385 1.935195
 C 1.842356 -3.173922 1.924298
 C 3.539189 0.079488 -0.376161
 C 2.719535 0.820313 -1.216936
 C 3.201861 1.889293 -2.005436
 C 4.523455 2.251423 -1.922783
 C 5.400361 1.592250 -1.020654
 C 4.906341 0.505369 -0.222525
 C 6.751665 2.007600 -0.875939
 C 7.585371 1.404857 0.037394
 C 7.091650 0.360480 0.854200
 C 5.791462 -0.077262 0.727866
 O 1.375144 0.496995 -1.339832
 P 0.290105 0.827160 -0.100985
 Pd -1.642913 -0.472587 -0.384326
 C -1.087871 -1.154136 -2.428010
 C -2.109394 -0.325170 -2.953469
 C -3.492436 -0.552691 -2.978690
 C -4.118592 -1.713611 -2.531786
 C -5.615497 -1.803255 -2.445691
 O 1.223676 0.351313 1.195732
 N 0.381237 2.496885 0.186013
 C -0.651089 3.380108 -0.252070
 C -0.932488 4.548277 0.487176
 C -0.129364 4.942922 1.715000
 C 0.852717 3.858363 2.177752
 C 1.458922 3.143355 0.970797

C -1.959482 5.387603 0.038673
 C -2.702653 5.100647 -1.103886
 C -2.398433 3.956652 -1.842932
 C -1.367910 3.116736 -1.429842
 N -3.159531 -0.132153 1.087165
 C -3.543332 0.837301 2.133754
 C -4.251058 0.119913 3.304647
 N -3.268785 -1.820372 -0.385924
 C -3.109295 -3.220807 0.162018
 C -4.437536 -3.998110 -0.002566
 C -4.032377 -0.980531 0.535982
 O -5.253726 -1.113979 0.693514
 C -2.002317 -3.966056 -0.602899
 C -2.732764 -3.215232 1.661254
 C -2.266897 1.498439 2.667059
 C -4.474296 1.909273 1.528384
 H -2.556546 -4.244907 1.994955
 H -1.822998 -2.633512 1.834131
 H -3.533381 -2.792708 2.273910
 H -4.329123 -4.997051 0.437662
 H -5.255416 -3.474032 0.493993
 H -4.696540 -4.127164 -1.058237
 H -1.922045 -4.990312 -0.220436
 H -2.217393 -4.039460 -1.674444
 H -1.029925 -3.480413 -0.473421
 H -4.512915 0.843355 4.086804
 H -5.161441 -0.374518 2.960557
 H -3.588400 -0.633247 3.747322
 H -4.751347 2.655143 2.284718
 H -3.974019 2.426302 0.702043
 H -5.386677 1.441507 1.148442
 H -2.511654 2.200570 3.473206
 H -1.575349 0.745619 3.063368
 H -1.758298 2.052672 1.874859
 H -1.267502 -2.219493 -2.349215
 H -1.792326 0.657150 -3.303352
 H -3.569187 -2.644333 -2.575424
 H -6.086597 -0.963381 -2.968392
 H -5.988281 -2.740436 -2.875754
 H -4.126356 0.298445 -3.221434
 H -0.061402 -0.884125 -2.653123
 H -5.930844 -1.757643 -1.396405
 H 0.405367 -1.692711 2.543260
 H 1.429110 -3.969482 2.538702
 H 3.074396 -5.541939 1.642481
 H 5.887828 -4.261863 -1.347258
 H 4.993488 -1.981916 -1.247871
 H 4.957848 -6.055036 0.117580
 H 4.908982 3.065044 -2.531876
 H 5.428013 -0.871756 1.368878
 H 7.111321 2.824416 -1.497257
 H 8.614936 1.735294 0.142643
 H 7.742987 -0.098380 1.593070
 H 2.508935 2.397928 -2.667837
 H -3.499314 5.767449 -1.420613
 H -1.105130 2.253965 -2.030768

H -2.178646 6.286942 0.610919
H -2.946358 3.725580 -2.752193
H 1.981337 3.854859 0.317258
H 2.172447 2.384476 1.282452
H 1.650096 4.302156 2.785785
H 0.344969 3.114037 2.800662
H 0.430488 5.859255 1.477157
H -0.810461 5.212455 2.531648

(XXII-si)₁

E0+ZPE = -2524.696790
E298 = -2524.648669
H298 = -2524.647724
G298 = -2524.778088
NImag = 1, (-181.7372)
C -1.401510 4.217054 -2.224015
C -0.613255 3.261368 -1.581164
C -0.265681 3.414495 -0.229299
C -0.651318 4.588498 0.453956
C -1.413335 5.544934 -0.218334
C -1.813921 5.361071 -1.543154
C -0.126238 4.803326 1.851283
C 1.320906 4.293596 1.888471
C 1.362089 2.793403 1.599859
N 0.486947 2.415493 0.448269
P 0.275925 0.783457 -0.005762
O 1.342378 0.504640 -1.270352
C 2.696676 0.774160 -1.107232
C 3.480201 -0.069301 -0.331973
C 4.860399 0.289948 -0.131975
C 5.398910 1.429973 -0.819813
C 4.552646 2.205272 -1.656291
C 3.220369 1.899108 -1.782190
C 6.763346 1.779837 -0.631409
C 7.568763 1.061593 0.221693
C 7.032195 -0.038028 0.932064
C 5.717799 -0.413423 0.760522
C 2.858755 -1.269424 0.298885
C 1.725323 -1.116649 1.084267
C 1.127211 -2.185976 1.785020
C 1.650571 -3.449674 1.664069
C 2.755936 -3.697404 0.807655
C 3.361232 -2.603980 0.100630
C 3.258145 -5.013506 0.620001
C 4.294557 -5.259999 -0.250362
C 4.867811 -4.191092 -0.978689
C 4.415990 -2.900928 -0.807631
O 1.161452 0.145702 1.249410
Pd -1.737390 -0.344508 -0.385727
N -3.126959 -0.150575 1.217613
C -4.055409 -0.949619 0.679558
O -5.240134 -1.138515 0.989073
N -3.418081 -1.633390 -0.439923
C -3.266229 -3.112067 -0.168391
C -2.258419 -3.723771 -1.155914
C -2.754434 -3.382885 1.264721

C -4.629382 -3.823245 -0.342507
 C -2.436483 0.284470 -2.786817
 C -1.399744 -0.654831 -2.557379
 C -3.824807 0.094589 -2.713865
 C -4.456441 -1.114119 -2.434537
 C -5.942033 -1.180721 -2.216154
 C -3.372500 0.639176 2.440225
 C -2.080512 1.381473 2.799927
 C -4.494368 1.668394 2.179107
 C -3.767368 -0.287974 3.610198
 H -2.609736 -4.461182 1.402400
 H -1.796463 -2.884719 1.439107
 H -3.469328 -3.038739 2.016574
 H -4.510597 -4.891299 -0.122047
 H -5.374438 -3.397216 0.330557
 H -4.996983 -3.735348 -1.369843
 H -2.166484 -4.799367 -0.965199
 H -2.578021 -3.607329 -2.197268
 H -1.267335 -3.273635 -1.041498
 H -3.935369 0.296637 4.523402
 H -4.682501 -0.834961 3.371317
 H -2.968500 -1.011626 3.811766
 H -4.670514 2.280127 3.073399
 H -4.213123 2.335618 1.356221
 H -5.421972 1.156624 1.912758
 H -2.216783 1.958957 3.722366
 H -1.254315 0.677903 2.953839
 H -1.801516 2.071302 1.997679
 H -1.610277 -1.711290 -2.674786
 H -2.121246 1.315179 -2.940045
 H -3.956125 -2.035115 -2.702786
 H -6.420599 -0.238222 -2.504238
 H -6.395917 -1.996376 -2.791842
 H -4.439110 0.993331 -2.712850
 H -0.389057 -0.365760 -2.829559
 H -6.160352 -1.350185 -1.155189
 H 1.782322 4.459719 2.868923
 H -0.725802 4.253631 2.591062
 H 1.916582 4.843895 1.149987
 H -0.181139 5.864169 2.119417
 H 0.265700 -1.978068 2.410084
 H 1.205014 -4.280740 2.204350
 H 2.794292 -5.827706 1.171680
 H 5.669080 -4.390082 -1.685154
 H 4.860101 -2.096241 -1.381818
 H 4.664889 -6.271708 -0.390274
 H 4.970170 3.062154 -2.178837
 H 5.322547 -1.252840 1.320256
 H 7.156101 2.638995 -1.170100
 H 8.608981 1.342215 0.361221
 H 7.661846 -0.589835 1.624709
 H 2.551540 2.498107 -2.391497
 H -2.416358 6.114227 -2.042466
 H -0.246938 2.406538 -2.139162
 H -1.695342 6.451794 0.312150
 H -1.666319 4.074824 -3.268494

H 2.386605 2.473515 1.390607
H 1.022283 2.247587 2.484138

(XXII-si)₂

E0 = -2525.5158787
E0+ZPE = -2524.693606
E298 = -2524.645578
H298 = -2524.644634
G298 = -2524.774214
NImag = 1, (-190.4489)
C 3.790490 3.583809 1.129195
C 2.723864 2.789038 0.722079
C 1.507868 3.356172 0.300065
C 1.382736 4.766669 0.316894
C 2.473541 5.540639 0.733057
C 3.677783 4.973238 1.133176
C 0.110004 5.482111 -0.091045
C -1.087084 4.538131 -0.078618
C -0.713256 3.256115 -0.811582
N 0.398837 2.543867 -0.127882
P 0.237679 0.854038 -0.224883
O 1.238232 0.274227 -1.439195
C 2.616209 0.153956 -1.353483
C 3.200154 -0.724863 -0.450656
C 4.639670 -0.730012 -0.358047
C 5.410726 0.053796 -1.281002
C 4.741620 0.852049 -2.246909
C 3.372470 0.921395 -2.268572
C 6.828871 0.040778 -1.196658
C 7.475472 -0.687075 -0.224388
C 6.719116 -1.427656 0.713526
C 5.342813 -1.449913 0.648491
C 2.344095 -1.583303 0.416626
C 1.343078 -1.009589 1.186736
C 0.557193 -1.745902 2.099532
C 0.752222 -3.099453 2.220208
C 1.695376 -3.771637 1.398467
C 2.488656 -3.016500 0.470238
C 1.847743 -5.183112 1.461399
C 2.719760 -5.840506 0.624885
C 3.471935 -5.105058 -0.320891
C 3.361126 -3.733769 -0.395436
O 1.103107 0.364680 1.102823
Pd -1.889385 -0.088199 -0.480361
N -3.223527 0.396094 1.125162
C -4.282177 -0.201002 0.565064
O -5.491034 -0.119284 0.823009
N -3.767456 -1.045657 -0.509941
C -3.885336 -2.511949 -0.159750
C -3.005289 -3.350617 -1.102256
C -3.430843 -2.792723 1.291099
C -5.355011 -2.970382 -0.311439
C -2.435754 0.526972 -2.945601
C -1.596508 -0.570725 -2.628383
C -3.834975 0.596845 -2.889831
C -4.674018 -0.461165 -2.542742

C -6.149476 -0.246825 -2.353610
 C -3.350090 1.273824 2.308002
 C -1.946160 1.677698 2.774146
 C -4.158558 2.535385 1.934655
 C -4.053878 0.525816 3.462465
 H -3.468218 -3.872387 1.479820
 H -2.405145 -2.449538 1.455817
 H -4.082914 -2.299908 2.017084
 H -5.437004 -4.025195 -0.021556
 H -6.013444 -2.372313 0.320004
 H -5.694004 -2.883235 -1.348704
 H -3.113886 -4.412654 -0.853525
 H -3.295751 -3.234933 -2.152167
 H -1.947807 -3.086618 -1.000657
 H -4.125151 1.171662 4.346506
 H -5.059776 0.220575 3.166917
 H -3.483625 -0.368218 3.741061
 H -4.244914 3.209784 2.796222
 H -3.665247 3.080166 1.121095
 H -5.161941 2.254907 1.604937
 H -2.011227 2.344741 3.641770
 H -1.362449 0.798303 3.066677
 H -1.395416 2.197295 1.985003
 H -2.003659 -1.572953 -2.685905
 H -1.926922 1.464834 -3.171017
 H -4.345655 -1.470239 -2.751967
 H -6.450681 0.737900 -2.728067
 H -6.736479 -1.014595 -2.871492
 H -4.281680 1.586773 -2.967169
 H -0.547126 -0.494895 -2.893205
 H -6.401505 -0.285772 -1.287074
 H -1.954297 4.995192 -0.569150
 H 0.229936 5.903224 -1.100648
 H -1.380028 4.296823 0.949209
 H -0.060073 6.335808 0.575784
 H -0.183380 -1.219211 2.690521
 H 0.163398 -3.676172 2.928565
 H 1.246597 -5.736466 2.178826
 H 4.140169 -5.627016 -1.000379
 H 3.937398 -3.189065 -1.133883
 H 2.822146 -6.920772 0.677813
 H 5.331854 1.433406 -2.950457
 H 4.781960 -2.014662 1.383730
 H 7.394813 0.632234 -1.912486
 H 8.560289 -0.683930 -0.166020
 H 7.227695 -1.980929 1.498365
 H 2.842489 1.555042 -2.971969
 H 4.505609 5.600550 1.450965
 H 2.843156 1.718229 0.748212
 H 2.356435 6.622538 0.742892
 H 4.712508 3.102777 1.443714
 H -1.569887 2.579059 -0.859302
 H -0.415124 3.495116 -1.843933

(XXII-*st*)₃

E0 = -2525.5149341

E0+ZPE = -2524.692800
 E298 = -2524.644762
 H298 = -2524.643818
 G298 = -2524.773288
 NImag = 1, (-187.6243)
 C -3.663023 -3.590269 0.222798
 C -2.742865 -2.867956 -0.587616
 C -2.017931 -3.595421 -1.591080
 C -2.278518 -4.980243 -1.774894
 C -3.192362 -5.641016 -0.987065
 C -3.879930 -4.937020 0.029257
 C -2.485316 -1.461874 -0.408774
 C -1.453085 -0.897911 -1.143683
 C -0.736042 -1.606260 -2.131948
 C -1.033871 -2.925934 -2.365883
 C -3.254370 -0.619395 0.551849
 C -2.580253 0.113384 1.520384
 C -3.250719 0.868411 2.509147
 C -4.621316 0.929793 2.505803
 C -5.372469 0.280606 1.490161
 C -4.688424 -0.487935 0.488488
 C -6.787032 0.403011 1.433178
 C -7.508984 -0.177685 0.416281
 C -6.835530 -0.900816 -0.596068
 C -5.466587 -1.052538 -0.561266
 O -1.195201 0.090685 1.582646
 P -0.215570 0.771912 0.402879
 Pd 1.898754 -0.207550 0.526984
 C 1.669165 -0.883217 2.626611
 C 2.540692 0.165524 3.014968
 C 3.938676 0.216842 2.918661
 C 4.746289 -0.817112 2.447550
 C 6.218747 -0.609943 2.229699
 O -1.112215 0.440787 -0.944287
 N -0.399420 2.459080 0.460174
 C -1.287134 3.289856 -0.302839
 C -0.800690 4.536551 -0.752132
 C 0.570176 4.973148 -0.303673
 C 0.703904 4.617631 1.181945
 C 0.596914 3.101592 1.373056
 C -1.632081 5.362037 -1.511754
 C -2.925075 4.968925 -1.855531
 C -3.403624 3.741731 -1.398757
 C -2.600279 2.913988 -0.614871
 N 3.179170 0.394460 -1.081051
 C 3.274542 1.402967 -2.156069
 C 3.976585 0.808182 -3.397387
 N 3.761415 -1.192216 0.398108
 C 3.837046 -2.617477 -0.098150
 C 5.305115 -3.104783 -0.064224
 C 4.250769 -0.252470 -0.607690
 O 5.452892 -0.146465 -0.887166
 C 2.989665 -3.534096 0.800829
 C 3.308458 -2.750927 -1.544900
 C 1.856730 1.827773 -2.555624
 C 4.063619 2.628530 -1.646127

H 3.323280 -3.807084 -1.839688
 H 2.279925 -2.385928 -1.623499
 H 3.928692 -2.193509 -2.251851
 H 5.357038 -4.128203 -0.455429
 H 5.941795 -2.456552 -0.667996
 H 5.695898 -3.119284 0.958308
 H 3.070773 -4.568332 0.446787
 H 3.330036 -3.523105 1.842113
 H 1.932581 -3.250808 0.774744
 H 4.018432 1.552349 -4.202499
 H 4.992952 0.493681 -3.152489
 H 3.420179 -0.060813 -3.767758
 H 4.130958 3.401316 -2.422687
 H 3.568487 3.064650 -0.769806
 H 5.075322 2.331418 -1.357841
 H 1.894568 2.596910 -3.335977
 H 1.286738 0.977576 -2.946130
 H 1.309224 2.234841 -1.701247
 H 2.058398 -1.892933 2.573995
 H 2.060339 1.087117 3.345769
 H 4.405470 -1.836185 2.570078
 H 6.551035 0.330179 2.683947
 H 6.807028 -1.432596 2.653355
 H 4.406690 1.187824 3.072764
 H 0.631177 -0.816031 2.935919
 H 6.434754 -0.552320 1.156102
 H 0.036127 -1.084858 -2.686429
 H -0.497269 -3.480777 -3.130964
 H -1.727200 -5.512067 -2.546600
 H -4.582385 -5.464712 0.668632
 H -4.191162 -3.070737 1.013686
 H -3.377669 -6.701494 -1.133009
 H -5.147272 1.501144 3.266268
 H -4.967811 -1.600109 -1.352096
 H -7.287860 0.979780 2.207107
 H -8.589584 -0.071730 0.380012
 H -7.402773 -1.336689 -1.413960
 H -2.656651 1.383712 3.256737
 H -3.553499 5.618368 -2.458382
 H -2.998493 1.975367 -0.257579
 H -1.250539 6.327235 -1.837791
 H -4.414481 3.422724 -1.637615
 H 1.571692 2.640958 1.177631
 H 0.329827 2.880871 2.415396
 H -0.087280 5.129407 1.742430
 H 1.663386 4.948127 1.596495
 H 0.701739 6.048505 -0.465230
 H 1.358785 4.462996 -0.874289

XXII-re-b

E0 = -2525.5182809
 E0+ZPE = -2524.696508
 E298 = -2524.648245
 H298 = -2524.647301
 G298 = -2524.778443
 NImag = 1, (-167.6885)

