Supporting Information

A Density Functional Investigation of the Mitsunobu Reaction

Stephan Schenk, Jennie Weston, and Ernst Anders*

Contents

1 Full Author Listing for References 31 and 32

(31) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Rega, N.; Salvador, P.; Dannenberg, J. J.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. “Gaussian98, Revision A.11-4”, **2002** Gaussian, Inc., Pittsburgh PA.

(32) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. “Gaussian03, Revision C.02”, **2004** Gaussian, Inc., Wallingford CT.

2 Carbonyl Subtituted Diazenes

2.1 Results

Before addressing the mechanism of the Mitsunobu reaction, we first assessed the energetical and structural properties of a series of four carbonyl substituted diazenes in a general manner. For the two simplest diazenes (formyldiazene **2a** and acetyldiazene **2b**), six different conformers are theoretically possible — four planar and two nonplanar ones (Chart S1). An extended search of the conformational hypersurface demonstrated that the *cis c* conformers of both diazenes are not stationary points. The remaining conformers are either energetically stable structures or, when steric interactions are present, transition structures for rotation about the C–N bond. The planar *trans a* conformer is the global minimum for **2a** whereas the nonplanar *trans c* is the most stable structure for **2b** (see Table S1 for their relative stabilities).

As the flexibility of the diazene grows [diformyldiazene **2c** and dimethylazodicarboxylate **2d** (DMAD)], the number of possible conformers increases accordingly. Only the energetically stable conformers of the latter two diazenes are given in Table S1. The conformers of interest are named according to Chart S1 with footnotes in the table defining the additional dihedral angles necessary to unambiguously define the three dimensional structure of the conformer. The same general structural pattern calculated for **2b** is also observed for **2c** and **2d**. As steric hindrance increases, the planar *a* and *b* conformers become transition structures for rotation about the C–N bonds. In the case of **2d**, only nonplanar *c/c* conformers are energetical minima.

Optimization of the different conformers of **2a**–**2d** in acetonitrile (Table S1) showed that the relative energies of the different conformers do not change significantly upon solvation. For all diazenes, a fast equilibrium between several different conformers is to be expected in solution. When bulkier substituents are present (**2b** and **2d**), there is a clear preference for a single *trans* conformation which is illustrated in Chart S2 for the experimentally relevant DMAD (**2d**). For the calculations performed in this article, only the most stable conformation of **2d** was considered further.

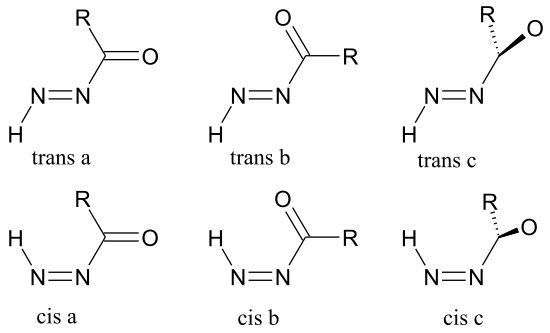


Chart S1: The six different possible conformations of the monsubstituted diazenes **2a** (R=H) and **2b** (R=CH_3).

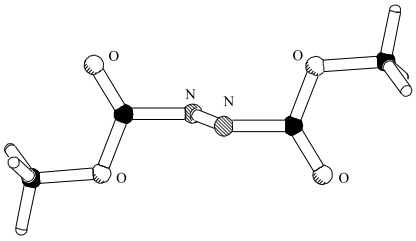


Chart S2: The most stable conformation of DMAD (**2d**).

The global minimum of all four carbonyl substituted diazenes is a *trans* conformation. This is in direct contrast to halogen substituted diazenes which prefer a *cis* conformation. Investigations on $X^1N{=}NX^2$ diazenes[S1] ($X^{1,2}$ = halogen or hydrogen) have shown that this *cis* preference can be interpreted as the sum of three different electronic interactions: (1) *negative hyperconjugation*. Partial delocalization of the lone pair on nitrogen (N1) into the σ^*_{N2-X} orbital leads to a significant stabilization of the *cis* form. (2) Electrostatic interactions between the two substituents X^1 and X^2. This stabilizes the cis form of unsymmetrical diazenes (X^1 = H; X^2 = halogen) and destabilizes that of symmetric diazenes. (3) Electrostatic interactions between the lone electron pairs on adjacent N atoms which destabilizes the *cis* conformer. In diazene itself (HN=NH), the hyperconjugative interactions are weak, leading to the domination of the electrostatic effects (2) and (3) thus resulting in a *trans* preference.[S1]

As with diazene, the hyperconjugative interactions, especially the $\pi_{N=N} \rightarrow \pi^*_{C=O}$ and the $n_N \rightarrow \sigma^*_{C-N}$ interactions in the carbonyl substituted derivatives **2a**–**2d**, are relatively small ($< 10\,\mathrm{kcal\,mol^{-1}}$). The *trans* preference is clearly determined by steric and electrostatic effects which increase as the size/number of substituents increases. The preference for a nonplanar conformation is also steric in origin due to strong electrostatic repulsions between the substituent on the carbonyl group(s) and the lone pair orbitals on the nitrogen atoms.

The successive replacement of H in diazene itself with carbonyl groups has quite some influence upon the electrophilicity of the diazene. The negative charge on nitrogen (q_N) is reduced considerably upon substitution (Table S2) thus facilitating the initial approach of a nucleophile. Carbonyl substitution also influences the $\pi^*_{N=N}$ orbital in a positive way since its energy is considerably lowered, i. e. the orbital is stabilized upon substitution. This increases the ability of this orbital to interact with a lone electron pair orbital on an incoming nucleophile such as triphenylphosphine.

2.2 Computational Details

As we have reported in the past, low level theoretical methods (semiempirical and HF methods) are not capable of properly describing the relative energies of the different conformers of simple diazenes.[S1] A correlated method combined with a large basis set has to be employed in order

(S1) Nordhoff, K.; Anders, E. *J. Org. Chem.* **1999,** *64,* 7485–7491.

Table S1: Relativ Gibbs' free enthalpies (kcal mol^{-1}) of the different conformers of carbonyl substituted diazenes in the gas phase (ΔG_{gas}) and in acetonitrile ($\Delta G_{soln.}$).

conformer	ΔG_{gas}	$\Delta G_{soln.}$	conformer	ΔG_{gas}	$\Delta G_{soln.}$
formyldiazene **2a**			acetyldiazene **2b**		
cis a	2.8[a]	3.6[a]	*cis a*	7.5[a]	6.7[a]
cis b	2.4	2.0	*cis b*	0.6	1.7
trans a	0.0	0.0	*trans a*	2.1[a]	1.9
trans b	4.8[a]	4.6[a]	*trans b*	3.9[a]	3.6
trans c	1.0	0.3	*trans c*	0.0	0.0
diformyldiazene **2c**[b]			DMAD **2d**[b]		
cis c/c[c]	3.2	3.1	*cis c/c*[c,d]	9.2	7.3
trans c/c[e]	1.6	1.2	*cis c/c*[c,f]	3.6	4.3
trans c/c[c]	1.0	0.7	*trans c/c*[c,g]	7.9	8.1
trans b/c[h]	1.0	0.5	*trans c/c*[c,g]	4.8	4.4
trans b/c[i]	0.3	0.0	*trans c/c*[c,d]	4.2	4.3
trans a/a[j]	0.0	0.3	*trans c/c*[c,g]	0.0	0.0

[a] First order transition structure for rotation about the C–N bond.
[b] Only energetically stable conformers for **2c** and **2d** are given.
[c] $\angle\mathrm{OCNN} = 90\,^\circ; -90\,^\circ$
[d] $\angle\mathrm{MeOCN} = 0\,^\circ; 0\,^\circ$
[e] $\angle\mathrm{OCNN} = 90\,^\circ; 90\,^\circ$
[f] $\angle\mathrm{MeOCN} = 0\,^\circ; 180\,^\circ$
[g] $\angle\mathrm{MeOCN} = 180\,^\circ; 180\,^\circ$
[h] $\angle\mathrm{OCNN} = 90\,^\circ; 180\,^\circ$
[i] $\angle\mathrm{OCNN} = 90\,^\circ; 0\,^\circ$
[j] $\angle\mathrm{OCNN} = 180\,^\circ; 180\,^\circ$

Table S2: Selected electronic properties of the most stable conformer of the substituted diazenes **2a**–**2d** as compared to HN=NH.

	diazene	**2a**	**2b**	**2c**	**2d**
q_{N1}[a]	-0.295	-0.213	-0.185	-0.168	-0.171
q_{N2}[a]	-0.295	-0.276	-0.286	-0.168	-0.171
$\varepsilon(\pi^*_{N=N})$[b]	$+12.1$	-2.6	-2.5	-2.7	-2.4

[a] Atomic charge (NBO analysis).
[b] Energy (eV) of the $\pi^*_{N=N}$ orbital.

to describe these compounds correctly with the best theoretical results being obtained using the BP86[S2,S3] density functional with the very large 6–311++G(3df,3pd)[S4] basis set.[S1] Since this level of theory is rather computationally demanding, especially when bulky substituents are present, we performed an extended conformational search at the HF/6–311+G(d,p) level for the series of diazenes considered here. The HF structures then served as starting geometries for full geometry optimizations and frequency calculations for all intermediates at the BP86/6-311++G(3df,3pd) level of theory.

3 Table of Electronic Properties

Table S3: Selected electronic (NBO) properties of the compounds involved in the diazene/phosphine reaction. Calculated at the BP86/6–311++G(3df,3pd) level of theory.

	q_P [a]	q_{N1} [a]	q_{N2} [a]	q_O [a]	ε_{N1} [b]	ε_{N2} [b]	ε_O [b]
PH_3	0.00						
3d	+0.99	−0.58	−0.49	−0.66	[c]	−9.5	−7.4
14b	+1.09	−0.60	−0.42	−0.74	−7.0	−10.1	−7.5
2d		−0.17	−0.17	−0.49	−11.7	−11.7	−8.5

[a] atomic chage

[b] Energy (eV) of the sp-hybridized orbital needed for deprotonation of an organic acid.

[c] Lone pair on N1 is involved in an $^-$O–C=N resonance structure.

(S2) Becke, A. D. *Phys. Rev. A: At., Mol., Opt. Phys.* **1988,** *38*, 3098–3100.

(S3) Perdew, J. P. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1986,** *33*, 8822–8824.

(S4) Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984,** *80*, 3265–3269.

4 Absolute Energies of Calculated Structures

All energies were calculated at the BP86/6-311++G(3df,3pd) level of theory corrected for zero point energy (ΔU) as well as thermodynamic effects (ΔG) using unscaled frequencies and standard temperature (298.15 K) and pressure (1 atm). Solvent effects were incorporated by the C-PCM model using acetonitrile ($\varepsilon = 36.64$) as solvent. N_{imag} denotes the number of imaginary frequencies.

Table S4: Absolute energies in solution [a. u.]