C 1.137986 3.176738 1.155233
 C 0.521611 3.403548 -0.084960
 C 0.859251 4.557042 -0.825819
 C 1.830032 5.426181 -0.325890
 C 2.488003 5.166140 0.878488
 C 2.132611 4.039238 1.618449
 N -0.432445 2.489195 -0.617164
 C -1.526869 2.992356 -1.505570
 C -1.388601 4.485111 -1.808245
 C 0.079431 4.837436 -2.085156
 P -0.273520 0.831863 -0.248749
 Pd 1.805233 -0.232211 -0.263031
 C 2.257835 0.665323 -2.248573
 C 3.200001 1.502550 -1.596667
 C 4.498590 1.187726 -1.169757
 C 5.132955 -0.035426 -1.358944
 C 6.460049 -0.331455 -0.721612
 O -1.238743 0.516538 1.076927
 C -2.597827 0.804686 1.053066
 C -3.039616 1.891343 1.840888
 C -4.371649 2.223122 1.851605
 C -5.302287 1.512996 1.046841
 C -4.848179 0.407676 0.250337
 C -3.463109 0.017068 0.306904
 C -6.670087 1.895190 0.997131
 C -7.560048 1.242210 0.176084
 C -7.108940 0.178417 -0.640215
 C -5.792963 -0.227805 -0.603916
 C -2.923932 -1.152635 -0.443253
 C -1.861213 -0.969056 -1.315771
 C -1.349266 -2.004633 -2.127521
 C -1.885715 -3.265166 -2.034337
 C -2.916320 -3.546968 -1.098981
 C -3.434371 -2.488702 -0.278448
 C -4.410630 -2.822905 0.701516
 C -4.872486 -4.113773 0.836379
 C -4.388247 -5.145798 -0.001535
 C -3.427269 -4.863966 -0.944656
 O -1.289185 0.292471 -1.454812
 N 2.542524 -1.024512 1.585047
 C 3.695107 -1.458754 1.065977
 O 4.746708 -1.825482 1.609428
 N 3.537430 -1.429731 -0.384074
 C 3.454658 -2.822985 -0.958646
 C 4.860074 -3.469704 -0.967136
 C 2.296598 -0.998193 3.042910
 C 3.251104 0.016094 3.710454
 C 0.844918 -0.575979 3.289050
 C 2.511907 -2.402447 3.649995
 C 2.500067 -3.726283 -0.144342
 C 2.934281 -2.758530 -2.404394
 H 2.899427 -3.769333 -2.827299
 H 1.923735 -2.339751 -2.439826
 H 3.584278 -2.158860 -3.051118
 H 4.787647 -4.489624 -1.364728
 H 5.550218 -2.910043 -1.606812

H 5.274533 -3.504158 0.041094
 H 2.414083 -4.702763 -0.636136
 H 2.874873 -3.890414 0.869357
 H 1.500726 -3.285754 -0.074126
 H 3.061153 0.071938 4.790140
 H 4.291081 -0.278883 3.550248
 H 3.102354 1.015362 3.283782
 H 2.318652 -2.382340 4.729835
 H 1.822248 -3.123127 3.195413
 H 3.536227 -2.741714 3.481802
 H 0.622008 -0.597264 4.362607
 H 0.658388 0.437675 2.923317
 H 0.149808 -1.247139 2.775067
 H 2.612074 -0.190013 -2.812656
 H 2.840842 2.488304 -1.307145
 H 4.843634 -0.646783 -2.203212
 H 6.914747 0.583396 -0.325746
 H 6.323939 -1.022371 0.119317
 H 4.978229 1.905705 -0.506951
 H 1.389576 1.152308 -2.685718
 H 7.155040 -0.791925 -1.433906
 H -2.030093 4.716484 -2.666561
 H 0.447361 4.228974 -2.925490
 H -1.746520 5.085182 -0.963015
 H 0.189664 5.886942 -2.378961
 H -0.543645 -1.774215 -2.816177
 H -1.507783 -4.069318 -2.660215
 H -3.030185 -5.650996 -1.581301
 H -5.611581 -4.342566 1.599298
 H -4.783631 -2.047693 1.360512
 H -4.765325 -6.158298 0.112062
 H -4.726033 3.050602 2.460949
 H -5.464729 -1.038746 -1.243352
 H -6.997695 2.726743 1.616623
 H -8.602219 1.547283 0.143072
 H -7.806449 -0.321251 -1.306976
 H -2.308167 2.437531 2.427392
 H -1.489613 2.428723 -2.440638
 H -2.495410 2.788779 -1.038946
 H 3.250559 5.848055 1.243347
 H 2.610206 3.833662 2.572295
 H 2.073591 6.320137 -0.896033
 H 0.842810 2.330266 1.765352

(XXII-*re-b*)₁

E0 = -2525.5150498
 E0+ZPE = -2524.693354
 E298 = -2524.645193
 H298 = -2524.644249
 G298 = -2524.774023
 NImag = 1, (-143.3195)
 C -2.900758 2.759865 -0.760311
 C -1.622806 3.342687 -0.722490
 C -1.485854 4.699192 -1.100998
 C -2.625439 5.409053 -1.500936
 C -3.886485 4.825011 -1.540663

C -4.014245 3.487530 -1.167126
 N -0.462310 2.602665 -0.303345
 C 0.697646 3.424200 0.117111
 C 1.024546 4.475455 -0.938655
 C -0.157353 5.432159 -1.073148
 P -0.196372 0.928165 -0.193048
 Pd 1.978460 0.068157 -0.225700
 C 2.175662 0.263901 -2.443578
 C 3.104114 1.309358 -2.227712
 C 4.466222 1.228117 -1.889818
 C 5.182538 0.050332 -1.738268
 C 6.585553 0.044966 -1.207124
 O -0.943477 0.278880 1.149331
 C -2.310402 0.145921 1.325618
 C -2.884798 0.884477 2.385310
 C -4.233719 0.800641 2.617316
 C -5.066769 0.017997 1.773485
 C -4.478014 -0.735505 0.702583
 C -3.046238 -0.717518 0.526232
 C -6.475510 -0.008288 1.955987
 C -7.288698 -0.718608 1.103233
 C -6.717392 -1.427275 0.020761
 C -5.353151 -1.436996 -0.173459
 C -2.358812 -1.549921 -0.500970
 C -1.516067 -0.957999 -1.431852
 C -0.936563 -1.678931 -2.499956
 C -1.160114 -3.028569 -2.611950
 C -1.923200 -3.719192 -1.633877
 C -2.514912 -2.982339 -0.553980
 C -3.201798 -3.717068 0.453029
 C -3.328444 -5.086795 0.376159
 C -2.780913 -5.803271 -0.713709
 C -2.089605 -5.129124 -1.693523
 O -1.249974 0.409997 -1.373738
 N 2.980094 0.082913 1.669929
 C 4.101011 -0.477799 1.201260
 O 5.228797 -0.582361 1.703762
 N 3.791304 -0.989773 -0.127019
 C 3.761865 -2.497588 -0.153025
 C 5.205408 -3.050463 -0.092314
 C 2.895551 0.647876 3.034163
 C 3.857124 1.850950 3.156000
 C 1.459366 1.116728 3.295091
 C 3.260417 -0.426717 4.082385
 C 2.958581 -3.076236 1.034424
 C 3.104559 -2.978194 -1.458003
 H 3.112266 -4.073934 -1.490052
 H 2.063722 -2.646724 -1.525721
 H 3.644682 -2.624712 -2.343859
 H 5.172865 -4.146936 -0.098537
 H 5.790395 -2.728090 -0.959992
 H 5.712135 -2.709355 0.811203
 H 2.898748 -4.166983 0.939466
 H 3.437013 -2.844241 1.989881
 H 1.939833 -2.676415 1.054820
 H 3.792869 2.295550 4.157429

H 4.886779 1.533247 2.976141
 H 3.596878 2.623789 2.422327
 H 3.186568 -0.011920 5.095458
 H 2.571013 -1.275963 4.011296
 H 4.279227 -0.787304 3.924167
 H 1.379042 1.526148 4.309323
 H 1.166432 1.902379 2.590491
 H 0.750285 0.290221 3.194957
 H 2.536300 -0.720142 -2.721085
 H 2.691446 2.317615 -2.247824
 H 4.845519 -0.835595 -2.259177
 H 7.001038 1.058577 -1.187662
 H 6.589153 -0.332602 -0.177057
 H 4.947235 2.153512 -1.577383
 H 1.228474 0.541992 -2.897373
 H 7.241747 -0.595266 -1.808873
 H 1.935615 5.015928 -0.656585
 H -0.151262 6.133260 -0.225410
 H 1.219518 3.972842 -1.894079
 H -0.057071 6.048151 -1.975118
 H -0.332872 -1.141011 -3.221707
 H -0.730721 -3.588530 -3.438627
 H -1.643291 -5.668057 -2.525876
 H -3.849065 -5.622469 1.165216
 H -3.617994 -3.187804 1.301917
 H -2.894559 -6.882462 -0.765593
 H -4.685743 1.357877 3.433738
 H -4.936589 -1.977342 -1.015205
 H -6.900551 0.559316 2.780398
 H -8.365181 -0.725813 1.249399
 H -7.360944 -1.966091 -0.669355
 H -2.234339 1.503149 2.994434
 H 0.465456 3.911630 1.074732
 H 1.548886 2.759291 0.284389
 H -4.751297 5.400835 -1.857540
 H -4.984587 2.999075 -1.182479
 H -2.503315 6.451099 -1.790200
 H -3.034373 1.727716 -0.478879

XXII-si-c

E0 = -2525.5148052
 E0+ZPE = -2524.693073
 E298 = -2524.644944
 H298 = -2524.644000
 G298 = -2524.774278
 NImag = 1, (-169.3682)
 C -4.321471 -4.273384 1.186798
 C -3.867310 -3.212748 1.973317
 C -2.613608 -2.656433 1.740772
 C -1.802908 -3.130229 0.695688
 C -2.243080 -4.215716 -0.091399
 C -3.502532 -4.767911 0.176681
 C -1.386814 -4.841129 -1.180968
 C -0.075444 -4.087274 -1.436238
 C 0.461913 -3.533365 -0.117694
 N -0.494958 -2.569698 0.471420

P -0.128661 -0.930333 0.188508
 O -1.020275 -0.411434 -1.122056
 C -2.408053 -0.323764 -1.116128
 C -3.055368 0.620502 -0.333131
 C -4.495785 0.597163 -0.305150
 C -5.205216 -0.291543 -1.180161
 C -4.472810 -1.157151 -2.035327
 C -3.102556 -1.190103 -1.989970
 C -6.625545 -0.306988 -1.160746
 C -7.332380 0.495026 -0.294434
 C -6.636910 1.343652 0.598067
 C -5.259914 1.395017 0.591875
 C -2.259264 1.592074 0.466347
 C -1.275429 1.133825 1.329866
 C -0.545157 1.993124 2.179411
 C -0.774169 3.345969 2.138083
 C -1.700754 3.894875 1.213018
 C -2.438703 3.017436 0.349637
 C -1.887343 5.299683 1.108247
 C -2.739139 5.833033 0.169106
 C -3.434681 4.974292 -0.714108
 C -3.290774 3.607082 -0.625971
 O -1.008572 -0.233763 1.420846
 Pd 2.180937 -0.489081 0.129432
 N 2.813178 1.161014 -1.083178
 C 4.088573 1.104254 -0.689510
 O 5.017565 1.914977 -0.815132
 N 4.259742 -0.173567 -0.006000
 C 5.114305 -1.122855 -0.810238
 C 4.996171 -2.545720 -0.237821
 C 4.680689 -1.163673 -2.293733
 C 6.597381 -0.687001 -0.741175
 C 2.472331 -1.656558 2.013861
 C 2.594187 -0.425907 2.704206
 C 3.703828 0.428558 2.777428
 C 4.942794 0.175754 2.197433
 C 6.024939 1.216408 2.183107
 C 2.288863 2.282589 -1.893566
 C 0.832367 1.986612 -2.261076
 C 2.355480 3.586235 -1.068153
 C 3.110668 2.433149 -3.192726
 H 5.274761 -1.914678 -2.828111
 H 3.622420 -1.427462 -2.389709
 H 4.836163 -0.198045 -2.781845
 H 7.204878 -1.373654 -1.343556
 H 6.719350 0.328983 -1.118215
 H 6.973367 -0.722009 0.286427
 H 5.636878 -3.226017 -0.810550
 H 5.319721 -2.599424 0.807426
 H 3.968255 -2.916828 -0.302593
 H 2.713838 3.256384 -3.799773
 H 4.159170 2.638498 -2.965581
 H 3.051849 1.514543 -3.788352
 H 1.941399 4.425154 -1.642028
 H 1.770658 3.480030 -0.147215
 H 3.390413 3.815982 -0.803228

H 0.433923 2.788509 -2.893973
 H 0.750268 1.040814 -2.807075
 H 0.206791 1.915854 -1.367964
 H 3.368616 -2.223686 1.790651
 H 1.679755 -0.054441 3.165177
 H 5.242754 -0.852394 2.045636
 H 5.786238 2.037521 2.868248
 H 6.995723 0.791969 2.465076
 H 3.531676 1.424663 3.181563
 H 1.602527 -2.265004 2.247048
 H 6.116272 1.642710 1.176453
 H 0.182901 1.561225 2.856003
 H -0.225297 4.015213 2.795291
 H -1.326651 5.947534 1.777729
 H -4.084563 5.397307 -1.475271
 H -3.822016 2.966524 -1.319693
 H -2.866884 6.909155 0.092330
 H -5.015081 -1.815682 -2.708868
 H -4.745738 2.044911 1.290206
 H -7.144773 -0.979568 -1.839457
 H -8.418484 0.469718 -0.284534
 H -7.193480 1.958787 1.300007
 H -2.527101 -1.865697 -2.613662
 H -0.233379 -3.249025 -2.125972
 H 0.663550 -4.751250 -1.900304
 H -1.968057 -4.923940 -2.108290
 H -1.155839 -5.873776 -0.882358
 H 1.421323 -3.027467 -0.257955
 H 0.613816 -4.342259 0.609394
 H -5.296521 -4.717223 1.367325
 H -2.250572 -1.851803 2.365024
 H -3.840033 -5.606519 -0.429636
 H -4.481682 -2.825066 2.781165

XXIII-*re*

E0 = -2638.6456731
 E0+ZPE = -2637.829427
 E298 = -2637.780314
 H298 = -2637.779370
 G298 = -2637.911726
 NImag = 1, (-190.2684)
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 C 5.579441 -0.935024 0.497404
 C 4.743063 -0.267826 -0.441368
 C 5.337178 0.742318 -1.270843
 C 6.731005 0.999170 -1.168336
 C 7.513584 0.317035 -0.265618
 C 4.518836 1.487978 -2.160335
 C 3.162570 1.282649 -2.204299
 C 2.585401 0.287007 -1.387352
 C 3.331871 -0.533291 -0.553634
 O 1.205011 0.116436 -1.478516
 P 0.198135 0.544650 -0.225801
 O 1.105508 0.038018 1.062941
 C 1.563521 -1.282351 1.025654

C 0.904871 -2.218727 1.850236
 C 1.326575 -3.525698 1.852472
 C 2.380581 -3.950009 0.999664
 C 3.040570 -2.990446 0.159287
 C 2.649551 -1.605962 0.225728
 C 2.774771 -5.314375 0.943548
 C 3.755792 -5.733766 0.075188
 C 4.379103 -4.798495 -0.784159
 C 4.033321 -3.465659 -0.742951
 Pd -1.937595 -0.328613 -0.453346
 N -3.062082 -0.113245 1.345180
 C -2.970179 0.422588 2.720589
 C -1.753873 1.352349 2.804944
 N -3.915186 -1.075288 -0.496959
 C -3.652243 -3.294872 -1.018275
 C -2.286108 -3.444255 -0.780485
 C -1.276790 -2.658780 -1.353766
 C -1.416338 -1.550725 -2.230320
 C -4.998370 -0.360730 -1.272941
 C -5.244537 1.065770 -0.729697
 C -4.594650 -0.245452 -2.752392
 C -6.323160 -1.155192 -1.183610
 C -4.080193 -0.882795 0.941821
 O -5.018590 -1.383269 1.576098
 C -4.664552 -4.077047 -0.228461
 C -4.239265 1.232380 3.066588
 C -2.805142 -0.740843 3.722965
 N 0.408259 2.235845 -0.012997
 C 1.370291 2.989362 0.727603
 C 1.061705 4.364845 0.600929
 C -0.100940 4.478929 -0.252466
 C -0.477900 3.170445 -0.624348
 H -5.392276 0.258102 -3.310561
 H -3.677451 0.340555 -2.869921
 H -4.443325 -1.224857 -3.218936
 H -7.108824 -0.609434 -1.720271
 H -6.228007 -2.142363 -1.647513
 H -6.623103 -1.287102 -0.143405
 H -5.983652 1.573127 -1.361191
 H -5.634261 1.040520 0.291119
 H -4.324885 1.659026 -0.731596
 H -2.705333 -0.356811 4.746095
 H -3.669491 -1.407592 3.677288
 H -1.905836 -1.323530 3.489369
 H -4.168707 1.632701 4.085510
 H -4.352502 2.077224 2.377621
 H -5.128486 0.601188 2.999816
 H -1.683985 1.794505 3.805614
 H -0.823373 0.810094 2.611964
 H -1.838284 2.167020 2.077571
 H -2.310645 -1.473265 -2.837308
 H -0.265441 -2.864436 -1.004307
 H -3.969847 -2.907252 -1.976793
 H -4.177241 -4.865106 0.356297
 H -5.184785 -3.417319 0.475697
 H -1.987236 -4.106898 0.029779

H -0.512806 -1.181350 -2.705564
 H -5.414933 -4.537184 -0.882400
 H 0.076980 -1.880189 2.462916
 H 0.837560 -4.256625 2.491069
 H 2.272538 -6.025169 1.595288
 H 5.134907 -5.135427 -1.488267
 H 4.514558 -2.765168 -1.415316
 H 4.043575 -6.780598 0.037073
 H 4.978710 2.246504 -2.788200
 H 5.144663 -1.671713 1.162662
 H 7.165356 1.760212 -1.812148
 H 8.576911 0.527155 -0.192322
 H 7.538111 -1.169432 1.313582
 H 2.514481 1.863363 -2.852093
 C 2.469411 2.573916 1.485568
 H 2.725572 1.530685 1.589420
 C 1.849291 5.328585 1.240254
 C 2.939727 4.916681 1.998358
 H 3.561475 5.652132 2.500867
 C 3.241135 3.551596 2.113011
 H 1.608991 6.383745 1.140762
 H 4.098330 3.239195 2.702967
 C -1.552258 2.950508 -1.491116
 H -1.842391 1.951022 -1.799258
 C -2.259713 4.060801 -1.953402
 H -3.100948 3.905225 -2.622937
 C -0.821554 5.579710 -0.729286
 C -1.903741 5.364809 -1.577065
 H -2.472810 6.209116 -1.955352
 H -0.534608 6.587796 -0.442504

XXIII-*re-b*

E0 = -2638.6439361
 E0+ZPE = -2637.827871
 E298 = -2637.778656
 H298 = -2637.777712
 G298 = -2637.910167
 NImag = 1, (-174.5907)
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 C -5.515288 -1.303965 -0.256243
 C -4.638498 -0.553554 0.577006
 C -5.221672 0.405830 1.472001
 C -6.635569 0.531878 1.536442
 C -7.453303 -0.228343 0.732636
 C -4.376815 1.233534 2.258391
 C -3.012167 1.156982 2.138354
 C -2.445875 0.212840 1.254938
 C -3.204441 -0.685714 0.519512
 O -1.055277 0.175988 1.183908
 P -0.222769 0.641161 -0.168592
 O -1.235011 0.063475 -1.350753
 C -1.585810 -1.286453 -1.271910
 C -0.987262 -2.166051 -2.199574
 C -1.301936 -3.502257 -2.162400
 C -2.181078 -4.012776 -1.170949
 C -2.790990 -3.110443 -0.235670

C -2.527813 -1.698352 -0.340514
 C -2.449890 -5.404871 -1.074891
 C -3.260435 -5.903220 -0.081409
 C -3.831413 -5.021611 0.866416
 C -3.605558 -3.664699 0.790915
 Pd 1.934254 -0.207712 -0.281747
 N 2.976439 -0.434922 1.571020
 C 2.868849 -0.153533 3.020336
 C 1.435519 0.290526 3.333697
 N 3.777818 -1.223005 -0.371534
 C 5.072539 0.065217 -1.819468
 C 4.318156 1.234316 -1.823420
 C 2.954210 1.318098 -2.141452
 C 2.058165 0.266670 -2.460735
 C 3.804854 -2.711352 -0.629569
 C 3.055934 -3.493718 0.473590
 C 3.127179 -3.019741 -1.975496
 C 5.267466 -3.212545 -0.687957
 C 4.096144 -0.916702 1.018222
 O 5.223606 -1.098673 1.496546
 C 6.485083 0.049640 -1.309648
 C 3.185877 -1.424937 3.837317
 C 3.852704 0.974998 3.402522
 N -0.548819 2.312989 -0.424278
 C -1.697791 2.976098 -0.959445
 C -1.477781 4.372938 -0.914936
 C -0.177504 4.595093 -0.321887
 C 0.370285 3.328929 -0.020800
 H 3.176655 -4.097420 -2.169753
 H 2.072553 -2.727422 -1.965091
 H 3.624287 -2.517648 -2.812849
 H 5.270854 -4.296054 -0.858968
 H 5.815533 -2.743838 -1.511959
 H 5.789581 -2.993706 0.244104
 H 3.037839 -4.559696 0.217310
 H 3.549313 -3.387719 1.443221
 H 2.022462 -3.146388 0.572138
 H 3.765863 1.211555 4.470610
 H 4.880290 0.672873 3.188168
 H 3.630406 1.886352 2.834812
 H 3.099553 -1.219350 4.911417
 H 2.479514 -2.224586 3.586551
 H 4.200517 -1.772371 3.628734
 H 1.326741 0.472390 4.409578
 H 1.181892 1.217873 2.809462
 H 0.713789 -0.475472 3.036120
 H 2.455294 -0.658706 -2.861832
 H 2.508601 2.305746 -2.030386
 H 4.773688 -0.748382 -2.466573
 H 6.849392 1.068104 -1.136444
 H 6.534614 -0.485415 -0.353878
 H 4.774711 2.128070 -1.401895
 H 1.092869 0.552514 -2.871400
 H 7.159402 -0.450851 -2.015228
 H -0.297041 -1.761276 -2.931267
 H -0.858442 -4.189161 -2.878412

H -1.987405 -6.072394 -1.797941
 H -4.449618 -5.419091 1.666636
 H -4.042056 -3.005390 1.531986
 H -3.452169 -6.970351 -0.013507
 H -4.827784 1.950716 2.939053
 H -5.096605 -2.003809 -0.969621
 H -7.059092 1.255885 2.228383
 H -8.532720 -0.118039 0.786729
 H -7.526527 -1.726147 -0.834296
 H -2.347792 1.799708 2.706022
 C 0.538166 5.760911 -0.026643
 C 1.789569 5.653703 0.571824
 H 2.356374 6.549317 0.809426
 C 2.320903 4.391184 0.875465
 H 3.295733 4.317042 1.349451
 C 1.623702 3.216361 0.589332
 H 0.116970 6.735220 -0.259535
 H 2.059562 2.254828 0.834298
 C -2.891130 2.461703 -1.476156
 H -3.081360 1.400301 -1.515753
 C -3.846708 3.362576 -1.945320
 H -4.777950 2.971939 -2.346041
 C -3.634800 4.748791 -1.909959
 C -2.449078 5.259352 -1.393798
 H -2.274755 6.331439 -1.358626
 H -4.399614 5.422892 -2.285001

XXIII-si

E0 = -2638.6444114
 E0+ZPE = -2637.828082
 E298 = -2637.778920
 H298 = -2637.777976
 G298 = -2637.910161
 NImag = 1, (-191.0133)
 C -3.294061 -3.071625 1.435666
 C -3.746347 -2.832591 -0.023125
 C -5.191156 -3.363329 -0.180011
 C -2.818442 -3.640656 -0.945783
 N -3.695063 -1.365803 -0.391074
 C -4.622811 -0.858376 -2.429539
 C -6.105964 -0.704387 -2.240872
 Pd -1.865896 -0.311784 -0.380723
 C -3.831625 0.227088 -2.805495
 C -2.430804 0.219592 -2.868804
 C -1.542765 -0.829492 -2.522483
 N -3.217124 0.136583 1.206479
 C -3.353320 0.991071 2.406698
 C -4.279596 2.186431 2.093011
 C -3.930083 0.171280 3.581522
 C -1.965161 1.511530 2.799049
 H -3.278157 -4.149039 1.639071
 H -2.288997 -2.674526 1.604573
 H -3.977755 -2.603146 2.148208
 H -5.222746 -4.417606 0.121081
 H -5.881166 -2.791473 0.441764
 H -5.527591 -3.304929 -1.220065

H -2.873559 -4.702105 -0.677799
 H -3.107992 -3.560088 -1.999206
 H -1.776981 -3.320047 -0.843121
 H -4.025968 0.801340 4.474314
 H -4.915319 -0.226158 3.326688
 H -3.265815 -0.665809 3.827034
 H -4.372203 2.838499 2.970813
 H -3.869511 2.781101 1.269158
 H -5.273916 1.831633 1.811166
 H -2.030782 2.108371 3.716127
 H -1.270694 0.683286 2.979904
 H -1.545489 2.147898 2.014910
 H -1.901598 -1.851078 -2.554283
 H -1.966051 1.173859 -3.117581
 H -4.252111 -1.856251 -2.620862
 H -6.446581 0.269065 -2.610560
 H -6.659868 -1.492682 -2.764723
 H -4.322883 1.193371 -2.907726
 H -0.497951 -0.709856 -2.789284
 H -6.360312 -0.759986 -1.175934
 P 0.232815 0.657297 -0.107611
 C 1.687426 2.987074 0.679104
 C -0.353709 3.341879 -0.312790
 C 1.547622 4.379027 0.470737
 C 0.263334 4.602148 -0.156761
 N 0.517652 2.327063 0.187913
 O 1.102553 0.064461 1.170593
 O 1.231824 0.230540 -1.368409
 C 1.415731 -1.297063 1.111239
 C 0.670714 -2.166847 1.935405
 C 2.450337 -1.725446 0.293097
 C 0.942869 -3.512562 1.911803
 C 2.678792 -3.144643 0.196513
 C 1.926616 -4.037795 1.032169
 C 2.160694 -5.436949 0.946322
 H -0.099271 -1.746343 2.572965
 H 0.385916 -4.194859 2.548363
 C 3.072594 -5.949844 0.053085
 C 3.595385 -3.713518 -0.731549
 C 3.784854 -5.076310 -0.801911
 H 1.590430 -6.097560 1.594933
 H 4.484887 -5.484352 -1.525820
 H 4.142257 -3.060233 -1.401229
 H 3.237323 -7.021927 -0.007911
 C 2.619978 0.207222 -1.275104
 C 3.254532 -0.725878 -0.467100
 C 4.689728 -0.646897 -0.357251
 C 3.323050 1.126298 -2.084262
 C 4.694046 1.148448 -2.048722
 H 5.246964 1.847802 -2.670247
 C 5.410040 0.289373 -1.173314
 C 5.434942 -1.431375 0.567509
 H 4.910492 -2.115775 1.223827
 C 6.825464 0.361276 -1.072374
 H 7.353467 1.069208 -1.706708
 C 7.514875 -0.430105 -0.182898

H 8.596618 -0.361126 -0.110402
 C 6.806081 -1.324665 0.652536
 H 7.347255 -1.931084 1.373703
 H 2.754980 1.799217 -2.717927
 C -4.246383 -0.534489 0.677890
 O -5.451914 -0.526934 0.958275
 C -1.634739 3.232331 -0.860363
 C -0.396819 5.764645 -0.570472
 C -1.665943 5.659417 -1.130767
 H -2.191857 6.552739 -1.455067
 C -2.276260 4.403401 -1.266571
 H -2.136519 2.276209 -0.947746
 H 0.076771 6.735273 -0.450299
 H -3.275414 4.334105 -1.687598
 C 2.826575 2.470881 1.303805
 H 2.941846 1.413289 1.487177
 C 2.558119 5.259314 0.873746
 C 3.822646 3.364948 1.694804
 H 4.713394 2.974159 2.178612
 C 3.698047 4.746222 1.482889
 H 2.447315 6.328573 0.714372
 H 4.491546 5.415901 1.802179

XXIII-si-c

E0 = -2638.6422386
 E0+ZPE = -2637.826399
 E298 = -2637.777089
 H298 = -2637.776145
 G298 = -2637.910064
 NImag = 1, (-179.9281)
 C 2.887660 4.934091 2.379405
 C 3.111286 3.564679 2.586117
 C 2.391337 2.589752 1.895822
 C 1.422281 3.012439 0.979861
 C 1.195773 4.393764 0.757112
 C 1.931073 5.353460 1.461391
 C 0.171714 4.513423 -0.258236
 C -0.203493 3.202385 -0.624436
 N 0.539996 2.267367 0.143274
 P 0.176470 0.580815 0.018339
 O 1.054330 0.082333 -1.289658
 C 2.439684 0.260313 -1.303365
 C 3.245605 -0.526993 -0.494323
 C 4.658525 -0.248831 -0.484773
 C 5.187319 0.738495 -1.383109
 C 4.305622 1.449598 -2.239676
 C 2.951157 1.233430 -2.187559
 C 6.582607 1.007693 -1.381239
 C 7.429172 0.359320 -0.512157
 C 6.906359 -0.585168 0.402198
 C 5.561081 -0.881978 0.415115
 C 2.626649 -1.589035 0.351048
 C 1.589910 -1.262424 1.212403
 C 0.988746 -2.194271 2.084164
 C 1.419483 -3.498120 2.077308
 C 2.425511 -3.924383 1.170504

C 3.024755 -2.971233 0.279582
 C 2.826624 -5.286288 1.109497
 C 3.757121 -5.710232 0.189551
 C 4.319295 -4.781991 -0.718132
 C 3.965134 -3.451490 -0.674455
 O 1.127525 0.057374 1.267867
 Pd -2.075293 0.029344 0.101654
 N -2.652749 -1.778937 -0.881073
 C -3.907185 -1.763293 -0.419767
 O -4.781492 -2.640570 -0.406468
 N -4.130646 -0.431545 0.134993
 C -5.095717 0.365965 -0.710156
 C -5.038451 1.850258 -0.310630
 C -4.758442 0.257903 -2.215117
 C -6.537987 -0.150002 -0.491448
 C -2.346667 1.390630 1.857227
 C -2.338162 0.246788 2.693926
 C -3.376463 -0.667148 2.925368
 C -4.658846 -0.567807 2.392082
 C -5.662016 -1.671941 2.566300
 C -2.090271 -2.941757 -1.603031
 C -0.671724 -2.597314 -2.066991
 C -2.036922 -4.161037 -0.656329
 C -2.956007 -3.269641 -2.839419
 H -5.434665 0.903342 -2.788173
 H -3.729337 0.574464 -2.412701
 H -4.876721 -0.766055 -2.578945
 H -7.226849 0.426683 -1.120824
 H -6.614318 -1.207166 -0.748536
 H -6.851771 -0.022422 0.549561
 H -5.756018 2.417971 -0.914293
 H -5.309717 2.004957 0.739603
 H -4.044218 2.274609 -0.481662
 H -2.537248 -4.128198 -3.378808
 H -3.979328 -3.508880 -2.540990
 H -2.979142 -2.415950 -3.527032
 H -1.602246 -5.026760 -1.172296
 H -1.413618 -3.935597 0.216799
 H -3.041569 -4.421280 -0.314615
 H -0.256034 -3.426533 -2.651646
 H -0.669339 -1.698542 -2.692571
 H -0.009566 -2.419848 -1.215168
 H -3.293279 1.859177 1.616014
 H -1.376256 -0.004487 3.141410
 H -5.041137 0.414332 2.149127
 H -5.322712 -2.391355 3.319856
 H -6.641019 -1.280905 2.867573
 H -3.112853 -1.593947 3.432131
 H -1.523487 2.091703 1.966642
 H -5.787050 -2.216820 1.622681
 H 0.195011 -1.858370 2.742137
 H 0.972201 -4.225758 2.749141
 H 2.368458 -5.991909 1.798177
 H 5.033395 -5.122866 -1.462721
 H 4.398053 -2.757744 -1.385329
 H 4.050050 -6.755465 0.147259

H 4.716443 2.190691 -2.920149
 H 5.177532 -1.601961 1.128541
 H 6.966871 1.750971 -2.075608
 H 8.493157 0.578684 -0.516226
 H 7.571658 -1.078755 1.105366
 H 2.256345 1.788665 -2.808657
 H 3.467453 5.666609 2.933639
 H 2.589491 1.542370 2.065512
 H 1.755538 6.411710 1.287086
 H 3.868266 3.247006 3.297935
 C -1.146689 2.973775 -1.631525
 H -1.423155 1.971538 -1.941514
 C -1.732376 4.083819 -2.242084
 H -2.468829 3.925238 -3.024740
 C -1.380766 5.391763 -1.873586
 C -0.424960 5.612643 -0.885984
 H -0.139966 6.624037 -0.608852
 H -1.851196 6.235402 -2.370349

XXIV-*re*

E0 = -2454.8279789
 E0+ZPE = -2454.108948
 E298 = -2454.063691
 H298 = -2454.062746
 G298 = -2454.187255
 NImag = 1, (-185.5026)
 C -4.345441 2.632213 -0.692718
 C -3.309812 2.278717 0.217185
 C -2.691439 3.331058 0.973648
 C -3.165367 4.663501 0.832563
 C -4.184967 4.964573 -0.040327
 C -4.768832 3.937131 -0.818326
 C -2.834079 0.927695 0.368182
 C -1.715939 0.722535 1.161870
 C -1.099831 1.751578 1.905852
 C -1.598508 3.028751 1.828765
 O -1.170868 -0.561490 1.265207
 P -0.226640 -1.062539 -0.010125
 N -0.228559 -2.725078 0.357319
 C 0.904938 -3.525807 -0.019199
 C -3.459970 -0.233557 -0.323929
 C -4.852273 -0.570310 -0.172804
 C -5.399361 -1.659030 -0.931805
 C -4.550653 -2.409686 -1.787505
 C -3.208458 -2.134723 -1.861797
 C -2.676162 -1.060314 -1.116374
 C -6.775279 -1.985872 -0.792121
 C -7.583408 -1.294762 0.080653
 C -7.039060 -0.247225 0.860291
 C -5.713036 0.105632 0.737228
 O -1.310071 -0.816011 -1.251766
 Pd 1.859311 -0.174250 -0.465128
 C 1.232355 0.680831 -2.418688
 C 1.186396 1.937490 -1.762765
 C 2.257570 2.785377 -1.444304
 C 3.591165 2.542184 -1.767772

C 4.690745 3.426967 -1.252504
 N 3.106292 -0.032256 1.258410
 C 4.112272 0.584904 0.626748
 O 5.105905 1.176416 1.068856
 N 3.845916 0.460548 -0.802988
 C 4.835230 -0.465568 -1.470024
 C 6.198260 0.247868 -1.633885
 C 3.089865 -0.224398 2.724945
 C 3.008375 1.150467 3.423602
 C 1.863732 -1.066712 3.095614
 C 4.361469 -0.971868 3.182596
 C 5.051202 -1.757551 -0.648256
 C 4.317841 -0.864091 -2.862408
 C -1.322891 -3.449761 0.949631
 H 5.045064 -1.524565 -3.348519
 H 3.365329 -1.400070 -2.794446
 H 4.182391 0.004725 -3.515940
 H 6.914782 -0.441659 -2.096993
 H 6.111724 1.124584 -2.284064
 H 6.583138 0.570755 -0.665742
 H 5.710943 -2.436383 -1.201445
 H 5.518142 -1.543255 0.316517
 H 4.104695 -2.274946 -0.460189
 H 2.958406 1.026318 4.512858
 H 3.884068 1.755353 3.176266
 H 2.111666 1.691841 3.098182
 H 4.344181 -1.121548 4.269232
 H 4.415167 -1.956910 2.705446
 H 5.257344 -0.403747 2.921997
 H 1.845345 -1.249895 4.176588
 H 0.934959 -0.555821 2.824477
 H 1.884025 -2.031767 2.581425
 H 2.074942 0.456037 -3.061843
 H 0.213407 2.237012 -1.373487
 H 3.809581 1.944981 -2.642918
 H 4.279691 4.333858 -0.795550
 H 5.266743 2.902257 -0.481287
 H 2.047112 3.605584 -0.760443
 H 0.287407 0.254284 -2.738905
 H 5.379305 3.717729 -2.054974
 H -0.244569 1.507705 2.525783
 H -1.141712 3.829547 2.404275
 H -2.693148 5.445762 1.421931
 H -5.556158 4.180086 -1.526605
 H -4.797935 1.860017 -1.303513
 H -4.533772 5.988128 -0.144417
 H -4.973880 -3.229134 -2.362323
 H -5.311604 0.903656 1.350663
 H -7.174471 -2.806877 -1.382853
 H -8.632284 -1.558463 0.183322
 H -7.671561 0.281084 1.568433
 H -2.538124 -2.722545 -2.478527
 H -0.928638 -4.140179 1.700754
 H -2.032344 -2.755323 1.396558
 H 0.561923 -4.446195 -0.500647
 H 1.557387 -2.957564 -0.686380

F 1.644211 -3.904631 1.099238
F -1.983380 -4.216938 -0.008539

XXIV-si

E0+ZPE = -2454.107716
E298 = -2454.062574
H298 = -2454.061630
G298 = -2454.185006
NImag = 1, (-175.7038)
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C -3.200922 2.345991 0.217130
C -2.544202 3.381622 0.963949
C -2.964012 4.730038 0.805465
C -3.967344 5.061496 -0.075296
C -4.588197 4.049170 -0.844153
C -2.780221 0.978777 0.386588
C -1.673164 0.739966 1.185554
C -1.018626 1.752327 1.919548
C -1.467139 3.046829 1.826971
O -1.177277 -0.562704 1.302622
P -0.249528 -1.101466 0.034820
N -0.276044 -2.759669 0.421462
C 0.898295 -3.562949 0.210837
C -3.454009 -0.164916 -0.290027
C -4.861560 -0.433697 -0.138023
C -5.460962 -1.500968 -0.887787
C -4.648655 -2.300762 -1.734229
C -3.294134 -2.094181 -1.805925
C -2.709831 -1.041397 -1.067729
C -6.851606 -1.758215 -0.748173
C -7.626000 -1.020488 0.117000
C -7.031411 0.005285 0.888703
C -5.689464 0.291360 0.764725
O -1.332875 -0.871628 -1.206353
Pd 1.786228 -0.106722 -0.427444
C 1.461435 -0.135717 -2.632710
C 2.353087 -1.233981 -2.716395
C 3.754844 -1.224190 -2.666549
C 4.543375 -0.079119 -2.583945
C 6.027065 -0.170528 -2.369460
N 3.152225 -0.166626 1.215097
C 4.175755 0.345849 0.521970
O 5.388524 0.380450 0.767404
N 3.609961 0.909910 -0.701036
C 3.646370 2.420709 -0.680720
C 5.091988 2.912229 -0.931768
C 3.317510 -0.740584 2.570034
C 4.006229 0.280254 3.502758
C 1.932744 -1.068671 3.141631
C 4.158562 -2.032736 2.484925
C 2.734972 2.984239 -1.784335
C 3.161221 2.988537 0.672914
C -1.439278 -3.483040 0.866461
H 3.149072 4.083804 0.622384
H 2.148641 2.643922 0.905704
H 3.823704 2.694753 1.491199