Compound	E_{SCF}	ΔU	ΔG	N_{imag}
10	−686.962476013	−686.836848	−686.873034	0
11	−571.571266547	−571.489161	−571.519480	0
12	−381.882991844	−381.781168	−381.813472	0
14a	−909.835944419	−909.685533	−909.725192	0
14b	−909.829091547	−909.688961	−909.728939	0
15	−910.255750309	−910.104077	−910.144967	0
16	−1139.03397000	−1138.833047	−1138.879485	0
17	−1025.62987298	−1025.424011	−1025.470827	0
18	−1025.60576013	−1025.414868	−1025.459526	0
19	−1025.61214736	−1025.406188	−1025.449945	0
20	−802.253784082	−802.088001	−802.128819	0
21	−686.953307579	−686.834158	−686.870009	0
22	−800.349384426	−800.220068	−800.257708	0
23	−800.341946316	−800.212207	−800.247940	0
2d	−566.615659920	−566.497371	−566.536266	0
3d	−909.813942497	−909.665735	−909.706077	0
4	−910.272667305	−910.111625	−910.151918	0
5	−573.551796686	−573.437388	−573.469160	0
6	−567.883269122	−567.740973	−567.779551	0
7	−458.172367348	−458.100238	−458.127741	0
8	−720.580600827	−720.398543	−720.441693	0
9	−268.494905633	−268.403711	−268.433832	0
AcOH	−229.187424534	−229.124436	−229.151828	0
AcO^-	−228.722072897	−228.672413	−228.700242	0
$E_{15\text{-}7}$	−1026.04261684	−1025.837744	−1025.881443	0
$E_{3d\text{-}17}$	−1025.60601413	−1025.416132	−1025.463744	0
$H_3P{=}O$	−418.468087544	−418.434720	−418.458356	0
MeOH	−115.774366174	−115.722937	−115.745705	0
MeO^-	−115.273983165	−115.237632	−115.258883	0
PH_3	−343.194058188	−343.167121	−343.188180	0

Table S4: (continued)

Compound	E_{SCF}	ΔU	ΔG	N_{imag}
$\mathbf{T_{15\text{-}7}}$	−1026.01190589	−1025.810167	−1025.853588	1
$\mathbf{T_{16\text{-}8}}$	−1139.01337092	−1138.813647	−1138.859968	1
$\mathbf{T_{17\text{-}5}}$	−1141.40157750	−1141.137570	−1141.182015	1
$\mathbf{T_{20\text{-}10}}$	−802.248438848	−802.091586	−802.131022	1
$\mathbf{T_{21\text{-}9Ret}}$	−686.918691118	−686.800884	−686.834122	1
$\mathbf{T_{22\text{-}23}}$	−800.340154516	−800.210447	−800.245095	1
$\mathbf{T_{23\text{-}12}}$	−800.332785801	−800.206220	−800.242639	1
$\mathbf{T_{3d\text{-}17}}$	−1025.60368840	−1025.415206	−1025.459890	1
$\mathbf{T_{4\text{-}7}}$	−1026.01679063	−1025.804197	−1025.848574	1
$\mathbf{T_{5\text{-}20}}$	−802.260327981	−802.102993	−802.148256	1
$\mathbf{T_{7\text{-}9Inv}}$	−686.895676091	−686.772652	−686.811787	1
$\mathbf{T_{7\text{-}9Ret}}$	−686.872544124	−686.758036	−686.794966	1

Table S5: Absolute energies in the gas phase [a. u.]

Compound	E_{SCF}	ΔU	ΔG	N_{imag}
10	−686.958687524	−686.839277	−686.875009	0
11	−571.502014104	−571.424694	−571.455174	0
12	−381.876541734	−381.781800	−381.815428	0
13	−909.796469553	−909.657466	−909.698616	0
14a	−909.831315114	−909.690093	−909.730247	0
14b	−909.831315114	−909.690093	−909.730247	0
15	−910.171945786	−910.018370	−910.058931	0
16	−1139.00497822	−1138.802758	−1138.851994	0
17	−1025.62124551	−1025.427602	−1025.476206	0
18	−1025.58567132	−1025.392967	−1025.438558	0
19	−1025.60451858	−1025.409010	−1025.453171	0
20	−802.183945930	−802.024880	−802.065078	0
21	−686.944451925	−686.824800	−686.860448	0
22	−800.342188385	−800.212097	−800.249620	0
23	−800.334179030	−800.204471	−800.239991	0
2d	−566.609079126	−566.499535	−566.538826	0
3d	−909.795762620	−909.657323	−909.698223	0
4	−910.208202376	−910.055160	−910.095611	0
5	−573.548901011	−573.439130	−573.470943	0
6	−567.872363778	−567.737693	−567.776277	0

Table S5: (continued)

Compound	E_{SCF}	ΔU	ΔG	N_{imag}
7	−458.100341864	−458.031684	−458.059247	0
8	−720.569686790	−720.399619	−720.444087	0
9	−268.491336229	−268.404775	−268.435505	0
AcO$^-$	−228.620357372	−228.574103	−228.601643	0
AcOH	−229.181758241	−229.122084	−229.149361	0
E$_{15\text{-}7}$	−1025.95914704	−1025.752427	−1025.798788	0
H$_3$P=O	−418.463508268	−418.433817	−418.457448	0
MeO$^-$	−115.157069645	−115.123885	−115.145103	0
MeOH	−115.770324916	−115.720726	−115.743543	0
PH$_3$	−343.193832543	−343.170667	−343.191727	0
T$_{15\text{-}7}$	−1025.93554723	−1025.731700	−1025.775161	1
T$_{16\text{-}8}$	−1138.98892211	−1138.788281	−1138.836102	1
T$_{17\text{-}5}$	−1141.39204993	−1141.145753	−1141.196938	1
T$_{21\text{-}9Ret}$	−686.904587452	−686.786691	−686.820323	1
T$_{22\text{-}23}$	−800.333810816	−800.203349	−800.237991	1
T$_{23\text{-}12}$	−800.321256574	−800.193812	−800.229888	1
T$_{4\text{-}7}$	−1025.95492856	−1025.752536	−1025.796909	1
T$_{5\text{-}20}$	−802.166359209	−802.009434	−802.051887	1
T$_{7\text{-}9Inv}$	−686.881234183	−686.764947	−686.800884	1
T$_{7\text{-}9Ret}$	−686.860442124	−686.745277	−686.781510	1

5 Cartesian Coordinates of Calculated Structures

All cartesian coordinates are given in Ångström. For convenience, coordinates of all compounds are also available in xyz-format packed together into a single ZIP-archive.

5.1 Coordinates in Solution

All structures were fully optimized at the BP86/6–311++G(3df,3pd) level of theory using the C-PCM solvation model and acetonitrile ($\varepsilon = 36.64$) as solvent.

10

16

P	−0.759277	−0.189987	−0.221506
O	1.598025	1.355692	0.088213
O	0.966023	−0.796369	−0.064175
O	−2.342751	0.341993	−0.468172
C	3.297297	−0.371696	0.165272
C	1.889419	0.159972	0.061606
C	−3.284263	−0.056061	0.525766
H	4.007663	0.453922	0.270356
H	3.542245	−0.960965	−0.729315
H	3.381043	−1.046644	1.028338
H	−4.258359	0.373855	0.262773
H	−3.383302	−1.156043	0.571125
H	−2.993776	0.313612	1.526534
H	−1.060243	−1.569163	−0.247747
H	−0.645464	0.359057	1.074807
H	−0.385735	0.478355	−1.397068

11

11

P	1.581378	−0.076035	0.000841
O	0.148450	−0.804946	−0.002615
O	−0.549207	1.334084	−0.000641
C	−2.244907	−0.436924	0.001196
C	−0.905396	0.183003	−0.001292
H	2.473066	−1.163629	0.002816
H	1.813697	0.707198	−1.146760

H	1.808426	0.706928	1.149718
H	−3.009681	0.344649	−0.004826
H	−2.349528	−1.074867	0.891538
H	−2.348766	−1.089332	−0.878476

12

13

O	1.293595	1.200419	−0.601234
O	−1.293525	1.200446	0.601239
O	−0.000018	−0.596934	−0.000071
C	2.346858	−0.786753	0.304465
C	1.216096	0.090901	−0.140355
C	−2.346905	−0.786708	−0.304442
C	−1.216091	0.090937	0.140336
H	3.302848	−0.300108	0.091071
H	2.294318	−1.759759	−0.202614
H	2.258001	−0.980963	1.383270
H	−3.302837	−0.299348	−0.092426
H	−2.295271	−1.759023	0.204084
H	−2.257219	−0.982505	−1.382875

14a

20

P	−0.187294	1.804836	0.110483
O	3.110259	−0.229790	−0.102627
O	1.617151	1.434206	−0.178242
O	−2.618893	0.101778	−0.133778
O	−1.564325	−1.894111	0.153572
N	0.844365	−0.697464	0.085159
N	−0.345883	0.071719	0.071515
C	3.357989	−1.650602	0.000326
C	1.828151	0.140867	−0.060715
C	−3.875964	−0.614538	−0.137952
C	−1.530610	−0.684590	0.046320
H	4.444700	−1.757987	−0.062302
H	2.986990	−2.035044	0.959177
H	2.868952	−2.185189	−0.824175

H	0.205785	2.485504	1.290200
H	−4.640975	0.154885	−0.277427
H	−4.024198	−1.136945	0.814940
H	−3.901767	−1.337689	−0.962035
H	−1.584287	1.993327	0.303701
H	−0.066095	2.683321	−0.995310

14b

20

P	−0.045105	1.607306	−0.282716
O	2.597896	0.376461	0.119476
O	1.905848	−1.784114	−0.145362
O	−2.776573	−1.099558	0.080457
O	−1.474767	0.666807	0.757789
N	0.467268	−0.021356	−0.547148
N	−0.639466	−0.915983	−0.674058
C	3.881682	−0.136690	0.574933
C	1.692085	−0.585384	−0.177996
C	−3.941327	−0.252178	0.274268
C	−1.604595	−0.436832	0.083264
H	4.503039	0.746189	0.748480
H	4.330039	−0.783863	−0.188641
H	3.749287	−0.703459	1.505742
H	0.907451	2.298963	−1.090382
H	0.089026	2.350765	0.912182
H	−4.803992	−0.912844	0.153374
H	−3.961254	0.536042	−0.492287
H	−3.936494	0.202423	1.271748
H	−1.181452	1.907293	−1.056745

15

21

P	0.188206	2.171819	−0.307340
O	2.632540	−0.656825	−0.360147
O	1.360656	1.100810	−0.664643
O	−2.767294	0.301703	0.857722

O	−1.565840	−1.151073	−0.434207
N	0.659737	−0.586890	0.840950
N	−0.459870	0.302803	0.941383
C	2.933017	−1.955525	0.240187
C	1.503763	−0.099952	0.001044
C	−2.797489	−1.690521	−1.000726
C	−1.728719	−0.200019	0.478190
H	3.884898	−2.250656	−0.208127
H	3.023475	−1.843922	1.327001
H	2.137976	−2.667985	−0.008170
H	0.731200	3.186163	−1.133574
H	0.177658	2.767379	0.973117
H	−3.397936	−2.148110	−0.205851
H	−3.363385	−0.890644	−1.492465
H	−2.468399	−2.440829	−1.724192
H	−1.112080	2.010731	−0.834434
H	−0.579502	0.608373	1.938498

16

28

P	0.826915	−1.467400	−0.748881
O	4.312541	0.411515	−0.195746
O	2.351143	−0.416194	−0.818544
O	0.438637	1.535713	−1.284189
O	−3.224540	−1.038629	1.475243
O	−2.537033	−0.466614	−0.633329
O	−0.702554	1.874554	0.661643
N	−1.010329	−0.699056	1.016561
N	−0.022127	−0.226796	0.158648
C	3.283722	−0.187646	0.112442
C	3.035948	−0.684806	1.520688
C	−3.912435	−0.537178	−1.087001
C	−2.349057	−0.749170	0.671650
C	−0.864598	3.272037	0.300097
C	−0.053008	1.128629	−0.249330
H	3.873715	−0.399860	2.164426
H	2.936092	−1.781195	1.533633
H	2.105031	−0.264999	1.926944
H	1.599449	−2.437111	−0.063814

H	0.967424	−1.455351	−2.154258
H	0.115638	3.758858	0.228955
H	−4.530265	0.186251	−0.540987
H	−4.308215	−1.549947	−0.942391
H	−3.874695	−0.286431	−2.151059
H	−1.455460	3.707796	1.110787
H	−1.394357	3.356646	−0.656551
H	−0.792105	−0.732343	2.026788
H	−0.367762	−2.264289	−0.727617