H 5.114977 4.008020 -0.887570
 H 5.774132 2.507817 -0.182863
 H 5.447791 2.611939 -1.922637
 H 2.788499 4.078971 -1.777403
 H 3.040441 2.653567 -2.783070
 H 1.690496 2.697837 -1.624790
 H 4.108676 -0.139033 4.511184
 H 4.997945 0.540830 3.127401
 H 3.406843 1.195555 3.576226
 H 4.309565 -2.457576 3.485644
 H 3.644032 -2.782593 1.875130
 H 5.135750 -1.818636 2.044567
 H 2.030024 -1.444001 4.167201
 H 1.299003 -0.175681 3.166090
 H 1.431139 -1.839244 2.552364
 H 1.817214 0.849094 -2.909961
 H 1.891102 -2.222546 -2.729572
 H 4.159927 0.842848 -2.999437
 H 6.379473 -1.198021 -2.512332
 H 6.573192 0.488466 -3.054739
 H 4.248568 -2.184871 -2.530050
 H 0.416428 -0.318448 -2.862218
 H 6.274757 0.123541 -1.342309
 H -0.174513 1.481079 2.543628
 H -0.981493 3.836119 2.394682
 H -2.462771 5.499652 1.387468
 H -5.361929 4.314874 -1.559244
 H -4.697241 1.969722 -1.306493
 H -4.274506 6.096895 -0.192770
 H -5.110484 -3.102663 -2.304110
 H -5.250440 1.073732 1.372460
 H -7.289787 -2.563644 -1.332709
 H -8.686804 -1.231073 0.219818
 H -7.637728 0.570139 1.591514
 H -2.651901 -2.722437 -2.412022
 H 0.642521 -4.458326 -0.363567
 H 1.666189 -2.974675 -0.294859
 H -2.202318 -2.788042 1.214284
 H -1.149806 -4.172315 1.664343
 F 1.413206 -4.002894 1.429117
 F -1.966888 -4.250825 -0.170975

XXV-re

E0+ZPE = -2851.107608
 E298 = -2851.059721
 H298 = -2851.058777
 G298 = -2851.188815
 NImag = 1, (-190.5372)
 C -5.646912 0.521948 0.696598
 C -4.814600 -0.166885 -0.229612
 C -5.400366 -1.226609 -1.000949
 C -6.784806 -1.512739 -0.855912
 C -7.564291 -0.810166 0.033486
 C -6.982095 0.207991 0.824547
 C -4.583073 -1.989366 -1.876461
 C -3.233082 -1.754729 -1.957987

C -2.667074 -0.712781 -1.194061
 C -3.413594 0.127684 -0.384262
 C -2.745927 1.258032 0.320569
 C -3.181624 2.624319 0.183370
 C -2.536138 3.650335 0.952995
 C -1.456190 3.307157 1.808885
 C -0.992934 2.016065 1.871719
 C -1.633994 1.014389 1.112685
 C -2.970853 4.997327 0.824512
 C -3.978435 5.336589 -0.048280
 C -4.589374 4.334484 -0.838388
 C -4.204309 3.016671 -0.725206
 O -1.121645 -0.287484 1.207082
 P -0.232482 -0.797313 -0.083077
 Pd 1.881736 0.046474 -0.455627
 N 3.861305 0.719232 -0.735560
 C 4.878826 -0.195867 -1.380471
 C 4.395788 -0.609093 -2.781143
 O -1.287882 -0.521356 -1.321015
 N -0.325364 -2.542250 0.213638
 C -1.406183 -3.309270 0.784371
 F -1.988571 -4.110588 -0.130449
 C 0.798533 -3.305091 -0.264022
 F 1.881447 -3.173898 0.523493
 C 1.308032 0.920583 -2.420564
 C 1.230045 2.178736 -1.769870
 C 2.284804 3.032891 -1.420441
 C 3.629056 2.792954 -1.702441
 C 4.708294 3.685623 -1.158528
 N 3.086570 0.210720 1.310266
 C 3.053889 0.011018 2.775692
 C 4.330764 -0.716910 3.250442
 C 4.094398 0.844409 0.701238
 O 5.071268 1.449367 1.162420
 C 6.233607 0.538342 -1.518994
 C 5.098290 -1.481682 -0.550266
 C 2.942054 1.380841 3.480320
 C 1.837483 -0.853899 3.127713
 H 5.145579 -1.258153 -3.247841
 H 3.453486 -1.164138 -2.730558
 H 4.260280 0.253913 -3.442542
 H 6.968595 -0.143149 -1.964429
 H 6.149062 1.410939 -2.174796
 H 6.594697 0.869612 -0.544557
 H 5.786948 -2.145309 -1.086416
 H 5.537582 -1.256701 0.425052
 H 4.159012 -2.019111 -0.390290
 H 2.876868 1.251515 4.568086
 H 3.813599 1.997472 3.248197
 H 2.044891 1.913424 3.143051
 H 4.297266 -0.874606 4.335587
 H 4.411745 -1.697417 2.767742
 H 5.220562 -0.131134 3.009270
 H 1.788826 -1.016146 4.210757
 H 0.904717 -0.376668 2.813959
 H 1.901860 -1.830101 2.637907

H 2.173521 0.701205 -3.034012
 H 0.242484 2.473402 -1.415018
 H 3.874665 2.198942 -2.572606
 H 4.278662 4.589992 -0.713822
 H 5.266857 3.165685 -0.371511
 H 2.049938 3.855049 -0.747027
 H 0.378825 0.490084 -2.779784
 H 5.415934 3.980321 -1.942700
 H -0.147614 1.741170 2.491370
 H -0.979388 4.087251 2.396342
 H -2.478159 5.759377 1.423385
 H -5.367088 4.607296 -1.546353
 H -4.677111 2.264601 -1.345610
 H -4.297115 6.370773 -0.142980
 H -5.036991 -2.783328 -2.463423
 H -5.216340 1.296808 1.319781
 H -7.213741 -2.311832 -1.455651
 H -8.619949 -1.042940 0.140665
 H -7.592669 0.744093 1.545849
 H -2.585021 -2.347232 -2.594674
 F -2.354453 -2.515239 1.275780
 F -0.958801 -4.095970 1.778600
 F 1.159904 -2.891094 -1.498269
 F 0.511868 -4.608882 -0.337977

XXV-si

E0 = -2851.7907517
 E0+ZPE = -2851.105603
 E298 = -2851.057674
 H298 = -2851.056730
 G298 = -2851.186198
 NImag = 1, (-181.3090)
 C -5.511000 0.889293 0.762139
 C -4.766481 0.143046 -0.193836
 C -5.474977 -0.813589 -0.996072
 C -6.882646 -0.942651 -0.851037
 C -7.572887 -0.186907 0.067926
 C -6.873174 0.727420 0.889683
 C -4.754726 -1.635042 -1.902918
 C -3.387084 -1.558589 -1.981319
 C -2.698914 -0.618430 -1.185648
 C -3.340568 0.283027 -0.350593
 C -2.557858 1.325285 0.372493
 C -2.864965 2.730128 0.276338
 C -2.130850 3.668335 1.077669
 C -1.087816 3.202479 1.921389
 C -0.741308 1.874020 1.939947
 C -1.469845 0.959735 1.150111
 C -2.441481 5.052544 0.993100
 C -3.412070 5.509913 0.132197
 C -4.108092 4.593412 -0.690390
 C -3.844199 3.243092 -0.619735
 O -1.078339 -0.383621 1.204207
 P -0.250655 -0.932598 -0.107981
 Pd 1.811250 0.067585 -0.452812
 N 3.565234 1.230904 -0.571531

C 3.518879 2.724587 -0.340995
 C 3.050042 3.075140 1.089436
 O -1.308602 -0.590645 -1.326474
 N -0.475854 -2.673585 0.195537
 C -1.660566 -3.341844 0.683180
 F -2.339054 -3.949427 -0.311673
 C 0.590455 -3.574221 -0.148752
 F 1.354258 -3.903369 0.908149
 C 1.485642 0.332644 -2.638720
 C 2.447062 -0.682768 -2.874572
 C 3.843222 -0.585131 -2.810900
 C 4.552365 0.588296 -2.559167
 C 6.040537 0.564851 -2.356991
 N 3.171229 -0.106314 1.187013
 C 3.372180 -0.865669 2.441470
 C 4.220110 -2.122100 2.150098
 C 4.166218 0.536104 0.566312
 O 5.378029 0.595919 0.809258
 C 4.929352 3.324928 -0.553243
 C 2.544607 3.378083 -1.334997
 C 4.076154 0.014217 3.499014
 C 2.002619 -1.279625 2.994724
 H 2.982151 4.164986 1.190371
 H 2.064413 2.648604 1.295754
 H 3.753105 2.709239 1.842274
 H 4.895914 4.402456 -0.351571
 H 5.652899 2.856717 0.115706
 H 5.270016 3.189638 -1.584534
 H 2.526691 4.461582 -1.170506
 H 2.844044 3.215441 -2.376170
 H 1.526781 2.998760 -1.199548
 H 4.195319 -0.545618 4.434714
 H 5.060140 0.330299 3.147977
 H 3.477377 0.907564 3.713315
 H 4.380133 -2.702357 3.067793
 H 3.712024 -2.765050 1.423675
 H 5.193777 -1.833194 1.745244
 H 2.127350 -1.824439 3.937677
 H 1.377061 -0.402069 3.190281
 H 1.471583 -1.934666 2.300987
 H 1.771827 1.368746 -2.775176
 H 2.052558 -1.686416 -3.022411
 H 4.107398 1.531225 -2.847378
 H 6.456373 -0.407750 -2.642094
 H 6.537420 1.347045 -2.943024
 H 4.401437 -1.519639 -2.809831
 H 0.455728 0.115214 -2.903939
 H 6.278239 0.726978 -1.298818
 H 0.077162 1.501889 2.545679
 H -0.543851 3.917660 2.532515
 H -1.882944 5.746936 1.616018
 H -4.855019 4.958225 -1.390061
 H -4.380464 2.558040 -1.265603
 H -3.635636 6.571258 0.071396
 H -5.299016 -2.349044 -2.515242
 H -4.992673 1.586698 1.409434

H -7.402671 -1.665411 -1.475054
H -8.648061 -0.299518 0.174702
H -7.414173 1.304292 1.634699
H -2.813657 -2.203707 -2.637918
F 1.398271 -3.020312 -1.069621
F 0.116790 -4.720719 -0.662212
F -2.498920 -2.494329 1.272890
F -1.324568 -4.293497 1.572538

XXVI-*re*

E0+ZPE = -2796.110542
E298 = -2796.055105
H298 = -2796.054161
G298 = -2796.199920
NImag = 1, (-205.4610)
C -0.046515 2.859686 -2.746670
C -0.036551 3.728790 -1.647634
C 0.139912 5.098259 -1.887366
C 0.315316 5.589075 -3.182703
C 0.315579 4.711499 -4.267488
C 0.131363 3.345179 -4.044104
C -0.304075 3.250602 -0.217431
C -1.808037 3.017590 -0.013331
N 0.567838 2.131784 0.255187
C 1.820050 2.579786 0.974178
C 1.467941 3.233676 2.315255
C 1.510085 4.619987 2.518702
C 1.183197 5.175495 3.759327
C 0.817120 4.351405 4.822283
C 0.782290 2.966753 4.636984
C 1.104026 2.416747 3.397201
P 0.232583 0.512866 -0.064589
Pd -1.950829 -0.317025 -0.475311
N -3.167289 -0.562665 1.302231
C -4.150420 -1.209824 0.668527
O -5.118708 -1.846242 1.111215
O 1.206156 -0.035965 -1.330279
C 2.588673 -0.076657 -1.303108
C 3.251698 -0.967580 -0.470141
C 4.690331 -0.903910 -0.423411
C 5.389184 -0.045028 -1.336660
C 4.646620 0.750726 -2.249366
C 3.274061 0.756734 -2.218400
C 5.460990 -1.634224 0.524263
C 6.835796 -1.545452 0.546254
C 7.522140 -0.726529 -0.380885
C 6.808507 0.009108 -1.298851
C 2.466106 -1.946080 0.330813
C 2.705623 -3.366673 0.252970
C 1.972933 -4.254254 1.110921
C 0.994704 -3.721990 1.991337
C 0.708944 -2.379811 1.991084
C 1.430528 -1.509537 1.144746
C 3.612123 -3.945206 -0.680020
C 3.811713 -5.307518 -0.731412
C 3.121036 -6.173305 0.148506

C 2.217666 -5.652605 1.045735
 O 1.105025 -0.154879 1.200839
 C 2.738831 3.438417 0.096461
 N -3.918511 -1.053945 -0.764512
 C -4.992883 -0.194505 -1.397678
 C -5.323373 1.041224 -0.529570
 C -1.395323 -1.119100 -2.457900
 C -1.251535 -2.383815 -1.825442
 C -2.264953 -3.284246 -1.479139
 C -3.621851 -3.085004 -1.742967
 C -4.659013 -4.031224 -1.204736
 C -4.526145 0.298863 -2.777813
 C -6.292101 -1.014728 -1.583085
 C -3.174912 -0.417663 2.774110
 C -1.970331 0.435465 3.185098
 C -4.464155 0.291923 3.244419
 C -3.077658 -1.807716 3.442179
 H -5.312775 0.914333 -3.229275
 H -3.620899 0.909735 -2.700766
 H -4.329588 -0.529569 -3.467174
 H -7.066296 -0.369778 -2.016783
 H -6.140907 -1.856069 -2.266722
 H -6.642115 -1.401754 -0.625530
 H -6.043948 1.675896 -1.058868
 H -5.767722 0.748309 0.424994
 H -4.428683 1.635624 -0.325745
 H -3.027846 -1.708184 4.534152
 H -3.947820 -2.413419 3.180247
 H -2.179361 -2.335282 3.102296
 H -4.450477 0.426580 4.333389
 H -4.544911 1.282069 2.781219
 H -5.345416 -0.294600 2.975556
 H -1.911445 0.513764 4.277164
 H -1.036382 0.002556 2.817673
 H -2.049971 1.449408 2.780270
 H -2.278812 -0.935925 -3.057096
 H -0.246641 -2.638370 -1.491444
 H -3.894693 -2.503462 -2.613788
 H -4.186124 -4.919392 -0.771307
 H -5.238413 -3.546200 -0.411097
 H -1.993157 -4.104720 -0.817825
 H -0.488025 -0.659322 -2.834095
 H -5.354321 -4.350903 -1.990359
 H -0.057788 -1.963879 2.632369
 H 0.451890 -4.396189 2.648653
 H 1.661048 -6.306332 1.712980
 H 4.503248 -5.720981 -1.460476
 H 4.142873 -3.301268 -1.370830
 H 3.293992 -7.244872 0.102561
 H 5.181256 1.379455 -2.956883
 H 4.952134 -2.260167 1.248165
 H 7.320666 0.657625 -2.005757
 H 8.606879 -0.671428 -0.357067
 H 7.398027 -2.106776 1.287553
 H 2.689157 1.383685 -2.883760
 H -0.042508 4.078526 0.447545

H 2.361170 1.663757 1.206802
 H 2.276082 4.372873 -0.228779
 H 3.643440 3.688291 0.662065
 H 3.036051 2.886777 -0.796867
 H -2.338582 3.949401 -0.238004
 H -2.198841 2.242669 -0.679426
 H -2.023854 2.727153 1.017619
 H 0.138464 5.792004 -1.048517
 H -0.197111 1.795795 -2.596573
 H 0.453741 6.655304 -3.341856
 H 0.120403 2.652786 -4.882088
 H 0.454183 5.087801 -5.277401
 H 1.812633 5.281528 1.712678
 H 1.075719 1.340503 3.259594
 H 1.222049 6.253621 3.892049
 H 0.507472 2.313160 5.460654
 H 0.566661 4.781660 5.788259

(XXVI-*re*)₁

E0 = -2797.056593
 E0+ZPE = -2796.103786
 E298 = -2796.048180
 H298 = -2796.047236
 G298 = -2796.193575
 NImag = 1, (-208.5725)
 C -1.157145 6.107396 0.482776
 C -1.148705 4.709519 0.738704
 C -2.035132 3.850257 0.005093
 C -2.846993 4.442267 -1.003388
 C -2.816503 5.799269 -1.240185
 C -1.975842 6.647098 -0.481822
 C -2.033884 2.432900 0.276870
 C -1.074064 1.947101 1.152742
 C -0.197277 2.787615 1.872877
 C -0.254491 4.145936 1.687079
 C -2.976137 1.493758 -0.393172
 C -2.481184 0.393610 -1.082755
 C -3.304581 -0.427600 -1.888793
 C -4.655180 -0.188194 -1.951003
 C -5.245445 0.840102 -1.168506
 C -4.405048 1.680577 -0.363837
 C -5.035077 2.650997 0.464869
 C -6.404349 2.804255 0.470573
 C -7.224981 2.000764 -0.355398
 C -6.652421 1.037365 -1.153465
 O -1.128343 0.111695 -1.096952
 P -0.207118 -0.352308 0.229784
 O -0.973560 0.577810 1.386997
 N -0.671575 -1.884052 0.778677
 C -1.837842 -2.048037 1.731585
 C -1.407510 -1.957353 3.205920
 C 0.317028 -2.945206 0.384018
 C 0.455253 -4.120205 1.364393
 C 0.151237 -3.467578 -1.046953
 C -1.087735 -3.773948 -1.621486
 C -1.165371 -4.299958 -2.913337

C -0.005223 -4.533341 -3.653639
 C 1.236751 -4.237299 -3.089491
 C 1.309722 -3.707894 -1.800226
 C -2.792471 -3.220025 1.468053
 C -2.782482 -4.398484 2.228460
 C -3.724721 -5.406612 2.012095
 C -4.711829 -5.251266 1.038644
 C -4.755896 -4.071153 0.294674
 C -3.811498 -3.067965 0.515633
 Pd 2.060892 0.050984 -0.280418
 N 4.122832 0.398680 -0.644094
 C 5.003905 -0.672831 -1.247732
 C 4.449725 -1.104441 -2.616008
 C 1.593543 0.812045 -2.300946
 C 1.695875 2.120672 -1.758114
 C 2.863245 2.842042 -1.479025
 C 4.158957 2.388720 -1.738461
 C 5.356167 3.167044 -1.265813
 N 3.337249 0.151247 1.449658
 C 3.331648 0.064606 2.923667
 C 4.468730 -0.857383 3.416928
 C 4.411293 0.577620 0.775906
 O 5.484565 1.047482 1.181797
 C 6.441368 -0.136267 -1.447247
 C 5.072120 -1.923972 -0.341738
 C 3.499892 1.471329 3.539392
 C 1.988408 -0.528767 3.358996
 H 5.100216 -1.876119 -3.044157
 H 3.441285 -1.519887 -2.528556
 H 4.423226 -0.275077 -3.331053
 H 7.070614 -0.934122 -1.860750
 H 6.458808 0.699814 -2.153611
 H 6.862724 0.200638 -0.499548
 H 5.650449 -2.709121 -0.843152
 H 5.558651 -1.700998 0.611137
 H 4.070997 -2.314079 -0.131019
 H 3.451878 1.421472 4.634742
 H 4.460447 1.898695 3.243933
 H 2.704213 2.139962 3.190794
 H 4.452705 -0.934321 4.511399
 H 4.349427 -1.865711 3.003446
 H 5.440241 -0.464407 3.108325
 H 1.942348 -0.623703 4.450409
 H 1.158677 0.104829 3.032559
 H 1.845562 -1.523052 2.921119
 H 2.413455 0.432620 -2.897982
 H 0.762259 2.579070 -1.433318
 H 4.310024 1.719143 -2.574756
 H 5.055553 4.151735 -0.890937
 H 5.853306 2.639151 -0.443854
 H 2.754494 3.738048 -0.870656
 H 0.610883 0.479724 -2.615774
 H 6.085899 3.307016 -2.072532
 H 0.504438 2.334616 2.563289
 H 0.407267 4.803428 2.244739
 H -0.487505 6.742081 1.058222

H -3.441149 6.220985 -2.022896
 H -3.489540 3.809946 -1.603915
 H -1.967691 7.716382 -0.673679
 H -5.293132 -0.802824 -2.581319
 H -4.422999 3.269494 1.110979
 H -7.271421 0.398615 -1.779169
 H -8.302695 2.137480 -0.347020
 H -6.858534 3.546914 1.120829
 H -2.834955 -1.229285 -2.449671
 H -2.437465 -1.155668 1.547257
 H 1.290682 -2.437946 0.402549
 H -0.432961 -4.752375 1.384649
 H 1.291253 -4.740082 1.024555
 H 0.685877 -3.777483 2.376775
 H -2.298618 -1.953437 3.844103
 H -0.772817 -2.787724 3.522320
 H -0.860646 -1.028995 3.374476
 H -2.044144 -4.536031 3.011263
 H -3.870914 -2.147250 -0.056119
 H -3.689874 -6.310542 2.614477
 H -5.533904 -3.922712 -0.449832
 H -5.447195 -6.033916 0.872836
 H -1.997444 -3.605531 -1.058546
 H 2.282505 -3.476156 -1.372743
 H -2.138558 -4.533257 -3.338493
 H 2.149523 -4.411330 -3.653404
 H -0.067919 -4.940925 -4.659109

(XXVI-*re*)₂

E0 = -2797.0616733
 E0+ZPE = -2796.108991
 E298 = -2796.053462
 H298 = -2796.052518
 G298 = -2796.198996
 NImag = 1, (-193.3571)
 C 2.355013 -5.539017 0.511884
 C 2.089170 -4.156018 0.702083
 C 2.759875 -3.187716 -0.118551
 C 3.629226 -3.669724 -1.137460
 C 3.850695 -5.018907 -1.307972
 C 3.220446 -5.966757 -0.468128
 C 2.497607 -1.783601 0.082683
 C 1.499830 -1.437726 0.981757
 C 0.842108 -2.385149 1.796490
 C 1.151706 -3.716583 1.674007
 C 3.231428 -0.723380 -0.662217
 C 2.529071 0.235114 -1.381784
 C 3.176599 1.172303 -2.221606
 C 4.545998 1.196866 -2.291941
 C 5.328888 0.324095 -1.489892
 C 4.671025 -0.635431 -0.649734
 C 5.482295 -1.438484 0.200586
 C 6.855554 -1.324458 0.194551
 C 7.500692 -0.405021 -0.664941
 C 6.747371 0.403026 -1.485385
 O 1.147487 0.265856 -1.371708

P 0.158387 0.549811 -0.026061
 O 1.141746 -0.098399 1.141994
 N 0.198585 2.162647 0.456513
 C 1.220451 2.874427 1.301460
 C 2.612884 2.929815 0.664017
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 C -0.179059 3.953688 -1.280630
 C 0.151642 5.287544 -1.006113
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 C 0.986450 5.592589 -3.258617
 C 0.648244 4.268713 -3.551595
 C 0.073528 3.460544 -2.570492
 C 1.242451 2.440948 2.774231
 C 2.254499 1.631578 3.307663
 C 2.280725 1.314270 4.666628
 C 1.296242 1.805130 5.525368
 C 0.287163 2.620445 5.011632
 C 0.267811 2.935053 3.652251
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 N -3.967526 -0.905716 -0.950260
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 C -3.721197 -2.863425 -2.112316
 C -4.811589 -3.805105 -1.684710
 N -3.246204 -0.614569 1.161058
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 C -4.230017 -1.185704 0.458042
 O -5.210992 -1.848478 0.827234
 C -5.206266 1.261387 -0.556993
 C -4.473391 0.626592 -2.856885
 C -3.071476 -2.109052 3.120286
 C -2.047730 0.190614 3.131795
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 H -6.697408 -1.086452 -0.825094
 H -5.878676 1.986327 -1.031162
 H -5.663660 0.936491 0.381364
 H -4.264111 1.766438 -0.321129
 H -5.217022 1.321108 -3.264661
 H -3.531213 1.171279 -2.736425
 H -4.325586 -0.162282 -3.602449
 H -3.004171 -2.152444 4.214985
 H -3.926143 -2.707160 2.794971
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 H -4.501257 -0.054123 4.309438
 H -4.651487 0.989196 2.881582
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 H -1.993792 0.176303 4.226315
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 H -2.252893 -0.655343 -3.187283

H -0.341493 -2.575656 -1.722296
 H -3.946476 -2.190517 -2.929084
 H -5.365372 -3.377371 -0.840669
 H -5.520151 -3.995487 -2.499587
 H -2.163083 -4.020979 -1.232713
 H -0.461233 -0.467142 -2.877923
 H -4.391351 -4.761100 -1.352908
 H 0.108350 -2.035147 2.512135
 H 0.659188 -4.452483 2.304164
 H 1.845595 -6.255948 1.151307
 H 4.512574 -5.357809 -2.100283
 H 4.114172 -2.960488 -1.797571
 H 3.409788 -7.027255 -0.608744
 H 5.048834 1.910134 -2.940159
 H 5.006701 -2.142304 0.873497
 H 7.226978 1.129366 -2.137386
 H 8.584531 -0.330294 -0.665081
 H 7.448158 -1.944519 0.861761
 H 2.563385 1.865339 -2.787463
 H 0.853972 3.904142 1.309774
 H -1.441685 2.320505 -0.802419
 H -1.258280 4.466554 1.372068
 H -2.526005 4.278679 0.159663
 H -2.259247 3.003532 1.367021
 H 3.264489 3.573485 1.265656
 H 3.079734 1.946183 0.596577
 H 2.549725 3.346515 -0.343680
 H 3.032018 1.237964 2.662682
 H -0.519803 3.578714 3.272084
 H 3.076551 0.683132 5.053729
 H -0.481970 3.019406 5.667809
 H 1.318601 1.559836 6.583855
 H -0.053917 5.711712 -0.027729
 H -0.185846 2.431096 -2.804924
 H 0.984831 7.129505 -1.747060
 H 0.822681 3.868256 -4.547005
 H 1.432486 6.225628 -4.020886

(XXVI-*re*)₃

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 G298 = -2796.197073
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 C 3.884223 -2.414964 0.766939
 C 4.963452 -2.887344 -0.032263
 C 5.606722 -4.069479 0.262857
 C 5.212812 -4.849136 1.375424
 C 3.184295 -1.185863 0.486096
 C 2.040631 -0.910256 1.220769
 C 1.619121 -1.713166 2.303574
 C 2.331792 -2.838853 2.633281
 C 3.619307 -0.254726 -0.590615

C 2.719435 0.107968 -1.583495
 C 3.112419 0.848519 -2.723343
 C 4.405188 1.296453 -2.836037
 C 5.343785 1.066979 -1.795252
 C 4.949014 0.296266 -0.650595
 C 5.890990 0.143742 0.405150
 C 7.152866 0.690315 0.319826
 C 7.549922 1.416857 -0.827294
 C 6.658709 1.601570 -1.859065
 O 1.402403 -0.314133 -1.532906
 P 0.279191 0.224260 -0.388132
 O 1.288842 0.231965 0.942490
 N 0.025104 1.882767 -0.541613
 C -1.154527 2.223716 -1.410465
 C -0.814764 2.226869 -2.911607
 C 1.023703 2.915611 -0.093390
 C 1.567074 3.785109 -1.234428
 C 0.540019 3.729877 1.117811
 C 0.315779 5.110878 1.064926
 C -0.074947 5.820067 2.203461
 C -0.240943 5.161780 3.421031
 C -0.006988 3.786531 3.491270
 C 0.382994 3.082412 2.353018
 C -1.939885 3.446450 -0.941283
 C -1.998874 4.635083 -1.678916
 C -2.775005 5.712253 -1.241479
 C -3.513221 5.611857 -0.063229
 C -3.476906 4.423925 0.672215
 C -2.701352 3.353898 0.232913
 Pd -1.651885 -1.109645 -0.571479
 N -3.472442 -2.175617 -0.739335
 C -4.656240 -1.570063 -1.457281
 C -4.276536 -1.241701 -2.911361
 C -0.945627 -2.062777 -2.438588
 C -0.611406 -3.195882 -1.649425
 C -1.472379 -4.196079 -1.180637
 C -2.838033 -4.260422 -1.459947
 C -3.718061 -5.279563 -0.793263
 N -2.833985 -1.285762 1.225824
 C -2.814101 -0.994335 2.674863
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 C -3.674856 -2.186039 0.705866
 O -4.494621 -2.939781 1.250952
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 C -5.130027 -0.264505 -0.778487
 C -2.329896 -2.241703 3.446415
 C -1.852852 0.172334 2.923209
 H -5.145555 -0.820041 -3.429455
 H -3.466094 -0.506860 -2.955575
 H -3.969023 -2.133084 -3.469257
 H -6.695213 -2.112898 -1.972534
 H -5.576347 -3.483561 -2.018658
 H -6.117321 -2.849055 -0.453538
 H -5.943289 0.177847 -1.365908
 H -5.504435 -0.452755 0.231174
 H -4.318771 0.467313 -0.712771

H -2.263708 -2.032938 4.522069
 H -3.022471 -3.072716 3.291430
 H -1.339413 -2.548787 3.090655
 H -4.189274 -0.341640 4.239396
 H -4.566407 0.306243 2.630681
 H -4.935864 -1.391019 3.009303
 H -1.782580 0.389455 3.995820
 H -0.851739 -0.054979 2.549944
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 H -4.350753 -4.792315 -0.042003
 H -1.079788 -4.871854 -0.422991
 H -0.119779 -1.511590 -2.874637
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 H 0.739797 -1.417542 2.861935
 H 2.020701 -3.455451 3.472440
 H 3.826659 -5.036738 3.000129
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 H 5.275021 -2.311941 -0.895749
 H 5.733848 -5.775331 1.601132
 H 4.717676 1.855700 -3.714250
 H 5.600901 -0.401235 1.295940
 H 6.942907 2.173621 -2.739159
 H 8.550393 1.836410 -0.884252
 H 7.848263 0.566375 1.145487
 H 2.374495 1.035224 -3.496773
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 H 1.867173 2.326552 0.271333
 H 0.807614 4.439413 -1.668303
 H 2.371190 4.420186 -0.847138
 H 1.985863 3.159548 -2.025213
 H -1.731361 2.355673 -3.498339
 H -0.115895 3.016330 -3.196458
 H -0.369258 1.266862 -3.189134
 H -1.447143 4.729362 -2.609069
 H -2.681312 2.430467 0.804016
 H -2.806152 6.625863 -1.829680
 H -4.056052 4.329630 1.586663
 H -4.119972 6.447269 0.275833
 H 0.432707 5.650771 0.131928
 H 0.574517 2.017117 2.421498
 H -0.249620 6.890584 2.132885
 H -0.120855 3.260494 4.435700
 H -0.543338 5.713775 4.307154

(XXVI-*re*)₄

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 E0+ZPE = -2796.107581
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 H298 = -2796.051328
 G298 = -2796.196191
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 C -1.173067 3.836392 -0.179445
 C -1.145345 5.234748 -0.259037
 C -2.177645 6.005238 0.282187
 C -0.063348 3.026261 -0.849745
 C -0.556232 2.470361 -2.199321
 N 0.591496 2.006496 0.026534
 C 1.558247 2.524044 1.076117
 C 2.385368 3.718454 0.596044
 C 2.108342 5.035620 0.990095
 C 2.914491 6.095963 0.568521
 C 4.016414 5.858995 -0.253838
 C 4.309267 4.551187 -0.646007
 C 3.503684 3.495010 -0.220373
 P 0.267142 0.359130 -0.162279
 Pd -1.903166 -0.493430 -0.576892
 C -1.285029 -1.400846 -2.491429
 C -1.158491 -2.628498 -1.785572
 C -2.184086 -3.507842 -1.423170
 C -3.531461 -3.323849 -1.746565
 C -4.588336 -4.240242 -1.195854
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 C 2.661076 -0.275278 -1.280416
 C 3.360686 0.493740 -2.239358
 C 4.733776 0.511612 -2.231770
 C 5.461168 -0.186413 -1.231068
 C 4.748832 -0.975577 -0.266301
 C 3.314545 -1.075604 -0.352593
 C 6.877653 -0.100989 -1.155913
 C 7.573959 -0.737586 -0.154685
 C 6.872853 -1.484265 0.821476
 C 5.501428 -1.602817 0.766074
 C 2.522583 -2.004620 0.500548
 C 1.450354 -1.531002 1.243526
 C 0.720176 -2.349094 2.132813
 C 1.033555 -3.680058 2.247596
 C 2.052472 -4.255902 1.444631
 C 2.795954 -3.420760 0.544271
 C 3.747879 -4.049010 -0.307873
 C 3.978699 -5.405835 -0.243610
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 O 1.093004 -0.184191 1.181726
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 C -4.145314 -1.324193 0.530802
 O -5.122092 -1.950184 0.970739
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 H 4.979691 -2.171726 1.526886
 H 7.401095 0.491937 -1.902297
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 H 7.421210 -1.965335 1.626769
 H 2.787690 1.049192 -2.974603
 H 2.268047 1.712668 1.236016
 H 0.737353 3.729581 -1.094164
 H -1.413198 1.798676 -2.089294
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 H 0.240122 1.935503 -2.727037
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 H -4.132602 3.493953 1.477868
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(XXVI-re)₅

E0 = -2797.0624834

E0+ZPE = -2796.109298

E298 = -2796.054024

H298 = -2796.053080

G298 = -2796.197988

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C 0.169388 3.710821 -0.706076

C 0.414736 3.148569 -1.969262

C 0.824342 3.936547 -3.043944

C -0.344516 2.805709 0.422476

C -0.905754 3.558265 1.633444

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C 2.548380 3.241556 1.407097

C 2.529688 4.313178 2.309904

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C -5.603764 -2.779588 -1.856306

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C 2.482748 -0.501080 -1.051623

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C 7.257943 -1.946831 -0.198758

C 6.441329 -2.800499 0.579479

C 5.068189 -2.698080 0.530846

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C 2.148699 -6.769350 -0.555822

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 H 7.290972 -0.309656 -1.582571
 H 8.339200 -2.043155 -0.156068
 H 6.901491 -3.541513 1.227438
 H 2.823594 1.160157 -2.378459
 H 2.503678 1.131561 1.401902
 H -1.202877 2.268790 -0.008426
 H -0.152871 4.155800 2.151613
 H -1.701333 4.234871 1.303043
 H -1.339654 2.848584 2.341137
 H 2.378889 1.803102 3.763594
 H 0.738516 2.434566 3.536512

H 1.058903 0.712346 3.304206
 H 1.952756 4.244865 3.226290
 H 3.400265 2.531130 -0.435043
 H 3.232015 6.293245 2.779362
 H 4.691239 4.584367 -0.887522
 H 4.610407 6.489593 0.715615
 H 0.145996 5.565429 0.399125
 H 0.279583 2.080868 -2.114830
 H 0.867653 6.957049 -1.489977
 H 1.000199 3.476910 -4.013515
 H 1.311122 5.932065 -3.714308

(XXVI-*re*)₆

E0+ZPE = -2796.098646
 E298 = -2796.043300
 H298 = -2796.042356
 G298 = -2796.187745
 NImag = 1, (-209.3673)
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 C 0.766234 4.316345 -0.534212
 C 1.193980 5.593176 -0.152074
 C 1.957226 6.385080 -1.015450
 C 2.298765 5.907013 -2.279891
 C 1.871564 4.635280 -2.675088
 C -0.107855 3.485242 0.404865
 C -1.526055 3.358733 -0.163038
 N 0.566240 2.210258 0.820212
 C 1.602395 2.492763 1.893338
 C 3.015740 1.940620 1.711580
 C 3.505792 0.848650 2.440172
 C 4.850955 0.484396 2.365718
 C 5.733764 1.207987 1.562915
 C 5.258611 2.295656 0.828874
 C 3.913866 2.656844 0.906043
 P 0.088320 0.710535 0.218213
 Pd -2.168910 0.195447 -0.372389
 N -3.515405 0.043333 1.319076
 C -4.534340 -0.439070 0.600528
 O -5.598971 -0.965450 0.959024
 O 1.024621 0.296035 -1.117962
 C 2.330563 -0.158260 -1.139030
 C 2.696932 -1.339723 -0.507659
 C 4.089590 -1.715773 -0.546530
 C 5.002060 -0.972118 -1.365695
 C 4.529166 0.160344 -2.079038
 C 3.231932 0.579688 -1.941542
 C 4.620466 -2.782377 0.231554
 C 5.956211 -3.117262 0.172186
 C 6.841608 -2.409442 -0.673283
 C 6.368423 -1.355745 -1.421416
 C 1.680167 -2.174599 0.190086
 C 1.521422 -3.582153 -0.096548
 C 0.612950 -4.368952 0.689173
 C -0.151183 -3.741180 1.707811
 C -0.072540 -2.385472 1.901308
 C 0.820161 -1.614937 1.125070