17

26

P	−1.521358	−1.107247	0.539000
O	2.782335	−1.294911	−1.387380
O	1.979819	−0.880769	0.717043
O	0.755888	2.084229	−0.426704
O	−2.656195	−0.473294	−0.462092
O	−1.093964	1.861896	0.904301
N	0.677081	−0.454533	−1.080715
N	−0.309074	0.069488	−0.264574
C	3.233346	−1.368291	1.242151
C	1.898073	−0.904343	−0.636640
C	0.812393	3.469155	−0.025034
C	−4.029925	−0.905213	−0.336128
C	−0.272035	1.384100	0.127390
H	4.068568	−0.756957	0.878242
H	3.393778	−2.414112	0.951463
H	3.143893	−1.283687	2.329354
H	1.669097	3.891103	−0.559788
H	0.959988	3.553967	1.059103
H	0.565234	−0.371994	−2.091704
H	−4.567106	−0.420299	−1.159253
H	−4.461255	−0.582371	0.621661
H	−4.122539	−1.995872	−0.431770
H	−2.481901	−2.053301	1.084751
H	−1.202090	−0.556315	1.805324
H	−0.605771	−2.128660	0.160278
H	−0.109748	3.992853	−0.307420

18

26

P	0.601544	−1.999671	0.081022
O	1.868839	−1.116209	−0.452727
O	1.277300	2.629428	0.390761
O	0.841084	0.866275	1.695263
O	−2.497508	0.559239	−0.239953
O	−2.295134	−1.696190	0.116438
N	0.061820	0.887383	−0.506392
N	−0.428636	−0.416450	−0.224214
C	3.194950	−1.687866	−0.436230
C	1.161359	3.314830	−0.878294
C	0.688437	1.423367	0.484315
C	−3.923350	0.383508	−0.109587
C	−1.767270	−0.591474	−0.104322
H	3.846682	−0.924011	−0.876161
H	3.522430	−1.903703	0.590222
H	3.244647	−2.604684	−1.039816
H	1.706521	4.254645	−0.745935
H	1.610487	2.711762	−1.677460
H	1.458178	−3.154539	0.308562
H	1.386270	1.467078	2.277847
H	0.106475	3.506147	−1.111840
H	0.081174	−2.036681	1.399110
H	−4.349419	1.384026	−0.239765
H	−4.309571	−0.296104	−0.881025
H	−4.181023	−0.012371	0.881813
H	−0.259717	−2.687573	−0.800184

19

26

P	−0.136271	1.371649	0.964258
O	2.769016	−0.175365	−0.688768
O	1.925212	−1.640460	0.851407
O	−2.774916	−1.331045	0.103349
O	−1.731891	0.579705	0.431964
O	−0.150669	2.345130	−0.402960

N	0.535964	−0.318686	−0.473270
N	−0.540195	−1.258492	−0.416680
C	4.109003	−0.498554	−0.244863
C	1.784620	−0.820587	−0.028823
C	−2.767835	−2.698142	−0.366650
C	−1.617610	−0.659863	0.029359
C	−1.368087	2.913663	−0.899629
H	4.772595	0.112001	−0.863507
H	4.311298	−1.565499	−0.398297
H	4.230056	−0.247651	0.815897
H	1.228415	1.751780	1.141406
H	0.611841	0.134475	−1.392750
H	−3.799466	−3.043887	−0.249592
H	−2.462548	−2.741405	−1.419724
H	−2.085912	−3.309646	0.237277
H	−2.012924	3.265960	−0.078090
H	−1.932139	2.196318	−1.512239
H	−1.079460	3.773621	−1.518437
H	−0.803344	2.249002	1.857235
H	−0.039301	0.247622	1.850306

20

21

P	−0.506553	−0.463700	−0.122951
O	3.494113	0.316261	−0.712666
O	1.274066	0.113102	−0.760972
O	−2.022977	−1.100735	0.400480
O	−1.088094	1.178577	−0.430474
C	2.470659	−0.703908	1.196720
C	2.429646	−0.054780	−0.181175
C	−3.180820	−0.747178	−0.328522
C	−1.325546	2.023122	0.670072
H	3.484231	−1.065304	1.403587
H	2.206334	0.042199	1.960377
H	1.749570	−1.528488	1.279872
H	0.101168	−1.773098	0.048699
H	−3.994125	−1.425270	−0.024572
H	−3.500307	0.293751	−0.137460
H	−3.033421	−0.856270	−1.419978

H	−2.391212	2.019706	0.974386
H	−1.046032	3.058519	0.410686
H	−0.745526	−0.652835	−1.523615
H	−0.730391	1.725779	1.558177
H	−0.122496	−0.044360	1.200589

21

16

P	−0.919115	0.925912	0.255804
O	1.293536	−0.870713	1.104541
O	0.735265	0.623304	−0.498049
O	−1.350183	−0.490250	−0.438518
C	2.954507	−0.217446	−0.533283
C	1.585869	−0.203134	0.112001
C	−2.706164	−0.974648	−0.271132
H	3.601594	−0.946258	−0.035119
H	3.405449	0.783118	−0.467117
H	2.865642	−0.462999	−1.600590
H	−3.437986	−0.255285	−0.663235
H	−2.921348	−1.187845	0.784791
H	−2.756029	−1.902885	−0.851657
H	−2.248600	1.147776	0.779453
H	−0.874759	2.130805	−0.481974
H	−0.281456	1.077529	1.509094

22

18

P	0.413461	1.597193	−0.000031
O	1.142781	0.167414	−1.072290
O	1.142742	0.166923	1.072760
O	−1.191215	0.763471	−0.000267
O	−0.898739	−1.503341	−0.000503
C	2.240477	−1.731977	−0.000110
C	1.466225	−0.466746	0.000146
C	−3.128535	−0.574715	0.000303
C	−1.615865	−0.507469	−0.000345
H	3.313514	−1.481669	0.003291

H	2.020675	−2.311070	−0.902837
H	2.015899	−2.314145	0.899486
H	1.735611	2.131141	0.000342
H	−3.526586	−0.053424	−0.881365
H	−3.524660	−0.062163	0.888022
H	−3.457925	−1.618589	−0.004139
H	−0.058562	2.340651	1.105957
H	−0.058247	2.341073	−1.105858

23

18

P	1.320990	−1.280274	0.002208
O	0.998745	0.084309	−1.068359
O	0.991040	0.083645	1.070281
O	−1.049026	−1.293658	−0.006291
O	−0.934703	0.975174	−0.005786
C	1.081286	2.303372	0.001615
C	0.606093	0.874961	−0.000300
C	−3.089019	−0.004332	0.003663
C	−1.596291	−0.181741	−0.005577
H	2.733475	−1.268079	0.006678
H	2.178109	2.306751	0.005210
H	1.079599	−2.193575	−1.058486
H	1.072832	−2.194029	1.060985
H	0.718448	2.822672	−0.893409
H	0.712718	2.822165	0.894591
H	−3.582907	−0.977251	−0.079259
H	−3.395542	0.649361	−0.824231
H	−3.392424	0.486776	0.939633

2d

16

O	2.423852	0.683440	0.117318
O	2.140310	−1.577830	−0.069542
O	−2.422733	−0.683855	−0.113531
O	−2.142138	1.578556	0.063647

N	0.349449	−0.218615	0.467452
N	−0.349748	0.219796	−0.469375
C	3.860150	0.535964	−0.080456
C	1.732753	−0.451125	0.102594
C	−3.859012	−0.537479	0.084934
C	−1.733162	0.451737	−0.104370
H	4.270920	−0.150531	0.669025
H	4.269320	1.541700	0.044031
H	4.058540	0.155994	−1.089237
H	−4.271408	0.145298	−0.667049
H	−4.266956	−1.544275	−0.034942
H	−4.057011	−0.153521	1.092282

3d

20

P	−0.026311	1.875941	−0.360152
O	2.137441	1.042310	0.497193
O	2.053021	−1.190516	−0.045135
O	−2.527016	−1.677139	−0.681120
O	−1.765596	0.046829	0.633313
N	0.363414	0.252558	−0.609622
N	−0.500279	−0.713128	−1.162995
C	3.354120	−1.377443	0.579405
C	1.588499	0.046290	−0.003270
C	−3.015184	−0.034777	1.341196
C	−1.634215	−0.864500	−0.439393
H	4.108109	−0.770468	0.065209
H	3.570440	−2.442744	0.464977
H	3.305578	−1.102390	1.639348
H	0.867150	2.788013	−0.962753
H	−3.860273	0.180192	0.673713
H	−3.148540	−1.033678	1.775806
H	−2.959518	0.716813	2.136549
H	−1.243917	2.036279	−1.044930
H	−0.228422	2.323572	0.961039

4

21

P	−0.374433	2.010238	−0.092492
O	2.665118	−0.998117	−0.397527
O	1.572257	0.521912	0.922378
O	−2.423776	0.711478	0.517591
O	−1.893678	−1.398768	−0.218901
N	0.571545	−0.382057	−0.920906
N	−0.531767	0.400492	−0.631442
C	3.853316	−0.879935	0.436628
C	1.639872	−0.239299	−0.039982
C	−3.123481	−1.940490	0.362015
C	−1.711264	−0.115729	−0.046417
H	4.583562	−1.552128	−0.020584
H	4.215284	0.154529	0.427815
H	3.621772	−1.194249	1.460626
H	0.839406	2.458854	−0.642144
H	0.732786	−0.596675	−1.912285
H	−3.989428	−1.486220	−0.131571
H	−3.140366	−1.739489	1.438817
H	−3.074592	−3.013267	0.162183
H	−1.378388	2.802280	−0.683419
H	−0.382005	2.244440	1.292582

5

14

P	0.000000	−0.394300	0.000025
O	1.711824	−0.513390	−0.000154
O	−1.711822	−0.513390	0.000079
C	2.399699	0.726752	0.000027
C	−2.399701	0.726752	−0.000030
H	3.479110	0.526614	−0.000052
H	2.153840	1.327952	0.897038
H	2.153672	1.328471	−0.896536
H	0.000140	0.422297	1.172085
H	0.000001	−1.803389	−0.000132
H	−3.479111	0.526611	−0.000218

H	−2.153867	1.328317	0.896688
H	−2.153648	1.328104	−0.896886
H	−0.000137	0.422747	−1.171734

6

18

O	2.661297	0.211595	0.483916
O	1.276270	−0.632503	−1.135771
O	−2.662152	0.212374	−0.483079
O	−1.276027	−0.631268	1.135827
N	0.656996	1.147810	0.203001
N	−0.656961	1.147925	−0.204061
C	3.679340	−0.723490	0.067173
C	1.507837	0.148139	−0.229722
C	−3.678692	−0.724715	−0.066996
C	−1.508244	0.149147	0.229784
H	4.530461	−0.538657	0.729436
H	3.962576	−0.544962	−0.977852
H	3.325052	−1.755828	0.179289
H	0.862466	1.619044	1.085365
H	−4.530152	−0.540794	−0.729069
H	−3.962139	−0.547574	0.978199
H	−3.322649	−1.756364	−0.179985
H	−0.862420	1.618919	−1.086545

7

9

P	−0.990058	0.092382	0.000002
O	0.420077	−0.584225	0.000133
C	1.664244	0.216973	0.000041
H	2.466284	−0.524580	−0.011842
H	1.706120	0.821680	0.913984
H	1.695817	0.839220	−0.902431
H	−1.922459	−0.961169	−0.008289
H	−1.223893	0.899452	1.139126
H	−1.217086	0.911633	−1.131887

8

23

O	2.346308	−0.785142	0.231068
O	0.570458	−1.867812	−0.681057
O	0.205253	2.672535	−0.147865
O	−2.967045	−0.213825	−0.522663
O	−1.609335	−0.204097	1.325226
N	0.484950	0.419227	−0.366682
N	−0.834206	0.368953	−0.770006
C	3.045641	−2.055046	0.295316
C	2.419599	1.910416	0.326375
C	1.117293	−0.854606	−0.296945
C	0.976869	1.734864	−0.060539
C	−4.076105	−0.590682	0.322869
C	−1.790641	−0.045469	0.131229
H	4.018673	−1.820933	0.736014
H	3.165389	−2.472715	−0.711221
H	3.097737	1.471546	−0.415123
H	2.634235	1.424442	1.286255
H	2.599417	2.986753	0.410325
H	2.492257	−2.759448	0.927189
H	−4.933453	−0.683133	−0.350417
H	−4.264554	0.182552	1.078115
H	−3.874303	−1.547913	0.819373
H	−1.011660	0.291456	−1.771190