C 2.194137 -4.228167 -1.172374
 C 2.016022 -5.571006 -1.424549
 C 1.158754 -6.351541 -0.614441
 C 0.469667 -5.756466 0.416585
 O 0.832788 -0.239585 1.364969
 C 1.014605 2.241965 3.288375
 N -4.202286 -0.242489 -0.808809
 C -5.116125 0.789428 -1.438561
 C -5.309902 2.018774 -0.521712
 C -1.621784 -0.523655 -2.377348
 C -1.682659 -1.842144 -1.848563
 C -2.823542 -2.618146 -1.616936
 C -4.128242 -2.214771 -1.913502
 C -5.305521 -3.048667 -1.487036
 C -4.525329 1.281814 -2.770517
 C -6.507117 0.170984 -1.717919
 C -3.588450 0.121385 2.792954
 C -2.307956 0.793580 3.298747
 C -4.799786 0.973463 3.234038
 C -3.708028 -1.294867 3.398319
 H -5.200378 2.022194 -3.215200
 H -3.550914 1.758107 -2.623249
 H -4.411535 0.471822 -3.498858
 H -6.946857 -0.217871 -0.798956
 H -7.166312 0.941373 -2.136591
 H -6.443433 -0.642407 -2.447423
 H -5.929077 2.762575 -1.037371
 H -5.812938 1.746845 0.409550
 H -4.351415 2.484144 -0.275152
 H -3.714091 -1.247272 4.494890
 H -4.630248 -1.770302 3.057620
 H -2.864555 -1.919931 3.084931
 H -4.834520 1.052107 4.328013
 H -4.724011 1.986984 2.822950
 H -5.732248 0.523126 2.886380
 H -2.306208 0.847717 4.393973
 H -1.420490 0.239996 2.979278
 H -2.226689 1.814280 2.907943
 H -2.437900 -0.179311 -3.000382
 H -0.740871 -2.260376 -1.498486
 H -4.278507 -1.549085 -2.753144
 H -4.974388 -4.027797 -1.123352
 H -5.842316 -2.556670 -0.667992
 H -2.695423 -3.514423 -1.013135
 H -0.643778 -0.153402 -2.664044
 H -6.009174 -3.201338 -2.314186
 H -0.682528 -1.880773 2.640288
 H -0.827700 -4.342316 2.309536
 H -0.212650 -6.336280 1.033500
 H 2.535912 -6.032948 -2.259399
 H 2.846679 -3.647004 -1.812434
 H 1.034447 -7.411301 -0.818729
 H 5.221461 0.715129 -2.707265
 H 3.962426 -3.331863 0.894238
 H 7.039728 -0.785798 -2.059715
 H 7.890440 -2.689477 -0.718880

H 6.332749 -3.931504 0.785594
 H 2.867146 1.471556 -2.438577
 H -0.218260 4.056736 1.334549
 H 1.738821 3.573454 1.803497
 H 0.812850 1.184260 3.463949
 H 1.709668 2.597545 4.057083
 H 0.071086 2.785257 3.401614
 H -1.920705 4.371716 -0.300646
 H -1.555504 2.860077 -1.136025
 H -2.182364 2.817404 0.522805
 H 0.924135 5.976892 0.830017
 H 0.792197 2.858477 -2.125387
 H 2.281591 7.372400 -0.697605
 H 2.127165 4.259096 -3.662466
 H 2.890112 6.519118 -2.955420
 H 2.838368 0.280032 3.077779
 H 3.556347 3.517173 0.345646
 H 5.209376 -0.366692 2.938274
 H 5.936000 2.871096 0.203099
 H 6.781080 0.924073 1.508508

(XXVI-*re*)₇

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 E0+ZPE = -2796.107105
 E298 = -2796.051510
 H298 = -2796.050566
 G298 = -2796.196413
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 C -1.723466 3.876885 -0.304994
 C -2.734809 3.448966 0.568840
 C -3.596123 4.363896 1.172482
 C -3.462141 5.730543 0.911707
 C -2.466342 6.168721 0.039795
 C -0.822515 2.826968 -0.955083
 C -0.083680 3.309487 -2.210823
 N 0.114530 2.185032 0.032376
 C 0.897882 3.118463 0.916724
 C 2.396768 3.264914 0.647404
 C 3.357213 2.422072 1.225135
 C 4.720365 2.663642 1.049754
 C 5.153158 3.755429 0.294722
 C 4.211016 4.607939 -0.281039
 C 2.849033 4.363859 -0.097995
 P 0.158282 0.509353 -0.116091
 Pd -1.914236 -0.540320 -0.550239
 N -3.233537 -0.697931 1.164300
 C -4.135295 -1.450161 0.522724
 O -5.077038 -2.130198 0.958563
 O 1.217185 0.066809 -1.350747
 C 2.598457 0.085802 -1.293359
 C 3.286434 -0.754802 -0.429015
 C 4.724740 -0.657990 -0.397529
 C 5.396806 0.178410 -1.349756
 C 4.629771 0.940195 -2.270520
 C 3.260002 0.917474 -2.226171

C 5.521855 -1.325008 0.575229
 C 6.895119 -1.205503 0.579637
 C 7.555017 -0.417147 -0.391926
 C 6.814697 0.262037 -1.332227
 C 2.538459 -1.693609 0.450927
 C 2.823652 -3.108135 0.482857
 C 2.159648 -3.943703 1.442644
 C 1.201953 -3.370625 2.319921
 C 0.862702 -2.045103 2.213959
 C 1.512573 -1.228906 1.262485
 C 3.710200 -3.732297 -0.439602
 C 3.955020 -5.087207 -0.389282
 C 3.333693 -5.898126 0.589256
 C 2.451723 -5.334006 1.481540
 O 1.108519 0.109903 1.191714
 C 0.586228 2.894633 2.404933
 N -3.832053 -1.374503 -0.902067
 C -4.895826 -0.609297 -1.655309
 C -5.287684 0.692925 -0.921473
 C -1.201217 -1.447230 -2.427786
 C -1.042711 -2.656636 -1.697153
 C -2.038470 -3.576104 -1.348617
 C -3.382284 -3.461871 -1.713379
 C -4.411735 -4.414456 -1.173345
 C -4.381443 -0.230348 -3.054517
 C -6.163918 -1.481139 -1.816965
 C -3.272673 -0.557337 2.637237
 C -2.174373 0.421673 3.066635
 C -4.636345 0.008854 3.093639
 C -3.031554 -1.931341 3.300640
 H -5.160312 0.322657 -3.592159
 H -3.494045 0.407895 -2.993752
 H -4.136950 -1.111463 -3.657761
 H -6.935572 -0.903238 -2.340356
 H -5.957781 -2.376458 -2.412168
 H -6.545606 -1.792246 -0.843891
 H -6.024513 1.241633 -1.520124
 H -5.733374 0.482732 0.054497
 H -4.419506 1.341753 -0.772990
 H -3.016342 -1.836747 4.394104
 H -3.822895 -2.629364 3.018198
 H -2.072138 -2.349248 2.975268
 H -4.645714 0.150461 4.181825
 H -4.820472 0.982773 2.624056
 H -5.446310 -0.669379 2.818146
 H -2.120443 0.480270 4.160322
 H -1.196750 0.112576 2.688160
 H -2.375680 1.427974 2.686543
 H -2.052508 -1.352913 -3.091190
 H -0.052096 -2.839874 -1.281665
 H -3.621314 -2.952798 -2.637620
 H -3.930765 -5.272171 -0.689902
 H -5.027712 -3.912154 -0.418059
 H -1.776824 -4.334478 -0.613144
 H -0.297364 -0.958672 -2.774096
 H -5.073272 -4.782450 -1.966395

H 0.106557 -1.601856 2.849616
 H 0.714426 -4.002525 3.057564
 H 1.948098 -5.947533 2.224699
 H 4.628565 -5.537871 -1.113069
 H 4.187645 -3.129524 -1.202810
 H 3.542488 -6.963740 0.623138
 H 5.144689 1.568391 -2.992579
 H 5.036765 -1.927875 1.333844
 H 7.304341 0.891743 -2.071425
 H 8.638663 -0.339394 -0.383885
 H 7.475772 -1.720326 1.340360
 H 2.659135 1.518441 -2.899759
 H -1.493759 2.017526 -1.276201
 H 0.466823 4.090967 0.669600
 H 0.930364 1.922844 2.761753
 H 1.077842 3.673729 2.997999
 H -0.492225 2.960705 2.570692
 H -0.788780 3.746059 -2.926982
 H 0.682730 4.055791 -1.983266
 H 0.411676 2.460620 -2.689854
 H -2.847612 2.386608 0.765807
 H -0.844950 5.610396 -1.251041
 H -4.376167 4.008676 1.840618
 H -2.356757 7.228340 -0.175773
 H -4.133422 6.445554 1.379640
 H 3.039568 1.573886 1.820326
 H 2.125071 5.057726 -0.519559
 H 5.446106 1.994489 1.503233
 H 4.532612 5.470672 -0.858984
 H 6.215674 3.942203 0.163230

XXVI-si

E0 = -2797.0617058
 E0+ZPE = -2796.108235
 E298 = -2796.052886
 H298 = -2796.051941
 G298 = -2796.196489
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 C -2.318616 3.569199 0.198794
 C -3.154902 4.237857 -0.738909
 C -3.216634 5.613476 -0.787639
 C -2.448897 6.403781 0.099393
 C -2.226976 2.131879 0.279287
 C -1.249928 1.592611 1.102157
 C -0.443917 2.383919 1.949864
 C -0.592619 3.748261 1.949713
 C -3.104732 1.236383 -0.523397
 C -2.538563 0.270934 -1.346151
 C -3.309599 -0.482309 -2.263559
 C -4.672501 -0.324920 -2.304953
 C -5.327836 0.549404 -1.398161
 C -4.542741 1.328280 -0.483342
 C -5.233550 2.137352 0.461963
 C -6.609918 2.198696 0.478603

C -7.377787 1.460101 -0.452082
 C -6.744718 0.650846 -1.367087
 O -1.169010 0.068597 -1.366228
 P -0.264520 -0.552494 -0.077813
 O -1.077508 0.211492 1.168020
 N -0.766736 -2.126357 0.264024
 C 0.011799 -3.342404 -0.111334
 C 1.517831 -3.255515 0.187037
 C -2.092722 -2.430744 0.922341
 C -3.034624 -3.228045 0.011766
 C -1.874875 -3.073940 2.297878
 C -2.176314 -4.416461 2.564301
 C -1.972702 -4.961255 3.836074
 C -1.469186 -4.168995 4.866270
 C -1.172384 -2.826249 4.616523
 C -1.372615 -2.287203 3.346966
 C -0.226283 -3.871637 -1.529871
 C -0.226673 -5.260887 -1.726709
 C -0.372037 -5.811039 -3.000479
 C -0.522029 -4.976549 -4.110008
 C -0.524642 -3.593192 -3.928764
 C -0.378577 -3.046644 -2.650185
 Pd 1.924375 0.282424 -0.437183
 N 3.754158 1.314419 -0.622902
 C 3.784885 2.828404 -0.625200
 C 3.267019 3.414472 0.707410
 C 1.752700 0.241147 -2.647417
 C 2.658245 -0.850280 -2.682380
 C 4.051803 -0.818393 -2.547696
 C 4.813973 0.342168 -2.416574
 C 6.284603 0.271245 -2.117718
 N 3.219832 0.269995 1.296480
 C 3.367027 -0.301529 2.653106
 C 4.271226 -1.552942 2.597525
 C 4.263991 0.781807 0.639020
 O 5.465457 0.844071 0.939457
 C 5.234609 3.323625 -0.844157
 C 2.900778 3.374343 -1.759002
 C 3.980565 0.739297 3.616877
 C 1.980355 -0.688664 3.179397
 H 3.250767 4.508802 0.637971
 H 2.252378 3.068518 0.921464
 H 3.914282 3.138218 1.543916
 H 5.250207 4.419876 -0.807456
 H 5.897362 2.929137 -0.072971
 H 5.618258 3.019219 -1.822952
 H 2.942881 4.469666 -1.757358
 H 1.855606 3.076934 -1.628607
 H 4.054556 0.322831 4.629410
 H 4.977615 1.032871 3.282554
 H 3.348865 1.634304 3.664011
 H 4.375033 -1.999902 3.594584
 H 3.845436 -2.306769 1.926351
 H 5.263266 -1.281635 2.228593
 H 2.066001 -1.171123 4.160049
 H 1.344459 0.195703 3.292755

H 1.471954 -1.380087 2.503234
 H 2.113893 1.228347 -2.908335
 H 2.209645 -1.842390 -2.724172
 H 4.447424 1.252816 -2.870817
 H 6.654687 -0.753998 -2.228446
 H 6.861094 0.928001 -2.780101
 H 4.552514 -1.770636 -2.380965
 H 0.725958 0.056402 -2.946028
 H 6.471158 0.579968 -1.082135
 H 0.278295 1.891266 2.589450
 H 0.012819 4.364658 2.608942
 H -0.993971 6.385833 1.673910
 H -3.858032 6.095686 -1.520322
 H -3.741943 3.652045 -1.435852
 H -2.513217 7.487412 0.055525
 H -5.268540 -0.892283 -3.015226
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 H -7.321472 0.061671 -2.076192
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 H -7.110463 2.817023 1.218767
 H -2.797342 -1.173792 -2.924297
 H -2.557332 -1.461088 1.099894
 H -0.368034 -4.109765 0.570526
 H -2.641727 -4.211986 -0.257137
 H -3.993464 -3.373577 0.521647
 H -3.222039 -2.680175 -0.912791
 H 1.975303 -4.224044 -0.041320
 H 2.029733 -2.495014 -0.406312
 H 1.683627 -3.037449 1.244017
 H -0.111626 -5.921306 -0.868988
 H -0.401427 -1.969552 -2.531351
 H -0.372709 -6.890794 -3.124797
 H -0.640316 -2.931805 -4.783766
 H -0.637806 -5.400181 -5.103816
 H -2.585792 -5.049996 1.783769
 H -1.140724 -1.243785 3.159838
 H -2.213835 -6.005525 4.017339
 H -0.786873 -2.195927 5.413594
 H -1.313418 -4.590063 5.855933
 H 3.240172 3.041162 -2.745901

(XXVI-si)₁

E0 = -2797.0585408
 E0+ZPE = -2796.105664
 E298 = -2796.050252
 H298 = -2796.049307
 G298 = -2796.194671
 NImag = 1, (-184.4069)
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 C -0.294941 -4.071667 -1.314263
 C -0.566724 -3.503681 -2.569287
 C -1.230864 -4.225552 -3.560767
 C 0.449382 -3.243136 -0.261082
 C 1.274632 -4.090843 0.715579

N -0.444270 -2.258709 0.435956
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 C -1.583987 -2.411628 2.718031
 C -2.538760 -1.526762 3.236292
 C -2.560297 -1.206552 4.594764
 C -1.627845 -1.768926 5.467359
 C -0.675674 -2.658552 4.968068
 C -0.661182 -2.976333 3.609469
 P -0.201603 -0.655834 -0.035070
 Pd 1.942606 0.211445 -0.525518
 C 1.652748 0.145603 -2.730835
 C 2.560172 -0.939964 -2.805558
 C 3.960354 -0.904645 -2.755428
 C 4.723828 0.257828 -2.682834
 C 6.210032 0.197884 -2.472568
 O -1.157204 -0.238458 -1.370193
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 C -3.065058 1.050371 -0.630222
 C -6.709567 0.503050 -1.491857
 C -7.334576 1.396014 -0.652212
 C -6.560469 2.179323 0.235210
 C -5.186159 2.077898 0.248946
 C -2.185963 1.973488 0.140427
 C -1.250097 1.465036 1.027860
 C -0.464308 2.283159 1.868863
 C -0.584714 3.648015 1.789063
 C -1.446110 4.243711 0.829906
 C -2.242171 3.405884 -0.021612
 C -3.023480 4.036388 -1.030234
 C -3.047944 5.407728 -1.161942
 C -2.297453 6.230903 -0.290265
 C -1.511090 5.655419 0.680813
 O -1.087594 0.085086 1.149486
 N 3.343912 0.167159 1.111800
 C 4.350068 0.687223 0.403540
 O 5.566436 0.743882 0.636868
 N 3.766561 1.232849 -0.817687
 C 3.790334 2.745228 -0.807953
 C 5.221840 3.249923 -1.108932
 C 3.550397 -0.413446 2.454254
 C 4.228154 0.608920 3.393838
 C 2.184022 -0.782383 3.039160
 C 4.430004 -1.677585 2.337965
 C 2.836214 3.291220 -1.883738
 C 3.350119 3.319230 0.558110
 C -2.939942 -2.729377 0.564329
 H 3.327640 4.414068 0.499045
 H 2.350535 2.969583 0.831469
 H 4.047112 3.037462 1.351809
 H 5.234420 4.346083 -1.067553
 H 5.931515 2.855392 -0.380406
 H 5.549284 2.952217 -2.110140

H 2.870514 4.386798 -1.879949
 H 1.802633 2.985264 -1.692348
 H 4.344593 0.182758 4.398294
 H 5.212134 0.890482 3.013303
 H 3.613250 1.512620 3.478639
 H 4.568134 -2.147888 3.320141
 H 3.962374 -2.408571 1.667908
 H 5.410042 -1.416247 1.931005
 H 2.300156 -1.260981 4.018168
 H 1.561581 0.108812 3.172943
 H 1.641511 -1.469020 2.384654
 H 1.996400 1.132813 -3.015223
 H 2.118052 -1.936624 -2.815313
 H 4.321339 1.165903 -3.111112
 H 6.582424 -0.822371 -2.617546
 H 6.741016 0.868052 -3.158902
 H 4.472775 -1.854069 -2.609748
 H 0.610651 -0.046858 -2.962712
 H 6.453558 0.495678 -1.445494
 H 0.214525 1.807646 2.567083
 H 0.004220 4.288957 2.439770
 H -0.910088 6.273401 1.343639
 H -3.646122 5.860515 -1.948023
 H -3.596489 3.422793 -1.715089
 H -2.332084 7.311257 -0.399823
 H -5.256788 -1.211363 -2.980877
 H -4.612694 2.680293 0.943535
 H -7.290949 -0.122138 -2.165505
 H -8.416776 1.491390 -0.658351
 H -7.054099 2.865512 0.918077
 H -2.796870 -1.556412 -2.820613
 H 1.176316 -2.625598 -0.800208
 H -1.333076 -3.910510 1.257984
 H 0.663231 -4.740822 1.348637
 H 1.961030 -4.732864 0.152619
 H 1.864668 -3.441112 1.365014
 H -3.682489 -3.293766 1.139630
 H -3.285150 -1.697105 0.490018
 H -2.895022 -3.146272 -0.444327
 H -3.273921 -1.074110 2.580168
 H 0.082300 -3.675777 3.239380
 H -3.311088 -0.515926 4.970119
 H 0.052171 -3.112864 5.635315
 H -1.646225 -1.520854 6.525272
 H -0.497877 -5.871274 -0.134828
 H -0.260209 -2.480471 -2.768410
 H -1.695148 -7.136160 -1.869113
 H -1.417485 -3.767348 -4.528672
 H -2.162784 -6.102625 -4.083376
 H 3.117710 2.963327 -2.890558

(XXVI-si)₂

E0 = -2797.0504258

E0+ZPE = -2796.097457

E298 = -2796.042062

H298 = -2796.041118

G298 = -2796.186365
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 C 2.771631 -3.245342 1.643083
 C 3.315451 -2.468930 0.564986
 C 4.309521 -3.074025 -0.254226
 C 4.764506 -4.349512 -0.000416
 C 4.257565 -5.093552 1.090664
 C 2.812844 -1.138802 0.325328
 C 1.712998 -0.727636 1.064396
 C 1.176809 -1.482466 2.130202
 C 1.719080 -2.707376 2.430224
 C 3.424086 -0.228452 -0.685283
 C 2.639661 0.355213 -1.672975
 C 3.196785 1.115242 -2.728714
 C 4.546553 1.354765 -2.765403
 C 5.391028 0.887991 -1.723247
 C 4.828177 0.104265 -0.660234
 C 5.690331 -0.276856 0.406756
 C 7.026195 0.061355 0.403213
 C 7.583375 0.797523 -0.668097
 C 6.776018 1.203722 -1.705408
 O 1.275373 0.154736 -1.714126
 P 0.166903 0.640151 -0.525959
 O 1.132737 0.512306 0.810660
 N 0.041903 2.340372 -0.509086
 C 0.897108 3.298958 0.302673
 C 2.366254 3.341435 -0.133453
 C -0.527342 3.035322 -1.710689
 C -1.200092 2.107371 -2.732267
 C -1.499501 4.153976 -1.340079
 C -2.682117 3.886183 -0.637464
 C -3.589956 4.907242 -0.357026
 C -3.332273 6.214448 -0.780593
 C -2.161645 6.491518 -1.486516
 C -1.253464 5.465879 -1.762873
 C 0.705708 3.242402 1.820931
 C 1.661726 2.704494 2.692706
 C 1.487577 2.766420 4.076228
 C 0.354761 3.375923 4.617743
 C -0.599966 3.927244 3.761988
 C -0.420757 3.862999 2.379577
 Pd -1.560167 -1.032997 -0.600829
 N -2.903118 -2.655431 -0.390961
 C -2.464387 -3.934667 0.291045
 C -2.096693 -3.702554 1.773834
 C -0.970387 -1.832958 -2.593468
 C -2.149689 -1.286882 -3.155882
 C -3.459775 -1.780304 -3.083469
 C -3.827405 -2.978353 -2.477771
 C -5.273323 -3.349496 -2.308371
 N -3.107249 -0.816419 0.877991
 C -3.642877 0.134510 1.871503
 C -4.842711 0.894563 1.264257
 C -3.795906 -1.885858 0.471930
 O -4.955840 -2.249372 0.713736

C -3.607246 -4.976856 0.235366
 C -1.230704 -4.515924 -0.419928
 C -4.092767 -0.602221 3.153299
 C -2.527866 1.116305 2.239763
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 H -1.315281 -2.944812 1.868760
 H -2.965450 -3.384240 2.355725
 H -3.292737 -5.883021 0.767699
 H -4.511138 -4.582815 0.702017
 H -3.841052 -5.262640 -0.794894
 H -0.936920 -5.451671 0.069524
 H -0.381112 -3.827964 -0.370813
 H -4.460000 0.118588 3.894511
 H -4.888063 -1.316631 2.930783
 H -3.248885 -1.142691 3.597652
 H -5.233350 1.636413 1.973001
 H -4.543939 1.416752 0.347644
 H -5.642309 0.192948 1.012955
 H -2.891362 1.867031 2.949979
 H -1.683474 0.595104 2.704585
 H -2.147292 1.637098 1.357742
 H -0.935494 -2.895071 -2.383989
 H -2.046605 -0.313540 -3.631766
 H -3.104301 -3.782348 -2.447518
 H -5.917998 -2.672027 -2.879296
 H -5.465243 -4.378286 -2.636149
 H -4.257543 -1.105336 -3.389590
 H -0.021858 -1.405606 -2.901087
 H -5.560564 -3.266550 -1.253484
 H 0.350631 -1.065210 2.695200
 H 1.324395 -3.293829 3.255554
 H 2.863034 -5.117720 2.718872
 H 5.516718 -4.790001 -0.649159
 H 4.701891 -2.523713 -1.101172
 H 4.631047 -6.095162 1.284589
 H 4.981463 1.928696 -3.579795
 H 5.283062 -0.833273 1.242525
 H 7.183672 1.788003 -2.527049
 H 8.639773 1.050909 -0.662006
 H 7.656639 -0.237019 1.236444
 H 2.530027 1.489803 -3.499146
 H 0.322144 3.507011 -2.227525
 H 0.470937 4.264598 0.019197
 H -2.063095 1.593047 -2.301922
 H -1.555220 2.720095 -3.567193
 H -0.505009 1.362668 -3.130343
 H 2.864008 4.190183 0.349118
 H 2.911175 2.433772 0.127448
 H 2.443831 3.477064 -1.216599
 H 2.553026 2.231223 2.296165
 H -1.165635 4.304344 1.723176
 H 2.243576 2.340797 4.731238
 H -1.481690 4.415882 4.168551
 H 0.221486 3.427301 5.695182
 H -2.890267 2.875212 -0.302813
 H -0.341520 5.688783 -2.313561

H -4.500563 4.680003 0.190781
H -1.950471 7.504104 -1.819902
H -4.040013 7.009262 -0.561229
H -1.431409 -4.751822 -1.470771

(XXVI-si)₃

E0 = -2797.0558315
E0+ZPE = -2796.102684
E298 = -2796.047157
H298 = -2796.046212
G298 = -2796.190818
NImag = 1, (-187.8447)
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C 1.491047 -4.292542 1.306006
C 2.286745 -3.524312 0.391206
C 3.124767 -4.233761 -0.514444
C 3.201470 -5.609216 -0.489258
C 2.449139 -6.358454 0.445372
C 2.181368 -2.085493 0.393977
C 1.194513 -1.514894 1.184112
C 0.409372 -2.265943 2.085890
C 0.579086 -3.625554 2.165093
C 3.072164 -1.230026 -0.439474
C 2.528427 -0.303921 -1.320912
C 3.321470 0.393687 -2.261732
C 4.682431 0.224042 -2.274264
C 5.315981 -0.604839 -1.311103
C 4.509632 -1.328074 -0.368825
C 5.179777 -2.088374 0.631000
C 6.555171 -2.156976 0.674655
C 7.343935 -1.475920 -0.281987
C 6.731959 -0.713982 -1.250704
O 1.161276 -0.097407 -1.377667
P 0.246131 0.571116 -0.129574
O 1.003140 -0.135449 1.175863
N 0.758144 2.163294 0.184608
C 1.634116 2.550451 1.356098
C 0.841582 3.328356 2.416640
C 0.353298 3.296054 -0.698295
C 0.349311 2.930289 -2.193461
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C -2.141923 3.413146 -0.039174
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C -3.250950 5.557289 0.195118
C -2.044947 6.201649 -0.084251
C -0.896507 5.450423 -0.339421
C 2.925847 3.253611 0.932328
C 3.065587 4.650274 0.926813
C 4.273320 5.251523 0.563817
C 5.370373 4.465297 0.210618
C 5.251069 3.074030 0.225957
C 4.041202 2.478970 0.582974
Pd -1.928264 -0.321725 -0.515547
N -3.678982 -1.502747 -0.664020
C -3.579523 -3.011428 -0.728990
C -2.970510 -3.595092 0.565079

C -1.847754 -0.184403 -2.736299
 C -2.846492 0.818115 -2.669638
 C -4.228519 0.662828 -2.486153
 C -4.890867 -0.557121 -2.385806
 C -6.348706 -0.623108 -2.028201
 N -3.213189 -0.363389 1.216924
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 C -4.559643 1.058551 2.740084
 C -4.190699 -1.058763 0.624265
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 C -4.981259 -3.632816 -0.936465
 C -2.680676 -3.425757 -1.906376
 C -3.497055 -1.072780 3.577834
 C -2.074684 0.908149 2.962712
 H -2.860736 -4.681031 0.458737
 H -1.982390 -3.170399 0.760833
 H -3.612470 -3.402739 1.428728
 H -4.887530 -4.725432 -0.966109
 H -5.651959 -3.350630 -0.124368
 H -5.424360 -3.312669 -1.884757
 H -2.610652 -4.518976 -1.943029
 H -1.668352 -3.025063 -1.794885
 H -3.571776 -0.721854 4.614695
 H -4.399449 -1.641175 3.337675
 H -2.634082 -1.745567 3.508052
 H -4.626280 1.450978 3.762890
 H -4.457233 1.909038 2.056948
 H -5.480952 0.525630 2.499446
 H -2.113738 1.246812 4.004871
 H -1.175323 0.299040 2.831058
 H -1.983270 1.789166 2.320474
 H -2.130653 -1.187337 -3.031198
 H -2.497260 1.849774 -2.658471
 H -4.467826 -1.418443 -2.885212
 H -6.797011 0.376549 -2.031217
 H -6.903386 -1.259517 -2.728613
 H -4.792075 1.562769 -2.246133
 H -0.853474 0.105848 -3.062192
 H -6.473942 -1.037440 -1.020946
 H -0.313075 -1.747134 2.704424
 H -0.011257 -4.210046 2.865703
 H 1.006030 -6.270692 2.028404
 H 3.842444 -6.123500 -1.200164
 H 3.699674 -3.680344 -1.247178
 H 2.525083 -7.442111 0.459585
 H 5.293888 0.749138 -3.003472
 H 4.593777 -2.608893 1.379313
 H 7.324322 -0.171048 -1.983629
 H 8.427296 -1.546281 -0.241493
 H 7.038664 -2.736693 1.456178
 H 2.825698 1.042655 -2.974600
 H 1.168517 4.015915 -0.590337
 H 1.933885 1.609921 1.810704
 H -0.392440 2.167885 -2.438334
 H 0.109356 3.824215 -2.778034
 H 1.333771 2.568411 -2.499820

H 1.495298 3.558889 3.265478
 H 0.429002 4.267924 2.040485
 H 0.007589 2.722274 2.776990
 H 2.233614 5.281712 1.224746
 H 3.964109 1.395904 0.602584
 H 4.356818 6.335299 0.567875
 H 6.100417 2.447210 -0.031652
 H 6.312646 4.932125 -0.064062
 H -2.200691 2.329041 -0.012799
 H 0.038828 5.962201 -0.559484
 H -4.226004 3.647813 0.432321
 H -1.994878 7.287356 -0.100204
 H -4.148294 6.135950 0.396898
 H -3.084378 -3.096800 -2.870464

(XXVI-si)₄

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 E0+ZPE = -2796.104076
 E298 = -2796.048115
 H298 = -2796.047171
 G298 = -2796.194330
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 C 3.273815 -3.962019 -0.436901
 C 3.391277 -5.333596 -0.380689
 C 2.688674 -6.079670 0.594417
 C 2.294472 -1.819567 0.441781
 C 1.311276 -1.258557 1.244387
 C 0.571322 -2.007842 2.184920
 C 0.784969 -3.359042 2.297271
 C 3.138278 -0.957601 -0.431642
 C 2.547525 -0.049553 -1.300781
 C 3.301044 0.705330 -2.229846
 C 4.666154 0.588172 -2.262623
 C 5.342726 -0.244309 -1.332735
 C 4.579174 -1.006417 -0.387093
 C 5.295367 -1.748334 0.594526
 C 6.673594 -1.769142 0.612468
 C 7.419898 -1.054382 -0.353457
 C 6.761540 -0.305442 -1.301647
 O 1.172610 0.082384 -1.368589
 P 0.161045 0.619861 -0.130858
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 N 0.302196 2.291865 0.048804
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 C 0.343076 3.497959 -2.163849
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 C 0.798191 2.908471 2.445460
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 C 3.523812 2.148796 1.279928
 C 4.907990 2.244405 1.130146
 C 5.471196 3.311886 0.428327
 C 4.638283 4.288108 -0.118143
 C 3.255007 4.189495 0.039517

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 C -1.021267 5.503878 -0.422574
 C -1.847567 6.482304 0.136939
 C -3.041643 6.120135 0.760170
 C -3.408056 4.773071 0.815324
 C -2.579530 3.799818 0.257897
 Pd -1.894653 -0.487502 -0.528286
 N -3.579278 -1.751973 -0.697925
 C -3.413150 -3.253415 -0.604725
 C -2.885587 -3.681877 0.783188
 C -1.640529 -0.543499 -2.746728
 C -2.682122 0.405381 -2.876606
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 C -6.162725 -1.134439 -2.359497
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 C -2.408155 -3.736913 -1.664270
 C -3.790784 -1.013914 3.478319
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 H 4.025846 -5.847473 -1.097591
 H 3.810767 -3.409273 -1.198370
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 H 7.319655 0.269209 -2.037179
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 H 1.143563 4.181492 -1.869577
 H 0.809805 2.629267 -2.635762
 H -0.105567 5.810714 -0.919782
 H -2.876326 2.754968 0.291717
 H -1.557207 7.528044 0.079070
 H -4.341487 4.478371 1.287151
 H -3.686126 6.880986 1.192069
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 H 2.620041 4.977251 -0.360046
 H 5.547210 1.479111 1.561173
 H 5.062030 5.133841 -0.653806
 H 6.549691 3.384067 0.315672
 H -2.742615 -3.514778 -2.683771

(XXVI-si)₅

E0 = -2797.0591568
 E0+ZPE = -2796.106210
 E298 = -2796.050839
 H298 = -2796.049895
 G298 = -2796.194899
 NImag = 1, (-178.2321)
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 C 2.826042 -3.507852 1.837833
 C 3.391627 -2.737805 0.766513
 C 4.421758 -3.338797 -0.010224
 C 4.890401 -4.601592 0.279811
 C 4.360398 -5.337900 1.365076
 C 2.872373 -1.421076 0.489956
 C 1.750871 -1.010237 1.193691
 C 1.189788 -1.763755 2.248036
 C 1.737398 -2.978004 2.579167
 C 3.471844 -0.532262 -0.543613
 C 2.675931 -0.019024 -1.559765
 C 3.220741 0.685055 -2.659901
 C 4.566835 0.948733 -2.707186
 C 5.416773 0.563871 -1.636654
 C 4.866939 -0.170424 -0.532773
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 C 7.059368 -0.113171 0.537986
 C 7.605357 0.575400 -0.570581
 C 6.795292 0.907913 -1.631761
 O 1.312553 -0.253934 -1.585356
 P 0.212204 0.347772 -0.450942
 O 1.164309 0.222547 0.910146
 N 0.133866 2.033270 -0.542386

C -0.977132 2.532415 -1.424133
 C -0.618306 2.476991 -2.921085
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 C 1.913275 3.731832 -1.211339
 C 0.886776 3.776946 1.140845
 C 0.845929 5.176069 1.106302
 C 0.555637 5.915619 2.255354
 C 0.308433 5.268729 3.465272
 C 0.358004 3.873706 3.516801
 C 0.647821 3.138807 2.367910
 C -1.573116 3.872437 -0.985394
 C -1.465956 5.033778 -1.761280
 C -2.072480 6.226994 -1.357795
 C -2.806029 6.275989 -0.173507
 C -2.933661 5.120801 0.601771
 C -2.326559 3.934940 0.195663
 Pd -1.650090 -1.093293 -0.571173
 N -3.122429 -2.602671 -0.459833
 C -2.727567 -4.005352 -0.059899
 C -2.118973 -4.048342 1.360594
 C -1.386158 -1.526527 -2.736878
 C -2.558656 -0.775015 -2.996786
 C -3.895894 -1.168864 -2.843945
 C -4.310798 -2.435364 -2.441526
 C -5.755405 -2.723908 -2.150758
 N -2.997368 -0.998092 1.103357
 C -3.368570 -0.115429 2.227016
 C -4.520466 0.817913 1.794488
 C -3.832643 -1.921083 0.617716
 O -4.994490 -2.214643 0.933681
 C -3.970910 -4.925893 -0.088901
 C -1.681414 -4.555652 -1.044161
 C -3.802617 -0.947431 3.454559
 C -2.141200 0.717214 2.611067
 H -1.795760 -5.072013 1.585149
 H -1.249594 -3.388912 1.439154
 H -2.849710 -3.749865 2.117351
 H -3.681461 -5.933768 0.232851
 H -4.748700 -4.546486 0.575268
 H -4.384889 -5.005062 -1.099266
 H -1.412057 -5.578508 -0.756637
 H -0.768823 -3.951127 -1.035690
 H -4.038732 -0.285947 4.297596
 H -4.682098 -1.550123 3.219671
 H -2.992489 -1.617756 3.765481
 H -4.796473 1.499162 2.609687
 H -4.223127 1.420583 0.928387
 H -5.398071 0.227746 1.518674
 H -2.392700 1.434871 3.400526
 H -1.335578 0.073683 2.980517
 H -1.753856 1.272369 1.752733
 H -1.444603 -2.608521 -2.747481
 H -2.408235 0.270366 -3.264454
 H -3.670637 -3.280511 -2.655925
 H -6.395796 -1.914535 -2.518771
 H -6.078083 -3.666080 -2.609230

H -4.648861 -0.384133 -2.893987
 H -0.438698 -1.128705 -3.086032
 H -5.908359 -2.798400 -1.067228
 H 0.336985 -1.359714 2.780731
 H 1.322068 -3.560881 3.396965
 H 2.911718 -5.361738 2.945354
 H 5.671501 -5.038428 -0.336441
 H 4.832512 -2.796558 -0.853359
 H 4.744481 -6.329571 1.587286
 H 4.993195 1.478159 -3.555476
 H 5.328705 -0.996530 1.418179
 H 7.195528 1.454023 -2.482757
 H 8.656390 0.850270 -0.574720
 H 7.692780 -0.352640 1.387770
 H 2.551384 0.990184 -3.457791
 H 2.018956 2.226019 0.273733
 H -1.777347 1.795116 -1.275801
 H 1.244582 4.481538 -1.639812
 H 2.789630 4.255293 -0.813990
 H 2.255208 3.067987 -2.007605
 H -1.497124 2.724082 -3.527646
 H 0.184558 3.165039 -3.193906
 H -0.290924 1.468447 -3.189352
 H -0.915855 5.020019 -2.696764
 H -2.432299 3.045649 0.807239
 H -1.974439 7.114571 -1.977586
 H -3.509770 5.141122 1.522661
 H -3.281198 7.201899 0.139319
 H 1.027221 5.707160 0.178610
 H 0.694683 2.056284 2.420041
 H 0.523064 7.000637 2.199193
 H 0.178989 3.355449 4.455497
 H 0.085308 5.843863 4.360157
 H -2.063148 -4.599226 -2.070373

(XXVI-si)₆

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 E0+ZPE = -2796.107299
 E298 = -2796.051832
 H298 = -2796.050888
 G298 = -2796.196165
 NImag = 1, (-178.1159)
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 C -1.983025 -5.698587 -1.721022
 C -1.406720 -5.028203 -0.638269
 C -1.042421 -3.680083 -0.734216
 C -1.262457 -3.027178 -1.958294
 C -1.830392 -3.693561 -3.043412
 C -0.336659 -2.928554 0.406795
 C 0.001416 -3.809453 1.616820
 N -0.994325 -1.635364 0.774317
 C -2.235507 -1.572631 1.634905
 C -3.254979 -2.681831 1.354589
 C -3.482673 -3.736908 2.248967
 C -4.456105 -4.705198 1.989475
 C -5.230211 -4.630238 0.832476