9

11

O	0.487475	−0.769313	0.000000
O	−1.190991	0.753164	0.000000
C	1.118610	1.504967	0.000000
C	0.000000	0.497883	0.000000
C	−0.510906	−1.814896	0.000000
H	1.754823	1.363137	0.884300
H	1.754823	1.363137	−0.884300
H	0.706123	2.517889	0.000000
H	0.049529	−2.754506	0.000000

H	−1.141699	−1.744097	0.895008
H	−1.141699	−1.744097	−0.895008

AcOH

8

O	0.789921	−1.041831	−0.001061
O	0.631318	1.213837	0.000173
C	0.089310	0.123476	−0.002281
C	−1.394000	−0.121309	−0.000517
H	1.743193	−0.803728	0.009888
H	−1.928910	0.830380	−0.061575
H	−1.681682	−0.649249	0.919763
H	−1.674375	−0.766459	−0.844177

AcO^-

7

O	−0.771527	−1.127061	0.002062
O	−0.756195	1.134930	0.002067
C	1.354010	−0.007539	−0.004888
C	−0.186861	−0.000026	−0.010718
H	1.759091	0.862382	−0.538937
H	1.754424	−0.933512	−0.437918
H	1.705379	0.053565	1.037458

$E_{15\text{-}7}$

27

P	0.493622	−1.411610	0.758918
O	2.081079	−1.383758	−0.685055
O	1.341574	2.296071	0.457810
O	1.075493	0.196692	1.063244
O	−2.532253	−1.550016	−0.900820
O	−2.447117	0.434076	0.230866
N	−0.537953	−0.364377	−0.771920
N	−0.069915	0.984688	−0.809954

C	3.446065	−1.359530	−0.171226
C	1.041136	3.409380	−0.434787
C	0.739203	1.152009	0.194893
C	−3.855486	0.312588	0.600768
C	−1.970909	−0.551583	−0.510109
H	4.134488	−1.285646	−1.021693
H	3.657485	−2.264449	0.414547
H	3.529448	−0.468606	0.457646
H	1.966191	−2.130036	−1.343231
H	1.611863	4.249558	−0.030615
H	1.450269	−1.940199	1.653585
H	1.366278	3.167664	−1.453777
H	0.142171	−2.584050	0.036916
H	−4.471431	0.290814	−0.305620
H	−4.065216	1.203434	1.197988
H	−4.005441	−0.601234	1.187465
H	−0.636853	−1.321127	1.607185
H	−0.344241	−0.826641	−1.696814
H	−0.034530	3.620791	−0.419821

$E_{3d\text{-}17}$

26

P	0.388269	0.800641	1.347225
O	2.619860	−0.093980	0.325518
O	1.878364	−1.096482	−1.605080
O	−2.701799	−1.109920	−1.208680
O	−1.407545	−1.568533	0.625839
O	−0.599338	2.567483	−0.475239
N	0.442164	−0.032644	−0.117362
N	−0.693631	−0.047007	−0.974757
C	3.980978	−0.525267	0.062572
C	1.679110	−0.479260	−0.579787
C	−2.430562	−2.492087	1.051538
C	−1.773875	3.345361	−0.216250
C	−1.658386	−0.919901	−0.572266
H	4.573237	−0.127337	0.891357
H	4.323660	−0.111875	−0.893447
H	4.029084	−1.620729	0.041815
H	1.107759	2.012298	1.422662

H	0.890035	−0.020753	2.383994
H	−3.389221	−1.976142	1.194159
H	−2.558134	−3.295636	0.314269
H	−2.500748	2.801913	0.412881
H	−2.273585	3.639459	−1.153515
H	−2.075344	−2.903838	2.002327
H	−1.462897	4.253660	0.315597
H	−0.961809	1.030083	1.649612
H	−0.865726	1.705210	−0.918964

$H_3P{=}O$

5

P	0.386719	0.000015	0.000016
O	−1.109092	0.000004	0.000026
H	1.024205	−0.622222	1.111911
H	1.024090	1.274116	−0.017427
H	1.023664	−0.652148	−1.094935

MeOH

6

O	−0.047617	−0.762170	0.000000
C	−0.047617	0.668053	0.000000
H	0.876630	−1.064839	0.000000
H	0.443337	1.082082	0.896968
H	0.443337	1.082082	−0.896968
H	−1.096661	0.989719	0.000000

MeO^-

5

O	0.000000	−0.000000	0.812540
C	−0.000000	0.000000	−0.569393
H	0.887917	−0.512639	−1.027989
H	0.000000	1.025278	−1.027989
H	−0.887917	−0.512639	−1.027989

PH_3

4

P	−0.000013	0.000001	−0.131014
H	0.597375	−1.033914	0.655019
H	0.597041	1.034094	0.655033
H	−1.194216	−0.000199	0.655158

$T_{15\text{-}7}$

27

P	0.888759	−1.601372	0.580551
O	2.083432	−0.865224	−0.618524
O	0.625359	0.265161	1.281572
O	0.607218	2.363023	0.574882
O	−2.334345	−1.852130	−0.660457
O	−2.203178	0.299253	0.099790
N	0.224321	0.648050	−0.962983
N	−0.339963	−0.684212	−0.834395
C	3.418405	−0.543054	−0.138499
C	0.446413	1.090631	0.331057
C	0.340427	3.335588	−0.492730
C	−3.593737	0.259949	0.558950
C	−1.762759	−0.807062	−0.467813
H	3.946772	−1.477219	0.086236
H	3.927584	−0.018617	−0.955702
H	3.374785	0.097127	0.753914
H	1.902369	−1.758152	1.554379
H	1.402770	0.102340	−1.048595
H	1.172725	3.327227	−1.205289
H	0.941118	−2.817504	−0.141340
H	0.282101	4.295978	0.025624
H	−4.252556	0.094618	−0.301006
H	−3.767065	1.240804	1.007967
H	−3.710888	−0.542052	1.296505
H	−0.601341	3.090441	−0.993630
H	−0.246353	−1.879703	1.389782
H	−0.214303	−1.178550	−1.759367

$T_{16\text{-}8}$

28

P	1.116144	−1.361292	−1.462509
O	2.820574	0.782972	0.814529
O	2.404747	−1.080805	−0.611996
O	0.896279	1.822155	−1.218780
O	−2.827382	−0.846117	1.616954
O	−2.031902	−0.923173	−0.528336
O	−0.798025	2.166871	0.275255
N	0.301292	0.139777	0.212715
N	−0.666985	−0.248098	1.154695
C	2.156953	−0.221460	0.763773
C	1.982169	−1.248243	1.849314
C	0.177065	1.421476	−0.306762
C	−3.322577	−1.424537	−0.953783
C	−1.924587	−0.677319	0.802396
C	−0.982612	3.485496	−0.291964
H	2.954760	−1.744527	1.977157
H	1.719437	−0.745341	2.788691
H	1.659433	−2.223491	−2.453502
H	1.224122	−2.001081	1.613632
H	0.559109	−0.320994	−2.230587
H	0.105183	−2.160788	−0.896430
H	−4.111280	−0.700140	−0.715938
H	−3.542087	−2.383131	−0.467072
H	−3.236432	−1.554796	−2.036841
H	−1.810171	3.928082	0.271047
H	−1.238029	3.412033	−1.356799
H	−0.627356	0.198163	2.086692
H	−0.071798	4.085937	−0.173136

$T_{17\text{-}5}$

32

P	−1.499736	−1.065787	−0.374233
O	2.969537	−0.035571	−1.871463
O	2.190520	−0.754375	0.158919
O	0.572979	2.506432	0.230358

O	−2.556540	−0.267626	−1.366312
O	−1.242915	1.660716	1.330623
O	−0.062242	−2.210972	0.839196
N	0.814499	0.403486	−1.233023
N	−0.184447	0.403487	−0.270541
C	3.507513	−1.314253	0.392400
C	2.065273	−0.111517	−1.054557
C	0.419952	3.697425	1.028292
C	−3.902694	−0.159023	−0.890957
C	−0.400899	−2.296932	2.237420
C	−0.352751	1.529737	0.493258
H	4.265237	−0.523481	0.355403
H	3.737345	−2.081948	−0.355920
H	3.462504	−1.753025	1.393927
H	1.223662	4.367698	0.705602
H	0.766819	−1.678609	0.732892
H	0.671452	0.926996	−2.099781
H	0.520751	3.467585	2.096905
H	0.365736	−2.875217	2.771012
H	−4.490401	0.318625	−1.684404
H	−4.332596	−1.153006	−0.678629
H	−3.953906	0.461979	0.017923
H	−2.228971	−2.316059	−0.301466
H	−1.907403	−0.612233	0.908300
H	−1.359261	−2.824902	2.303300
H	−0.587580	−1.513100	−1.371659
H	−0.558035	4.163428	0.851478
H	−0.498750	−1.298183	2.687856

$T_{20\text{-}10}$

21

P	−0.636811	−0.394231	−0.068030
O	3.340096	−0.226974	−0.792000
O	1.119959	−0.153701	−0.781211
O	−2.217170	−0.571219	0.546490
O	−0.955428	1.788822	−0.598801
C	2.269354	−0.369252	−0.178565
C	2.267180	−0.788525	1.282122
C	−3.089636	−1.372428	−0.240502

C	−0.564435	2.565730	0.484617
H	3.278293	−1.084013	1.580383
H	1.940216	0.049955	1.913876
H	1.571079	−1.620437	1.459040
H	0.512067	2.437250	0.759583
H	−4.059229	−1.426662	0.273419
H	−3.247593	−0.936251	−1.243994
H	−2.700078	−2.400899	−0.364403
H	−1.146364	2.362105	1.417326
H	−0.992390	−0.467882	−1.440235
H	−0.697144	3.647960	0.273130
H	−0.278772	−1.762261	0.163814
H	−0.222366	0.206027	1.146663

$T_{21\text{-}9Ret}$

16

P	1.617852	−0.327601	0.089997
O	0.389727	−1.326949	0.149515
O	0.091465	0.830563	−0.547331
O	−1.587394	−0.849480	−1.149031
C	−1.603449	−0.178734	1.179223
C	−0.982156	−0.461145	−0.168457
C	−0.119033	2.151133	−0.045559
H	2.602943	−1.265460	0.526195
H	2.234298	0.077307	−1.115142
H	1.828010	0.663122	1.081047
H	0.607497	2.822500	−0.527191
H	0.009293	2.209367	1.048998
H	−2.420372	0.545163	1.058578
H	−2.031182	−1.119933	1.550544
H	−1.133154	2.485320	−0.308674
H	−0.887672	0.196033	1.919223

$T_{22\text{-}23}$

18

P	0.963759	−1.467851	0.005576

O	1.050390	−0.009650	−1.065366
O	1.024943	−0.006437	1.074150
O	−1.075666	−1.100536	−0.018750
O	−0.847772	1.149922	−0.020480
C	1.442946	2.174254	0.005940
C	0.871967	0.791779	0.001207
C	−3.053673	0.242494	0.010641
C	−1.558717	0.075933	−0.019337
H	2.538488	2.093331	0.018955
H	2.365513	−1.681364	0.022193
H	1.131611	2.715875	−0.894064
H	1.110512	2.718469	0.896772
H	0.631467	−2.319708	−1.076168
H	0.606151	−2.316278	1.081947
H	−3.536719	−0.577719	−0.532866
H	−3.386303	0.200190	1.059295
H	−3.347401	1.211806	−0.406837

$T_{23\text{-}12}$

18

P	1.857444	−1.075620	−0.069548
O	1.096956	−0.032014	−0.968617
O	0.771833	0.433252	1.302655
O	−1.162677	−1.497220	0.134671
O	−1.080199	0.773174	−0.120572
C	0.713922	2.338209	−0.213845
C	0.367804	0.922075	0.199545
C	−3.211352	−0.232941	−0.109309
C	−1.716102	−0.418035	−0.011787
H	2.964458	−0.603260	0.662274
H	2.444653	−1.899375	−1.058859
H	1.797593	2.479015	−0.127099
H	1.139346	−1.974616	0.734701
H	0.391535	2.551362	−1.239251
H	0.210048	3.032850	0.472218
H	−3.703859	−1.207869	−0.177970
H	−3.570914	0.297774	0.784582
H	−3.467457	0.385037	−0.980108

$T_{3d\text{-}17}$

26

P	0.783307	0.954154	1.342113
O	2.297762	−1.089829	0.240447
O	0.848710	−1.784523	−1.389596
O	0.039686	2.560293	0.026860
O	−3.026294	0.276158	−1.025083
O	−2.000822	−1.050566	0.528730
N	0.305651	−0.054824	0.048964
N	−0.764903	0.415012	−0.769646
C	3.218489	−2.153291	−0.117770
C	1.138133	−1.059996	−0.458126
C	1.017530	3.158031	−0.834519
C	−3.294372	−1.616185	0.830682
C	−1.998768	−0.095587	−0.450293
H	4.076451	−2.024111	0.548171
H	3.522195	−2.049547	−1.166410
H	2.746834	−3.130508	0.042659
H	2.000758	3.185661	−0.332504
H	1.896801	1.825759	1.278952
H	1.278320	−0.028632	2.237699
H	1.117674	2.595721	−1.776567
H	0.720926	4.192014	−1.061362
H	−3.986403	−0.840216	1.183128
H	−3.718834	−2.106695	−0.055061
H	−3.111939	−2.351214	1.621545
H	−0.515687	1.762611	−0.539842
H	−0.320350	1.445444	2.061955

$T_{4\text{-}7}$

27

P	0.390032	1.250804	1.087102
O	1.987169	−2.152580	−0.277803
O	1.781821	0.010351	0.418744
O	0.520281	2.084906	−0.533629
O	−2.736257	1.078665	0.054627
O	−2.549506	−1.188870	−0.179235

N	−0.681674	0.123143	−0.293807
N	−0.001051	−1.103667	−0.405538
C	3.394303	−2.131489	0.123644
C	1.770662	2.531648	−1.113169
C	1.292514	−1.062782	−0.071228
C	−3.993973	−1.325091	−0.056728
C	−2.092290	0.064883	−0.112876
H	3.923325	−1.344047	−0.423964
H	3.769056	−3.119205	−0.153340
H	3.467873	−1.974058	1.205113
H	2.356835	1.683782	−1.487011
H	2.335872	3.077631	−0.347451
H	1.511196	3.215489	−1.928925
H	1.438610	2.006450	1.658620
H	0.207749	0.264911	2.098537
H	−4.488140	−0.763759	−0.857720
H	−4.319161	−0.954970	0.922022
H	−4.186118	−2.396546	−0.153110
H	−0.752055	2.033556	1.366456
H	−0.451335	−1.905678	−0.858768
H	−0.140471	1.155258	−0.931050

$T_{5\text{-}20}$

21

P	−0.999026	−0.312105	−0.225264
O	4.730724	−0.025040	−0.345146
O	2.589652	0.406706	−0.931469
O	−2.258479	−1.339245	0.078207
O	−1.978996	1.101150	−0.521009
C	3.480040	0.022625	−0.112798
C	2.998939	−0.397655	1.288846
C	−3.664138	−1.028047	−0.029749
C	−2.416062	1.871674	0.593232
H	3.759567	−0.980199	1.823732
H	2.781353	0.507356	1.877128
H	2.065344	−0.971918	1.219330
H	−4.158743	−1.951050	−0.358462
H	−4.059892	−0.736789	0.953860
H	−3.845200	−0.228444	−0.756123

H	−3.369571	1.505145	1.009730
H	−2.553252	2.910769	0.262327
H	−1.659236	1.862309	1.403070
H	−0.522390	−0.123345	−1.547804
H	−0.333843	0.411673	0.815393
H	−0.174623	−1.484075	−0.005072

$T_{7\text{-}9Inv}$

16

P	−3.294723	−0.206516	0.017319
O	2.177885	1.258909	0.002044
O	1.593824	−0.926603	−0.034624
O	−2.053620	0.708428	−0.015859
C	3.928599	−0.377052	0.029849
C	2.447050	0.028013	−0.007077
C	−0.542710	0.007372	−0.026375
H	4.481074	0.154378	−0.757589
H	4.364116	−0.069040	0.991959
H	4.063723	−1.458513	−0.091480
H	0.091987	0.894653	−0.019773
H	−4.468085	0.575649	0.033507
H	−3.411933	−1.077042	−1.094213
H	−3.365192	−1.054692	1.149852
H	−0.542366	−0.563531	−0.952651
H	−0.534834	−0.579990	0.889730

$T_{7\text{-}9ret}$

16

P	−1.676739	−0.956474	0.231516
O	1.762469	0.656786	1.144484
O	0.490289	0.078137	−0.630451
O	−2.111352	0.407187	−0.310296
C	2.663419	−0.885360	−0.483523
C	1.575453	0.022521	0.086818
C	−0.618259	1.954093	−0.245314
H	3.371575	−1.170185	0.303133

H	3.208003	−0.331869	−1.263590
H	2.232124	−1.778804	−0.951945
H	0.226794	1.990259	0.439609
H	−2.820457	−1.637926	0.729297
H	−1.563509	2.330237	0.133756
H	−1.123947	−1.880877	−0.683322
H	−0.807766	−0.957218	1.346608
H	−0.426667	2.099078	−1.304068

5.2 Coordinates in the Gas Phase

All structures were fully optimized at the bp86/6–311++G(3df,3pd) level of theory.

10

16

P	0.000000	0.927335	−0.000000
O	1.273677	−0.380605	0.000000
O	−0.997376	2.294896	−0.000000
O	−0.363214	−1.931468	0.000000
C	1.947989	−2.665838	0.000000
C	0.829841	−1.647151	0.000000
C	−2.400099	2.049287	−0.000000
H	2.585029	−2.522511	0.883575
H	2.585029	−2.522511	−0.883575
H	1.531049	−3.677371	0.000000
H	1.114577	1.778898	−0.000000
H	−2.913319	3.018765	−0.000000
H	−2.711192	1.481982	0.896639
H	−2.711192	1.481982	−0.896639
H	−0.525534	0.385186	1.193293
H	−0.525534	0.385186	−1.193293

11

11

P	1.542632	0.376761	−0.000000
O	0.000000	0.823823	−0.000000
O	−0.289248	−1.415583	0.000000
C	−2.295159	0.001249	−0.000000

C	−0.861197	−0.357895	0.000000
H	2.219233	1.608961	−0.000000
H	1.918520	−0.352353	1.144621
H	1.918520	−0.352353	−1.144621
H	−2.897092	−0.911839	0.000000
H	−2.523268	0.615064	0.883830
H	−2.523268	0.615064	−0.883830

12

13

O	1.276567	1.160555	0.697925
O	0.000010	−0.615370	−0.000067
O	−1.276628	1.160535	−0.697911
C	2.353991	−0.744945	−0.349162
C	1.211471	0.085098	0.168150
C	−2.353949	−0.744976	0.349205
C	−1.211461	0.085037	−0.168207
H	3.303599	−0.277062	−0.074381
H	2.298326	−1.765629	0.051330
H	2.279152	−0.820893	−1.443534
H	−3.303592	−0.277841	0.073274
H	−2.297552	−1.766150	−0.049913
H	−2.279836	−0.819472	1.443739

13

20

P	0.029849	2.158491	−0.074096
O	2.727998	0.354178	−0.846953
O	1.641766	−1.150086	0.492933
O	−2.809765	0.180661	0.953716
O	−1.600378	−1.061480	−0.538994
N	0.483597	0.586303	−0.389752
N	−0.573654	0.582580	0.707469
C	2.871280	−1.904824	0.600280
C	1.734120	−0.047778	−0.272442
C	−2.797432	−1.822803	−0.805643
C	−1.757708	−0.083586	0.393350

H	3.660611	−1.289732	1.049909
H	3.196866	−2.246184	−0.390206
H	2.629023	−2.755180	1.244026
H	0.925258	2.932582	−0.888984
H	0.237293	2.814899	1.162063
H	−3.602673	−1.167826	−1.162244
H	−3.133613	−2.340463	0.102033
H	−2.515698	−2.544235	−1.579002
H	−1.192935	2.604344	−0.629052

14a

20

P	−0.167783	2.029805	0.000422
O	2.662010	0.839845	−0.000716
O	1.898988	−1.306129	0.000355
O	−2.901860	−0.740802	−0.000390
O	−1.856899	1.241763	−0.000945
N	0.382180	0.381057	0.000369
N	−0.583771	−0.654057	0.000498
C	3.279852	−1.731703	−0.000216
C	1.742982	0.036521	0.000046
C	−2.779961	−2.180791	0.000232
C	−1.745062	−0.069472	−0.000307
H	3.798719	−1.362786	0.893450
H	3.797876	−1.363130	−0.894513
H	3.238459	−2.825052	0.000015
H	1.166427	2.526528	0.001160
H	−3.808158	−2.554453	0.000000
H	−2.241835	−2.519348	0.895267
H	−2.241169	−2.520063	−0.894132
H	−0.593986	2.738063	1.152869
H	−0.593229	2.739416	−1.151481

14b

20

P	−0.167783	2.029805	0.000422

O	2.662010	0.839845	−0.000716
O	1.898988	−1.306129	0.000355
O	−2.901860	−0.740802	−0.000390
O	−1.856899	1.241763	−0.000945
N	0.382180	0.381057	0.000369
N	−0.583771	−0.654057	0.000498
C	3.279852	−1.731703	−0.000216
C	1.742982	0.036521	0.000046
C	−2.779961	−2.180791	0.000232
C	−1.745062	−0.069472	−0.000307
H	3.798719	−1.362786	0.893450
H	3.797876	−1.363130	−0.894513
H	3.238459	−2.825052	0.000015
H	1.166427	2.526528	0.001160
H	−3.808158	−2.554453	0.000000
H	−2.241835	−2.519348	0.895267
H	−2.241169	−2.520063	−0.894132
H	−0.593986	2.738063	1.152869
H	−0.593229	2.739416	−1.151481

15

21

P	0.095638	2.131660	−0.303299
O	2.646803	−0.594030	−0.383738
O	1.300335	1.111831	−0.704466
O	−2.737952	0.346219	0.789323
O	−1.541565	−1.219720	−0.380760
N	0.704244	−0.548558	0.871644
N	−0.438138	0.310677	0.939728
C	3.023339	−1.869470	0.240872
C	1.516415	−0.071723	−0.009752
C	−2.772374	−1.790742	−0.943031
C	−1.721511	−0.217235	0.458801
H	3.964062	−2.138696	−0.242893
H	3.155505	−1.719703	1.317755
H	2.242699	−2.612585	0.046727
H	0.566572	3.143661	−1.174488
H	0.128766	2.793380	0.942150
H	−3.365665	−2.231578	−0.135109

H	−3.344889	−1.007625	−1.451129
H	−2.429390	−2.554585	−1.643707
H	−1.234409	1.962853	−0.748318
H	−0.596739	0.595763	1.914665

16

28

P	0.885312	−1.515142	−0.746140
O	4.285493	0.349428	−0.121630
O	2.351530	−0.515381	−0.807992
O	0.453096	1.476401	−1.375682
O	−3.198539	−0.894647	1.542747
O	−2.574256	−0.492286	−0.626005
O	−0.644285	1.869751	0.589430
N	−0.990052	−0.703041	0.981344
N	−0.010531	−0.254958	0.101604
C	3.235973	−0.185134	0.170391
C	2.853327	−0.499717	1.607249
C	−3.970202	−0.526232	−1.004546
C	−2.352022	−0.700156	0.691928
C	−0.768682	3.258874	0.198434
C	−0.022728	1.093356	−0.331264
H	3.706795	−0.284017	2.256816
H	2.562808	−1.553754	1.732033
H	1.999749	0.119963	1.916041
H	1.613595	−2.502947	−0.026489
H	1.029059	−1.587686	−2.149680
H	0.223859	3.711352	0.085232
H	−4.530732	0.248303	−0.467022
H	−4.402294	−1.508986	−0.779602
H	−3.979794	−0.335651	−2.081524
H	−1.324424	3.735961	1.010775
H	−1.315021	3.340070	−0.749137
H	−0.775429	−0.636459	1.973621
H	−0.322089	−2.305096	−0.709682