C -5.029984 -3.572064 -0.056818
 C -4.058282 -2.609111 0.207837
 P -0.216676 -0.247212 0.214385
 Pd 2.067217 -0.183966 -0.343088
 C 1.722114 -0.374485 -2.530902
 C 2.217928 -1.701129 -2.467995
 C 3.552780 -2.124757 -2.400925
 C 4.660009 -1.281165 -2.444114
 C 6.046395 -1.807861 -2.206824
 O -1.049562 0.412326 -1.099081
 C -2.311065 0.979936 -1.040360
 C -3.323725 0.356597 -1.807639
 C -4.596370 0.870864 -1.811068
 C -4.923637 1.997030 -1.010539
 C -3.890714 2.641032 -0.250355
 C -2.535510 2.157799 -0.338450
 C -6.256590 2.482683 -0.933663
 C -6.579210 3.541734 -0.116906
 C -5.572194 4.154459 0.665199
 C -4.266470 3.719574 0.598733
 C -1.392605 2.869912 0.295916
 C -0.535118 2.183571 1.141462
 C 0.524760 2.811442 1.831906
 C 0.752829 4.152441 1.647584
 C -0.028676 4.900872 0.728229
 C -1.099438 4.255263 0.023039
 C -1.798245 5.012811 -0.958561
 C -1.487764 6.334034 -1.195919
 C -0.462817 6.978524 -0.464731
 C 0.252233 6.270340 0.473140
 O -0.736129 0.824775 1.378666
 N 3.396417 -0.483108 1.324367
 C 4.505116 -0.425934 0.578989
 O 5.669378 -0.771591 0.825529
 N 4.119802 0.149491 -0.705651
 C 4.639325 1.561157 -0.852784
 C 6.157648 1.530137 -1.147842
 C 3.418829 -0.962995 2.721681
 C 4.450430 -0.170322 3.555947
 C 2.031068 -0.743620 3.334415
 C 3.770826 -2.466364 2.748866
 C 3.921886 2.264691 -2.017348
 C 4.406256 2.398033 0.426146
 C -1.882090 -1.437512 3.125713
 H 4.740150 3.427762 0.250415
 H 3.346172 2.421722 0.695375
 H 4.970745 1.999471 1.273449
 H 6.532405 2.558099 -1.226230
 H 6.695426 1.011209 -0.353071
 H 6.368670 1.025957 -2.096257
 H 4.312597 3.283091 -2.125584
 H 2.844464 2.333509 -1.836572
 H 4.435006 -0.509150 4.599463
 H 5.456500 -0.305470 3.154523
 H 4.209543 0.899256 3.543339
 H 3.776095 -2.847010 3.778421

H 3.037535 -3.042701 2.173082
 H 4.759145 -2.627907 2.310927
 H 1.995328 -1.142075 4.355282
 H 1.788232 0.323309 3.379056
 H 1.255583 -1.237204 2.743404
 H 2.365126 0.406545 -2.918761
 H 1.469338 -2.487272 -2.371269
 H 4.572062 -0.340340 -2.970519
 H 6.058285 -2.902875 -2.244854
 H 6.756290 -1.421590 -2.947733
 H 3.725016 -3.169019 -2.145568
 H 0.670350 -0.238178 -2.761700
 H 6.393594 -1.508490 -1.210388
 H 1.136359 2.215669 2.499165
 H 1.557142 4.649218 2.183737
 H 1.059062 6.744258 1.027058
 H -2.032891 6.884327 -1.958007
 H -2.578900 4.535494 -1.538582
 H -0.233599 8.023042 -0.656400
 H -5.375498 0.403031 -2.407553
 H -3.510799 4.195275 1.212825
 H -7.022714 1.987876 -1.525949
 H -7.603417 3.899514 -0.060243
 H -5.831491 4.973698 1.330275
 H -3.063037 -0.522699 -2.387466
 H 0.633903 -2.615560 -0.001796
 H -2.723788 -0.637757 1.347576
 H -0.883726 -4.242740 2.086754
 H 0.648319 -4.633092 1.296503
 H 0.547214 -3.229629 2.362775
 H -2.799384 -1.312585 3.712332
 H -1.346821 -2.307987 3.512352
 H -1.254571 -0.558681 3.277371
 H -2.911636 -3.807387 3.168755
 H -3.920236 -1.783843 -0.482075
 H -4.612113 -5.512726 2.700162
 H -5.636085 -3.492546 -0.955428
 H -5.989373 -5.381167 0.630348
 H -1.254044 -5.571213 0.287661
 H -0.996485 -1.979972 -2.063135
 H -2.263359 -6.743248 -1.614234
 H -1.981452 -3.164431 -3.981183
 H -2.639446 -5.559867 -3.772088
 H 4.084813 1.753839 -2.972921

(XXVI-si)₇

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 E0+ZPE = -2796.097649
 E298 = -2796.042036
 H298 = -2796.041092
 G298 = -2796.187038
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 C -1.687327 4.474918 -0.969218

C -1.357621 5.801609 -1.141536
 C -0.431708 6.434019 -0.279285
 C -1.423979 2.305544 0.276051
 C -0.643730 1.601115 1.181040
 C 0.319556 2.217160 2.009746
 C 0.545678 3.566376 1.899725
 C -2.534798 1.631826 -0.452559
 C -2.324273 0.443264 -1.141757
 C -3.323613 -0.141980 -1.954625
 C -4.563535 0.433400 -2.044679
 C -4.883667 1.581403 -1.273911
 C -3.873897 2.172097 -0.444419
 C -4.262143 3.254650 0.394046
 C -5.549089 3.748251 0.379321
 C -6.526228 3.193785 -0.479273
 C -6.194564 2.127923 -1.283952
 O -1.087833 -0.174604 -1.171269
 P -0.166997 -0.715928 0.131941
 O -0.820694 0.226291 1.335122
 N -0.765804 -2.204535 0.657026
 C -0.174922 -3.501265 0.191899
 C 1.098566 -3.401491 -0.657507
 C -1.799508 -2.448394 1.743749
 C -1.200681 -2.246441 3.142932
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 C -3.594768 -0.679960 2.277275
 C -4.911392 -0.223765 2.195854
 C -5.844687 -0.899889 1.408982
 C -5.449455 -2.036149 0.701993
 C -4.133187 -2.489538 0.786492
 C -1.197297 -4.355006 -0.560122
 C -1.809064 -3.882828 -1.729804
 C -2.693148 -4.689521 -2.445203
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 C -2.377791 -6.464096 -0.839299
 C -1.490036 -5.652922 -0.126532
 Pd 2.103381 -0.109467 -0.351441
 N 4.079930 0.601747 -0.590147
 C 4.442850 2.031144 -0.241725
 C 4.251883 2.319712 1.265177
 C 1.665975 0.493510 -2.437477
 C 2.307834 -0.685292 -2.894391
 C 3.680939 -0.939133 -2.993791
 C 4.682924 -0.011991 -2.703340
 C 6.129039 -0.421872 -2.685981
 N 3.568400 -0.813963 1.082806
 C 3.753014 -1.661468 2.279917
 C 4.403548 -3.005307 1.882630
 C 4.612184 -0.325805 0.405642
 O 5.827318 -0.545124 0.519060
 C 5.922810 2.306139 -0.600377
 C 3.553653 3.007432 -1.029541
 C 4.636757 -0.948426 3.327278
 C 2.374786 -1.917531 2.896880
 H 4.445847 3.381945 1.456898
 H 3.231031 2.093077 1.583123

H 4.945648 1.735315 1.874766
 H 6.180979 3.329319 -0.300890
 H 6.579955 1.604992 -0.084491
 H 6.097457 2.223267 -1.677661
 H 3.824810 4.037184 -0.769452
 H 2.495792 2.865896 -0.789252
 H 4.743740 -1.572500 4.223396
 H 5.629636 -0.747190 2.919406
 H 4.180951 0.002059 3.628059
 H 4.529062 -3.648267 2.763426
 H 3.778733 -3.539546 1.157577
 H 5.382802 -2.827924 1.432078
 H 2.462812 -2.551005 3.787666
 H 1.898856 -0.975297 3.191551
 H 1.715099 -2.417296 2.182738
 H 2.196399 1.435074 -2.508430
 H 1.655440 -1.532131 -3.106143
 H 4.470612 1.037141 -2.859325
 H 6.251847 -1.430939 -3.094929
 H 6.749349 0.271055 -3.267147
 H 3.982517 -1.972811 -3.154816
 H 0.594200 0.565678 -2.584195
 H 6.504463 -0.435445 -1.656063
 H 0.859779 1.601671 2.721004
 H 1.274147 4.054835 2.541243
 H 0.903195 6.173487 1.378104
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 H -2.392458 4.006175 -1.645034
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 H -5.328060 -0.006147 -2.680156
 H -3.533812 3.689117 1.068188
 H -6.939185 1.672175 -1.932565
 H -7.534304 3.598947 -0.489832
 H -5.815152 4.570243 1.038563
 H -3.075966 -1.043613 -2.503666
 H -1.988357 -3.519881 1.643627
 H 0.100932 -4.046960 1.104823
 H -0.915220 -1.209185 3.323648
 H -1.930391 -2.546159 3.903245
 H -0.308473 -2.867188 3.264978
 H 1.444055 -4.421835 -0.855944
 H 0.905037 -2.931542 -1.625208
 H 1.901743 -2.853611 -0.161378
 H -1.595897 -2.873977 -2.072057
 H -1.018192 -6.034918 0.776702
 H -3.158863 -4.309813 -3.351042
 H -2.596141 -7.467759 -0.484372
 H -3.673005 -6.610822 -2.557690
 H -2.888416 -0.145030 2.901743
 H -3.841584 -3.386278 0.247243
 H -5.206974 0.663729 2.748642
 H -6.167646 -2.578709 0.092375
 H -6.869439 -0.543472 1.349054
 H 3.685264 2.905180 -2.112349

XXVII-re

E0 = -2797.0619468
 E0+ZPE = -2796.108471
 E298 = -2796.053171
 H298 = -2796.052227
 G298 = -2796.197327
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 C -0.145357 -3.393330 -1.115977
 C 1.051803 -3.414547 -1.840031
 C 1.050654 -3.617107 -3.223990
 C -0.193029 -3.222212 0.406930
 N -0.853573 -1.940407 0.823165
 C -1.961092 -2.010583 1.850841
 C -3.001341 -3.091783 1.555268
 C -2.923251 -4.386823 2.091379
 C -3.908319 -5.339385 1.820740
 C -5.000093 -5.011913 1.016168
 C -5.101061 -3.722443 0.489914
 C -4.112724 -2.775209 0.760573
 P -0.229632 -0.481268 0.247493
 Pd 2.056370 -0.137125 -0.261888
 C 1.603961 0.525211 -2.317774
 C 1.688668 1.861160 -1.841345
 C 2.846304 2.607628 -1.592294
 C 4.148279 2.153765 -1.819086
 C 5.334405 2.966593 -1.378393
 O -1.119979 0.043077 -1.081007
 C -2.460776 0.377410 -1.053132
 C -3.330758 -0.411250 -1.841479
 C -4.670850 -0.115200 -1.883083
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 C -6.602411 1.196457 -1.057617
 C -7.119927 2.187940 -0.256356
 C -6.252256 2.960772 0.550828
 C -4.891184 2.748862 0.524013
 C -1.904926 2.401167 0.285804
 C -0.952203 1.883855 1.151928
 C -0.035604 2.697978 1.852054
 C -0.039322 4.055271 1.650892
 C -0.920414 4.644820 0.706652
 C -1.851506 3.814058 -0.003630
 C -2.653408 4.427330 -1.007556
 C -2.570579 5.779018 -1.261630
 C -1.684372 6.600311 -0.526135
 C -0.874620 6.038655 0.433410
 O -0.908659 0.514465 1.405884
 N 3.331445 0.086169 1.481403
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 O 5.471605 0.979819 1.155767
 N 4.117922 0.220522 -0.628527
 C 5.020834 -0.864374 -1.173571
 C 6.457726 -0.326456 -1.375436

C 3.349999 0.092347 2.960389
 C 3.547123 1.531514 3.487848
 C 2.011223 -0.457816 3.463581
 C 4.486500 -0.810267 3.490378
 C 5.084967 -2.076752 -0.216412
 C 4.494320 -1.356802 -2.532034
 C -1.404089 -2.100268 3.279964
 H 5.150740 -2.149001 -2.910695
 H 3.483130 -1.763682 -2.444848
 H 4.483442 -0.561274 -3.284941
 H 7.094937 -1.135405 -1.753716
 H 6.478463 0.483643 -2.111233
 H 6.866556 0.046736 -0.436243
 H 5.687944 -2.871749 -0.671229
 H 5.543514 -1.808227 0.738598
 H 4.085772 -2.476541 -0.015978
 H 3.506692 1.548022 4.584622
 H 4.511567 1.924958 3.160810
 H 2.761091 2.192514 3.105850
 H 4.485602 -0.824305 4.587667
 H 4.352522 -1.839520 3.137508
 H 5.456925 -0.444461 3.146830
 H 1.977209 -0.439956 4.559467
 H 1.173925 0.133356 3.082063
 H 1.869252 -1.491213 3.133739
 H 2.432003 0.125315 -2.889788
 H 0.748066 2.325398 -1.547156
 H 4.311553 1.446894 -2.621567
 H 5.020845 3.963320 -1.048737
 H 5.834222 2.481677 -0.532022
 H 2.724880 3.532086 -1.030762
 H 0.627141 0.167962 -2.622576
 H 6.065107 3.078797 -2.188649
 H 0.655162 2.228226 2.540731
 H 0.655491 4.690498 2.194007
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 H -5.343970 -0.705299 -2.500227
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 H -8.190535 2.370906 -0.231575
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 H -4.207499 -1.773804 0.353577
 H -3.823124 -6.335823 2.246080
 H -5.954734 -3.448184 -0.124451
 H -5.769324 -5.751024 0.809198
 H -2.284717 -3.606296 -1.264821
 H 1.998593 -3.278131 -1.329743

H -2.293100 -3.973432 -3.709564
H 1.993759 -3.629630 -3.763960
H -0.149877 -3.972210 -4.980447
H -0.882799 -3.993606 0.755282
C 1.146322 -3.475798 1.112982
H 1.889566 -2.705538 0.887266
H 1.003263 -3.485692 2.196634
H 1.550842 -4.449922 0.815436

(XXVII-re)₁

E0 = -2797.0568793
E0+ZPE = -2796.103641
E298 = -2796.048385
H298 = -2796.047441
G298 = -2796.192674
NImag = 1, (-211.6041)
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C -1.224497 -4.381920 -1.359879
C -2.119026 -3.644590 -0.513048
C -2.961236 -4.383849 0.365095
C -2.947939 -5.761429 0.376268
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C -2.102880 -2.202807 -0.544177
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C -0.237284 -2.307378 -2.138804
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C -3.074488 -1.384471 0.233756
C -2.605902 -0.407829 1.101947
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C -7.321235 -1.745545 -0.153457
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O -0.987784 -0.195753 -1.305589
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C -1.731331 3.677530 4.578244
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C -0.343037 2.423532 3.038332
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C -0.487262 4.705637 -3.740309
C -1.139725 5.933790 -3.602621
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Pd 1.958648 -0.173090 0.470749

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 C 6.304180 -0.673269 1.663951
 C 1.395501 -1.276469 2.299264
 C 1.386949 -2.457706 1.508084
 C 2.485031 -3.218442 1.092041
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 C 4.264872 -0.710081 -0.679846
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 C 3.384135 -0.960280 -3.570383
 C 2.015607 1.079342 -3.030638
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 H 6.716003 -0.876197 0.674858
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 H 4.242964 1.973631 0.751958
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 H 3.440432 0.823132 2.944283
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 H 3.364894 -0.692366 -4.634550
 H 4.306530 -1.504269 -3.356732
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 H 5.442298 0.695058 -2.737621
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 H 1.953171 1.998337 -2.438562
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 H 2.301967 -3.965458 0.322208
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 H 4.553162 -4.582038 0.242276
 H 0.481008 -1.755877 -2.732437
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 H -5.489060 0.729207 2.499100
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 H -7.428025 -0.321698 1.445734
 H -8.398766 -1.844081 -0.251071
 H -6.889477 -3.115457 -1.778581
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 H -3.327279 0.965630 -0.930984
 H -0.227010 2.719087 -2.951547
 H -2.992083 5.233905 -0.836131
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 H -2.555868 7.070805 -2.438155
 H -0.944839 6.738350 -4.306549
 H -1.674184 5.148442 1.513322
 H 0.309663 1.575971 2.851128
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 H 1.874653 4.042911 1.073264

(XXVII-re)₂

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 C -0.349757 -3.695949 -2.184506
 C -0.250880 -2.327858 -2.140257
 C -1.122927 -1.586680 -1.313025
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 C -3.086039 -1.343191 0.210876
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 C -3.441379 0.405764 1.903996
 C -4.802226 0.245386 1.824280
 C -5.374715 -0.661931 0.892878
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 C -6.784050 -0.777747 0.753674
 C -7.338141 -1.612037 -0.189610
 C -6.494838 -2.360783 -1.043540
 C -5.124373 -2.285457 -0.922676
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 C 1.477056 3.204999 0.520984
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 C -0.025428 2.260838 3.050832

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 C -2.023682 4.055880 3.799807
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 C -2.205532 6.225050 -2.270376
 C -1.249814 6.181769 -3.286049
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 H 4.276212 -1.457280 -3.435234
 H 2.508758 -1.585807 -3.435496
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 H -2.783701 7.129833 -2.101838
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XXVII-si

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 G298 = -2796.192769
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 C 4.880323 -2.489007 0.021534
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 C 3.087033 -0.789116 0.493846
 C 1.922208 -0.522161 1.196875
 C 1.467407 -1.328653 2.262791
 C 2.176433 -2.450017 2.614801
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 C 2.701793 0.536060 -1.582897
 C 3.148847 1.285645 -2.697788
 C 4.448491 1.720892 -2.756678
 C 5.343900 1.469797 -1.683233
 C 4.896328 0.691098 -0.563935
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(XXVII-si)₁

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 G298 = -2796.189124
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 C 1.563705 5.745684 -3.007407
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 H 1.742865 -7.532228 0.553097
 H 5.486854 0.344269 -2.859911
 H 4.357316 -2.997678 1.443512
 H 7.381542 -0.823171 -1.845621
 H 8.304156 -2.343182 -0.118830
 H 6.770229 -3.396621 1.544572
 H 3.065057 0.923140 -2.845355
 H 0.139617 4.156311 0.322899
 H -1.880405 4.144238 -0.923097
 H -1.716059 2.452638 -1.394726
 H -1.951962 2.867005 0.305054
 H 0.867933 5.893798 -0.974798
 H 0.668551 1.985476 -2.751336
 H 1.819510 6.800063 -3.071153
 H 1.589442 2.891785 -4.853103
 H 2.181660 5.302508 -5.026400
 H 2.282482 5.366380 1.645838
 H 0.919834 1.571012 3.123767
 H 1.764003 6.410849 3.829370
 H 0.407260 2.607170 5.311977
 H 0.823465 5.032528 5.676709
 H -3.093490 -3.355762 -2.392634
 H 2.341151 3.578342 0.233971
 H 3.070364 1.029761 1.737201
 H 3.591938 1.480460 0.099034
 H 4.037139 2.486994 1.480190