17

26

P	1.604892	−1.115206	−0.651002
O	2.621059	−0.508609	0.499477
O	1.113106	1.850531	−0.952407
O	−2.764361	−1.153375	1.470578
O	−2.109128	−0.877430	−0.707377
O	−0.706767	1.997437	0.433059
N	0.302550	−0.019001	0.080850
N	−0.608635	−0.571435	0.969337
C	4.023611	−0.818382	0.525115
C	0.298534	1.328678	−0.201868
C	−3.449675	−1.231256	−1.108750
C	−1.919405	−0.877904	0.636590
C	−0.764359	3.405660	0.124012
H	4.589032	0.056242	0.175580
H	4.292757	−1.044722	1.564513
H	4.261319	−1.685553	−0.110781
H	2.659586	−1.994838	−1.136733
H	1.375326	−0.527347	−1.919876
H	0.694263	−2.184248	−0.423992
H	0.175956	3.900807	0.397822
H	−4.176614	−0.523160	−0.691405
H	−3.699987	−2.244466	−0.769310
H	−3.445847	−1.180227	−2.201891
H	−1.595060	3.797762	0.719054
H	−0.951305	3.558894	−0.946639
H	−0.473713	−0.377203	1.960159

18

26

P	−0.540761	−1.918151	−0.455206
O	2.486571	0.711121	0.196508
O	2.461061	−1.531202	−0.204634
O	−1.813971	0.666002	−1.429703
O	−1.658582	2.531700	−0.205533
O	−1.407052	−1.351253	0.827635

N	0.490398	−0.323443	−0.246183
N	−0.020760	0.939075	0.080052
C	3.912930	0.582275	0.342472
C	1.851343	−0.466041	−0.081599
C	−2.603831	−2.033600	1.239594
C	−1.087327	1.336015	−0.492016
C	−0.961625	3.342380	0.763985
H	4.370030	0.204640	−0.581813
H	4.270698	1.594160	0.560938
H	4.164820	−0.099342	1.165603
H	0.691380	−2.604666	−0.373446
H	0.050005	3.575232	0.408549
H	−3.400762	−1.931603	0.488291
H	−2.915397	−1.545058	2.170445
H	−2.577100	1.227230	−1.662655
H	−2.420978	−3.100606	1.430730
H	−1.562572	4.252056	0.862251
H	−1.370368	−3.117393	−0.505588
H	−0.890047	2.810188	1.721166
H	−0.798906	−1.579103	−1.802279

19

26

P	0.604724	−1.548581	0.768424
O	1.621829	−1.813187	−0.558185
O	1.596497	2.229974	0.419383
O	1.333560	0.130133	1.012007
O	−2.619479	−1.289949	−1.016928
O	−2.381612	0.546865	0.321756
N	0.032565	1.021129	−0.739270
N	−0.555167	−0.286666	−0.767301
C	3.005581	−1.454401	−0.514475
C	1.211070	3.355708	−0.399898
C	0.939430	1.079834	0.204507
C	−3.783882	0.446695	0.667244
C	−1.955966	−0.392977	−0.535699
H	3.512465	−2.070454	−1.269222
H	3.446768	−1.666477	0.473544
H	3.162359	−0.391100	−0.749811

H	1.832830	4.185278	−0.048929
H	1.440927	−2.113695	1.765969
H	1.404702	3.146240	−1.459667
H	0.145798	3.582280	−0.266753
H	−4.404588	0.552521	−0.230922
H	−3.991449	−0.520389	1.141149
H	−3.966162	1.269365	1.364315
H	−0.420049	−1.076498	1.651860
H	−0.330427	−0.770810	−1.641524
H	−0.149583	−2.678624	0.335285

20

21

P	−0.589328	−0.457970	−0.134194
O	3.383253	0.207427	−0.745072
O	1.151064	0.117414	−0.720796
O	−2.140385	−1.094153	0.339302
O	−1.125186	1.228182	−0.243242
C	2.382402	−0.947375	1.100165
C	2.327934	−0.160722	−0.213073
C	−3.299905	−0.563715	−0.252637
C	−0.594420	2.177664	0.639707
H	3.391491	−1.355374	1.231159
H	2.162130	−0.270102	1.938566
H	1.634212	−1.752316	1.123698
H	0.243655	2.737816	0.180712
H	−4.137053	−1.254861	−0.047707
H	−3.557606	0.437691	0.143021
H	−3.199134	−0.463837	−1.353026
H	−1.381974	2.898046	0.931224
H	−0.893028	−0.515311	−1.534690
H	−0.212295	1.710618	1.573498
H	−0.204006	−0.201442	1.234420
H	−0.052501	−1.807446	−0.094485

21

16

P	−0.891212	0.961230	0.233509
O	1.195816	−0.860703	1.106179
O	0.731394	0.682859	−0.483529
O	−1.325806	−0.449337	−0.478412
C	2.901959	−0.282366	−0.514646
C	1.535971	−0.205781	0.131500
C	−2.601086	−1.064979	−0.245792
H	3.533628	−0.987571	0.033573
H	3.369591	0.711432	−0.528665
H	2.799273	−0.606632	−1.559428
H	−3.321145	−0.359243	0.197038
H	−2.980027	−1.409953	−1.215846
H	−2.466511	−1.921776	0.428339
H	−2.238984	1.161460	0.738029
H	−0.867100	2.183382	−0.479372
H	−0.292852	1.146638	1.503416

22

18

P	−0.429150	1.596540	−0.000096
O	1.172806	0.783419	−0.000149
O	0.873828	−1.486623	−0.000417
O	−1.139125	0.168010	−1.073399
O	−1.138823	0.168048	1.073791
C	3.103164	−0.565895	0.000229
C	1.589249	−0.495020	−0.000238
C	−2.158975	−1.773366	0.000161
C	−1.432484	−0.477510	0.000284
H	3.502363	−0.047791	−0.882169
H	3.501194	−0.052717	0.886066
H	3.424461	−1.611811	−0.002277
H	0.030593	2.353223	1.102694
H	0.030197	2.353066	−1.103149
H	−3.240997	−1.572117	−0.011540
H	−1.913258	−2.338336	0.904117

H	−1.896253	−2.346787	−0.893721
H	−1.756247	2.123085	0.000188

23

18

P	1.309925	−1.303167	0.003867
O	1.006320	0.097049	−1.073907
O	0.991010	0.096931	1.078403
O	−1.048275	−1.291576	−0.011039
O	−0.931541	0.982974	−0.011839
C	1.084258	2.311026	0.003102
C	0.614313	0.877368	−0.000428
C	−3.088668	−0.002996	0.006787
C	−1.590154	−0.175017	−0.010612
H	2.728072	−1.297659	0.013773
H	2.182980	2.316611	0.010491
H	1.067193	−2.209122	−1.068082
H	1.052157	−2.209530	1.071975
H	0.721869	2.827996	−0.895854
H	0.709828	2.827503	0.897402
H	−3.573931	−0.971785	−0.161651
H	−3.399437	0.722606	−0.758926
H	−3.396211	0.395575	0.986818

2d

16

O	2.439194	−0.690225	−0.118343
O	2.138241	1.571604	0.060037
O	−2.439210	0.690219	0.118400
O	−2.138215	−1.571593	−0.060128
N	0.356233	0.187436	−0.477063
N	−0.356229	−0.187422	0.477037
C	3.868106	−0.523398	0.089271
C	1.734345	0.445087	−0.107644
C	−3.868122	0.523377	−0.089204
C	−1.734339	−0.445078	0.107618

H	4.289802	−1.526969	−0.009853
H	4.281315	0.153967	−0.667653
H	4.056383	−0.117218	1.090068
H	−4.289838	1.526931	0.010009
H	−4.281303	−0.154061	0.667669
H	−4.056405	0.117275	−1.090033

3d

20

P	−0.022484	1.886066	−0.340111
O	2.127838	1.030333	0.507095
O	2.028219	−1.198858	−0.059597
O	−2.524438	−1.653849	−0.692120
O	−1.734393	0.052462	0.645569
N	0.359476	0.262631	−0.633985
N	−0.508016	−0.669919	−1.212825
C	3.312523	−1.405562	0.583240
C	1.572592	0.043238	−0.012885
C	−2.963811	−0.077310	1.377302
C	−1.627284	−0.857045	−0.468758
H	4.086253	−0.809184	0.085112
H	3.513520	−2.474079	0.470408
H	3.255567	−1.129045	1.642824
H	0.859442	2.828274	−0.919344
H	−3.830641	0.143852	0.739019
H	−3.073578	−1.096732	1.769524
H	−2.904541	0.641138	2.204128
H	−1.238243	2.060475	−1.024454
H	−0.232662	2.334713	0.981138

4

21

P	−0.433430	2.018148	−0.073529
O	2.682360	−0.947015	−0.416976
O	1.544997	0.507160	0.946598
O	−2.406119	0.687335	0.521255
O	−1.864112	−1.418034	−0.230645

N	0.590659	−0.334879	−0.949448
N	−0.535597	0.412823	−0.661361
C	3.864966	−0.881799	0.444736
C	1.648279	−0.215851	−0.038905
C	−3.080119	−1.995892	0.366542
C	−1.698387	−0.136557	−0.055790
H	4.597547	−1.528322	−0.042692
H	4.225471	0.150915	0.501567
H	3.612016	−1.254614	1.442757
H	0.777230	2.497916	−0.604883
H	0.763677	−0.553651	−1.929472
H	−3.959955	−1.553425	−0.111473
H	−3.082885	−1.800715	1.443761
H	−3.006892	−3.064087	0.154615
H	−1.442040	2.811800	−0.652485
H	−0.433594	2.221372	1.315540

5

14

P	0.000079	−0.000061	−0.116359
O	1.601123	0.608245	−0.228213
O	−1.601219	−0.608151	−0.228170
C	2.619243	−0.246172	0.262623
C	−2.619293	0.246220	0.262626
H	3.592408	0.199863	0.019641
H	2.568098	−1.250191	−0.204720
H	2.552401	−0.374129	1.360121
H	0.383486	−1.232790	−0.707259
H	0.000566	−0.001188	1.308121
H	−3.592574	−0.196921	0.014659
H	−2.564840	1.252082	−0.200629
H	−2.555843	0.369913	1.360845
H	−0.383817	1.233238	−0.705832

6

18

O	2.625166	0.172616	−0.490125

O	1.241153	−0.559819	1.187086
O	−2.625206	0.172703	0.490078
O	−1.241132	−0.559935	−1.186982
N	0.665174	1.209964	−0.190274
N	−0.665166	1.209937	0.190203
C	3.601905	−0.809101	−0.079840
C	1.486581	0.173726	0.251361
C	−3.601901	−0.809128	0.079866
C	−1.486574	0.173725	−0.251378
H	4.447440	−0.677504	−0.761550
H	3.911162	−0.633218	0.958244
H	3.187734	−1.821158	−0.168467
H	0.843395	1.572267	−1.123663
H	−4.445691	−0.680377	0.764277
H	−3.914315	−0.630697	−0.956851
H	−3.186264	−1.820906	0.164490
H	−0.843420	1.572428	1.123503

7

9

P	−0.749284	−0.668949	0.000000
O	0.000000	0.702213	0.000000
C	1.479421	0.838736	0.000000
H	1.884637	0.379254	0.908602
H	1.884637	0.379254	−0.908602
H	1.649391	1.917564	0.000000
H	−2.120799	−0.357394	0.000000
H	−0.467571	−1.467278	1.133410
H	−0.467571	−1.467278	−1.133410

8

23

O	2.366651	−0.764852	0.226952
O	0.617056	−1.878758	−0.701658
O	0.183818	2.672202	−0.282355
O	−2.961915	−0.269774	−0.506489
O	−1.600233	−0.131979	1.336655

N	0.483513	0.407709	−0.392815
N	−0.836137	0.330124	−0.794112
C	3.064376	−2.032294	0.315653
C	2.344915	1.941213	0.431544
C	1.133645	−0.853659	−0.310324
C	0.943806	1.746354	−0.092314
C	−4.058702	−0.621441	0.363919
C	−1.786499	−0.047449	0.139711
H	4.033305	−1.792556	0.763175
H	3.192092	−2.468566	−0.682303
H	3.096716	1.544445	−0.261253
H	2.503392	−2.729128	0.949408
H	2.485086	3.018553	0.561430
H	2.483846	1.425354	1.389241
H	−4.918317	−0.762257	−0.298149
H	−4.252663	0.184977	1.082286
H	−3.834969	−1.547094	0.908985
H	−1.012388	0.150386	−1.778300

9

11

O	1.185616	0.762178	0.000000
O	−0.484532	−0.775792	0.000000
C	0.523358	−1.811892	0.000000
C	0.000000	0.498146	0.000000
C	−1.130371	1.499256	0.000000
H	1.156149	−1.732356	0.893126
H	1.156149	−1.732356	−0.893126
H	−1.765183	1.352080	0.884057
H	−1.765183	1.352080	−0.884057
H	−0.719288	2.512634	0.000000
H	−0.029238	−2.756227	0.000000

AcO^-

7

O	1.118447	0.800302	0.000000

O	−1.161072	0.711696	0.000000
C	0.041859	−1.357648	0.000000
C	0.000000	0.212117	0.000000
H	1.073227	−1.740314	0.000000
H	−0.491691	−1.741244	0.885243
H	−0.491691	−1.741244	−0.885243

AcOH

8

O	0.166251	1.357933	0.000000
O	−1.245386	−0.411424	0.000000
C	1.081800	−0.893092	0.000000
C	0.000000	0.155917	0.000000
H	2.062141	−0.409648	0.000000
H	0.978994	−1.537396	0.883711
H	0.978994	−1.537396	−0.883711
H	−1.877848	0.335412	0.000000

$E_{15\text{-}7}$

27

P	0.421893	−1.141446	1.140306
O	1.868565	−1.940812	−0.612414
O	1.563607	2.357893	0.335493
O	1.388100	0.252220	0.967904
O	−2.601314	0.456630	0.078792
O	−2.358841	−1.637151	−0.822486
N	−0.507034	−0.285155	−0.530435
N	−0.091332	1.076777	−0.639985
C	3.295712	−1.656065	−0.726917
C	1.125660	3.496446	−0.475432
C	0.904103	1.239208	0.182361
C	−4.051908	0.273805	0.208540
C	−1.958116	−0.557006	−0.462388
H	3.859697	−2.168476	0.062998
H	3.652222	−1.969024	−1.716115
H	3.408970	−0.574464	−0.618479

H	1.799300	4.307364	−0.191274
H	1.744476	−2.901219	−0.715617
H	1.378084	−1.681374	2.027117
H	1.223933	3.250829	−1.538585
H	0.085334	3.740491	−0.234450
H	−4.488245	0.130504	−0.785587
H	−4.407732	1.197983	0.668137
H	−4.257887	−0.594644	0.843254
H	−0.586926	−0.674421	2.012991
H	−0.176122	−2.340046	0.666934
H	−0.148579	−0.831730	−1.328274

$H_3P{=}O$

5

P	−0.384012	0.000002	−0.000007
O	1.107296	0.000001	0.000006
H	−1.032746	1.168443	−0.500194
H	−1.032743	−0.151025	1.261993
H	−1.032702	−1.017462	−0.761739

MeO^-

5

O	−0.000000	−0.000000	0.794791
C	0.000000	0.000000	−0.536911
H	0.895770	−0.517173	−1.045622
H	0.000000	1.034346	−1.045622
H	−0.895770	−0.517173	−1.045622

MeOH

6

O	−0.046927	−0.761946	0.000000
C	−0.046927	0.667844	0.000000
H	0.874639	−1.064203	0.000000

H	0.440094	1.085429	0.898102
H	0.440094	1.085429	−0.898102
H	−1.097846	0.981848	0.000000

PH_3

4

P	−0.000000	−0.000078	−0.131470
H	1.032621	−0.596285	0.657607
H	0.000430	1.192993	0.656834
H	−1.033051	−0.595540	0.657607

$T_{15\text{-}7}$

27

P	0.900153	−1.557652	0.644939
O	2.075044	−0.878840	−0.620049
O	0.668172	0.288130	1.275581
O	0.613676	2.379773	0.560311
O	−2.344618	−1.838608	−0.761035
O	−2.223577	0.263641	0.144402
N	0.227206	0.651156	−0.964988
N	−0.344481	−0.677703	−0.806331
C	3.447702	−0.614555	−0.212880
C	0.463147	1.110796	0.324176
C	0.319115	3.359520	−0.496229
C	−3.631395	0.206532	0.566217
C	−1.785251	−0.811860	−0.481074
H	3.952255	−0.164268	−1.074957
H	3.932866	−1.565826	0.033723
H	3.480751	0.067964	0.647244
H	1.931373	−1.707741	1.597968
H	1.399291	0.102672	−1.040522
H	1.166797	3.404357	−1.187756
H	0.930177	−2.792317	−0.047240
H	0.205042	4.305111	0.038031
H	−4.267778	0.104990	−0.319002
H	−3.807430	1.154689	1.077838

H	−3.773357	−0.644525	1.240198
H	−0.597025	3.076675	−1.022636
H	−0.225176	−1.814030	1.471341
H	−0.198639	−1.192509	−1.684022

$T_{16\text{-}8}$

28

P	1.197963	−1.425442	−1.441529
O	2.874262	0.755684	0.503239
O	2.297108	−1.470701	−0.341442
O	0.823818	1.779209	−1.346801
O	−2.849551	−0.754884	1.620745
O	−2.080306	−0.977660	−0.524500
O	−0.770276	2.189980	0.239461
N	0.287043	0.136225	0.155882
N	−0.678947	−0.231240	1.113121
C	2.179032	−0.167526	0.782333
C	2.006751	−0.878004	2.091026
C	0.155059	1.406146	−0.390948
C	−3.394063	−1.461277	−0.884037
C	−1.957659	−0.651617	0.796136
C	−0.919574	3.508308	−0.329680
H	2.944160	−1.416873	2.284674
H	1.861261	−0.134563	2.885444
H	1.736237	−2.325884	−2.405365
H	1.177788	−1.589205	2.079977
H	1.030555	−0.229120	−2.173544
H	0.027273	4.060075	−0.275249
H	−4.155867	−0.704283	−0.661200
H	−3.631575	−2.381596	−0.335602
H	−3.346790	−1.653808	−1.960490
H	−1.689673	3.998993	0.273764
H	−1.235415	3.441588	−1.378722
H	−0.661824	0.278160	1.996455
H	−0.059959	−2.005962	−1.184816

$T_{17\text{-}5}$

32

P	−1.631746	−0.924483	−0.319865
O	2.861985	−0.172501	−2.002346
O	2.123276	−0.887932	0.046760
O	0.793142	2.404131	0.226760
O	−2.601950	−0.024606	−1.301112
O	−1.011048	1.691340	1.439093
O	−0.187586	−2.236350	0.997449
N	0.737074	0.320294	−1.300671
N	−0.208492	0.409049	−0.288986
C	3.425148	−1.495966	0.225089
C	1.986033	−0.227760	−1.159608
C	0.824190	3.567971	1.077123
C	−4.007730	−0.025344	−1.021856
C	−0.409217	−2.126329	2.414587
C	−0.206808	1.514468	0.530557
H	4.210132	−0.733060	0.167716
H	3.602701	−2.258515	−0.542921
H	3.400411	−1.948393	1.221448
H	1.657768	4.173696	0.707186
H	0.991508	3.281442	2.123582
H	0.642714	−1.754349	0.768801
H	0.621266	0.897751	−2.131528
H	0.394245	−2.633685	2.969196
H	−4.480192	0.622745	−1.769576
H	−4.430857	−1.039820	−1.100773
H	−4.212202	0.379617	−0.017255
H	−2.496085	−2.088395	−0.227366
H	−1.921280	−0.462001	0.988704
H	−1.359297	−2.628836	2.630339
H	−0.743843	−1.532451	−1.250556
H	−0.474517	−1.074446	2.732675
H	−0.118613	4.125653	1.007722

$T_{21\text{-}9Ret}$

16

P	1.618988	−0.349065	0.077896
O	0.421555	−1.334026	0.252754
O	0.102500	0.846085	−0.539349
O	−1.563826	−0.852187	−1.184203
C	−1.678827	−0.165826	1.143781
C	−1.045445	−0.443043	−0.192129
C	−0.072055	2.155425	−0.024067
H	2.660152	−1.231539	0.512897
H	2.176071	−0.003007	−1.175074
H	1.900305	0.706149	0.987098
H	0.673236	2.823393	−0.485362
H	0.046569	2.204048	1.074892
H	−2.516600	0.530845	1.006406
H	−2.078384	−1.116527	1.519207
H	−1.073340	2.528349	−0.287982
H	−0.976694	0.235941	1.880353

$T_{22\text{-}23}$

18

P	0.982600	−1.452528	0.005788
O	1.048375	−0.004342	−1.065293
O	1.021437	−0.001165	1.074716
O	−1.071344	−1.113905	−0.019455
O	−0.852334	1.139226	−0.021140
C	1.415034	2.182963	0.006017
C	0.854913	0.793998	0.001190
C	−3.051176	0.225655	0.010992
C	−1.553212	0.058091	−0.019765
H	2.510356	2.111762	0.020084
H	2.385724	−1.659347	0.023418
H	1.097688	2.719147	−0.894413
H	1.074821	2.722391	0.896083
H	0.657766	−2.311305	−1.072947
H	0.631246	−2.307961	1.078926
H	−3.534957	−0.618962	−0.491446

H	−3.378985	0.234135	1.061008
H	−3.345087	1.175299	−0.448772

$T_{23\text{-}12}$

18

P	1.808970	−1.074721	−0.041836
O	1.138271	−0.049833	−1.011896
O	0.775705	0.403656	1.278265
O	−1.154694	−1.492855	0.086205
O	−1.063184	0.786677	−0.126987
C	0.733226	2.340893	−0.199437
C	0.354017	0.934054	0.207713
C	−3.198638	−0.212875	−0.080544
C	−1.702398	−0.413613	−0.021633
H	2.916423	−0.648740	0.718128
H	2.427046	−1.945585	−0.975779
H	1.818047	2.459167	−0.106272
H	1.057801	−1.962301	0.743536
H	0.417576	2.561956	−1.224462
H	0.240621	3.041529	0.488938
H	−3.696722	−1.183827	−0.156467
H	−3.532525	0.302615	0.831221
H	−3.468840	0.424098	−0.932605

$T_{4\text{-}7}$

27

P	0.394939	1.270803	1.102469
O	1.997292	−2.188285	−0.237500
O	1.856082	0.045277	0.256133
O	0.412854	2.139557	−0.497885
O	−2.739673	1.021250	0.099791
O	−2.509372	−1.240000	−0.195641
N	0.032473	−1.105502	−0.405608
N	−0.660811	0.112005	−0.258438
C	3.425054	−2.185994	0.098346
C	1.597282	2.729092	−1.095597

C	1.344471	−1.056382	−0.104660
C	−3.959935	−1.416346	−0.084981
C	−2.081939	0.026709	−0.090626
H	3.958525	−1.497240	−0.565031
H	3.743784	−3.216487	−0.070120
H	3.558177	−1.899689	1.146835
H	2.277574	1.951800	−1.461829
H	2.095397	3.350109	−0.341458
H	1.468269	2.029938	1.618846
H	1.247415	3.366115	−1.914905
H	0.349979	0.220003	2.063088
H	−4.456823	−0.854352	−0.882731
H	−4.297190	−1.062437	0.894836
H	−4.122262	−2.490643	−0.196333
H	−0.753981	1.985945	1.498160
H	−0.507332	−1.963728	−0.515576
H	−0.174306	1.168249	−0.896582

$T_{5\text{-}20}$

21

P	−0.777028	−0.464538	−0.197917
O	4.141599	0.155039	−0.542582
O	1.894259	0.136884	−0.840399
O	−2.185936	−1.303370	0.150538
O	−1.603070	1.089936	−0.506123
C	2.959648	−0.017357	−0.155422
C	2.751704	−0.453769	1.324985
C	−3.490965	−0.747545	−0.008608
C	−1.707907	2.034899	0.524351
H	3.710713	−0.678812	1.811527
H	2.252312	0.356782	1.880591
H	2.094156	−1.335903	1.376760
H	−4.196070	−1.569111	0.190137
H	−3.687332	0.067933	0.705515
H	−3.654753	−0.362146	−1.025210
H	−2.710240	2.035057	1.003450
H	−1.519327	3.044702	0.121725
H	−0.959464	1.847961	1.325663
H	−0.481352	−0.420505	−1.577748

H	−0.156291	0.167344	0.920698
H	−0.086640	−1.710508	0.032347

$T_{7\text{-}9Inv}$

16

P	−2.093633	−0.748190	−0.000003
O	1.660292	1.205816	−0.000037
O	0.813932	−0.907406	−0.000032
O	−2.242811	0.790614	0.000033
C	3.196623	−0.628669	0.000031
C	1.771877	−0.071686	−0.000036
C	−0.554060	1.424774	0.000012
H	3.941714	0.174581	−0.000695
H	3.337287	−1.265294	0.884798
H	3.336902	−1.266659	−0.883804
H	−3.395775	−1.307956	−0.000003
H	−1.446361	−1.305634	−1.122481
H	−1.446338	−1.305686	1.122436
H	−0.715605	2.502826	0.000032
H	−0.272648	0.969006	−0.934738
H	−0.272614	0.968975	0.934738

$T_{7\text{-}9Ret}$

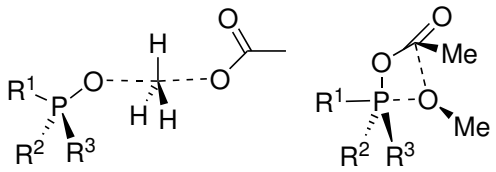
16

P	−1.545951	−0.972764	0.109945
O	1.447275	0.241796	1.332843
O	0.486652	0.192850	−0.709187
O	−2.122074	0.385236	−0.277882
C	2.742950	−0.564510	−0.541997
C	1.485400	−0.003483	0.118489
C	−0.630767	1.945870	−0.077678
H	3.413989	−0.977594	0.218649
H	3.258416	0.253463	−1.066581
H	2.491955	−1.324950	−1.291970
H	0.125822	1.890105	0.703597
H	−2.611407	−1.774042	0.611018

H	−1.615090	2.278673	0.234123
H	−1.023066	−1.798962	−0.911350
H	−0.609805	−1.016203	1.171080
H	−0.321868	2.234649	−1.076827

6 Effect of Substitution on Phosphorus

The transition states for inversion $\mathbf{T_{7X\text{-}9}}$ and retention $\mathbf{T_{21X\text{-}9}}$ (Chart S3) for different substituents on phosphorus have been calculated. Geometries were optimized at the BP86/6–311++G(3df,3pd) level of theory. A smaller basis set [6–311+G(d,p) except for the phenyl substituents for which the 6–31G(d) basis was employed] was used for the calculations of the two transition structures of the PPh_3 system. Solvent effects were incorporated by the C-PCM model using acetonitrile ($\varepsilon = 36.64$) as solvent.



$\mathbf{T_{7X\text{-}9}}$ inversion $\quad$ $\mathbf{T_{21X\text{-}9}}$ retention

	R^1	R^2	R^3
inversion			
$\mathbf{T_{7m1\text{-}9}}$	Me	H	H
$\mathbf{T_{7m2\text{-}9}}$	Me	Me	H
$\mathbf{T_{7m3\text{-}9}}$	Me	Me	Me
$\mathbf{T_{t7p3\text{-}9}}$	Ph	Ph	Ph
retention			
$\mathbf{T_{21m1\text{-}9}}$	Me	H	H
$\mathbf{T_{21m2\text{-}9}}$	Me	Me	H
$\mathbf{T_{21m3\text{-}9}}$	Me	Me	Me
$\mathbf{T_{21p3\text{-}9}}$	Ph	Ph	Ph

Chart S3: Compounds used in the investigation of stereochemical control

6.1 Absolute Energies of Calculated Structures

Table S6: Absolute energies in solution [a. u.]

Compound	E_{SCF}	ΔU	ΔG	N_{imag}
$\mathbf{T_{21m1\text{-}9}}$	-726.259794757	-726.114703	-726.149781	1
$\mathbf{T_{21m2\text{-}9}}$	-765.598984748	-765.426404	-765.463473	1
$\mathbf{T_{21m3\text{-}9}}$	-804.930672338	-804.730029	-804.768753	1
$\mathbf{T_{21p3\text{-}9}}$	-1380.02213901	-1379.667383	-1379.721320	1
$\mathbf{T_{7m1\text{-}9}}$	-726.261076973	-726.118401	-726.157669	1
$\mathbf{T_{7m2\text{-}9}}$	-765.607395596	-765.437404	-765.478521	1
$\mathbf{T_{7m3\text{-}9}}$	-804.947674154	-804.749227	-804.794129	1
$\mathbf{T_{7p3\text{-}9}}$	-1380.04494601	-1379.691780	-1379.752441	1

6.2 Cartesian Coordinates of Calculated Structures

All cartesian coordinates are given in Ångström. For convenience, coordinates of all compounds are also available in xyz-format packed together into a single ZIP-archive.

$T_{21m1\text{-}9}$

19

P	1.261897	0.321767	−0.115203
O	0.432844	−1.039746	−0.002893
O	−1.644393	−1.323393	−1.086159
O	−0.651651	0.905237	−0.555294
C	2.922465	−0.345096	0.261522
C	−1.694265	−0.716355	1.255806
C	−1.241098	2.027619	0.087534
C	−1.111921	−0.766668	−0.138994
H	3.642392	0.486593	0.225719
H	3.212410	−1.098949	−0.482299
H	2.943658	−0.796134	1.262181
H	1.526700	0.920803	−1.369614
H	1.166877	1.303856	0.904697
H	−2.722256	−0.334863	1.210327
H	−2.337979	1.934682	0.073197
H	−1.727358	−1.746226	1.638828
H	−1.105536	−0.106136	1.950060
H	−0.963526	2.940684	−0.462589
H	−0.909329	2.135405	1.137095

$T_{21m2\text{-}9}$

22

P	−1.103051	0.013363	−0.227133
O	1.841835	−0.788161	1.484998
O	0.647916	1.025132	0.200690
O	−0.077916	−1.151874	0.200462
C	2.118410	−0.885127	−0.913878
C	1.357662	−0.635097	0.371316
C	1.170311	1.974568	−0.713428
C	−2.499963	−1.104204	−0.642349
C	−1.867675	1.099871	1.016029

H	3.076644	−0.351572	−0.885089
H	2.328626	−1.963032	−0.970287
H	2.268872	2.007916	−0.638972
H	1.561062	−0.593196	−1.811348
H	0.899370	1.746031	−1.762497
H	0.780305	2.975452	−0.465033
H	−3.338471	−0.503374	−1.023785
H	−2.958972	0.990189	1.006726
H	−2.834555	−1.659183	0.244745
H	−2.192308	−1.819530	−1.416172
H	−1.580763	2.141137	0.834589
H	−1.478225	0.805654	2.000093
H	−0.952981	0.642224	−1.501322

$T_{21m3\text{-}9}$

25

P	1.005997	−0.092266	0.008614
O	−2.147855	−1.133681	−1.166372
O	−0.680155	0.901985	−0.467008
O	−0.150682	−1.247504	−0.023949
C	2.325924	−1.361780	0.299114
C	1.699902	0.670971	−1.497654
C	1.270531	0.901824	1.512806
C	−2.203624	−0.557299	1.175505
C	−1.542372	−0.765595	−0.168689
C	−1.146495	2.176594	−0.079785
H	3.306989	−0.875937	0.391991
H	2.793819	0.581721	−1.494890
H	2.360993	−2.065593	−0.543572
H	2.351720	1.062286	1.622820
H	2.119399	−1.928327	1.216781
H	1.396235	1.718938	−1.584824
H	1.298587	0.122432	−2.361152
H	0.929001	0.316499	2.378042
H	0.756565	1.866283	1.500065
H	−3.119724	0.031407	1.044372
H	−2.485436	−1.544989	1.571150
H	−2.078635	2.402813	−0.624339
H	−1.550909	−0.066181	1.904842

H	−1.352936	2.251470	1.004346
H	−0.409279	2.956464	−0.343985

$T_{21p3\text{-}9}$

46

P	0.036426	−0.221697	0.285093
O	0.270871	−2.143333	0.357778
O	0.186861	−0.381115	1.961145
O	−0.176215	−2.253999	3.195997
C	3.937375	−0.101893	−2.295111
C	3.678479	0.895190	−1.339096
C	3.017409	−1.148961	−2.478138
C	2.491700	0.862379	−0.588519
C	2.098831	−1.843743	2.477411
C	1.849111	−1.208301	−1.701947
C	1.562923	−0.190881	−0.760663
C	0.605704	−1.636199	2.494402
C	−4.134763	−0.786432	−1.723908
C	−4.024418	−0.432306	−0.367404
C	−2.973535	−0.971853	−2.493734
C	−2.759123	−0.251973	0.215718
C	−1.702982	−0.817427	−1.910850
C	−1.591852	−0.447426	−0.554344
C	−0.770344	−3.111104	0.326690
C	−0.662236	3.803286	−0.598261
C	−0.506319	4.478477	0.626176
C	−0.499237	2.410507	−0.659450
C	−0.179346	3.748622	1.779652
C	−0.169538	1.659724	0.494569
C	−0.008120	2.352610	1.714279
H	4.858774	−0.066391	−2.892459
H	4.397459	1.710033	−1.179147
H	3.216112	−1.936630	−3.217581
H	2.558246	−1.474355	1.553366
H	2.524584	−1.286301	3.331384
H	2.325007	−2.909994	2.611999
H	2.296990	1.654766	0.141487
H	1.168032	−2.055978	−1.810087
H	0.253367	1.800180	2.622873

H	−5.125104	−0.915766	−2.181048
H	−4.927293	−0.285444	0.241065
H	−3.050816	−1.243260	−3.555479
H	−2.686736	0.045922	1.270889
H	−1.518748	−2.961821	1.128990
H	−1.298123	−3.120187	−0.643785
H	−0.916237	4.362019	−1.509674
H	−0.807645	−0.976844	−2.522914
H	−0.639573	5.567779	0.678065
H	−0.632455	1.906595	−1.626007
H	−0.299704	−4.099575	0.475744
H	−0.052977	4.264517	2.741721

$T_{7m1\text{-}9}$

19

P	−2.767757	−0.422343	−0.003373
O	2.786969	1.333006	−0.005485
O	2.116146	−0.828976	−0.006035
O	−1.589891	0.575924	−0.002548
C	4.468393	−0.383212	0.010634
C	3.011305	0.095331	−0.004596
C	0.098252	−0.072256	−0.004213
C	−4.352957	0.416621	0.012024
H	5.029225	0.113536	−0.793198
H	4.933326	−0.085943	0.962215
H	4.546866	−1.470787	−0.101165
H	0.571454	0.903198	−0.002657
H	0.046452	−0.624732	0.927418
H	0.046235	−0.621265	−0.937862
H	−5.149814	−0.341806	0.010837
H	−4.440416	1.047127	−0.882249
H	−4.430029	1.033487	0.916694
H	−2.752962	−1.289770	−1.131545
H	−2.739726	−1.306429	1.111559

$T_{7m2\text{-}9}$

22

P	−2.478534	0.023388	0.276969
O	3.157760	−1.243405	−0.471966
O	2.388024	0.759546	0.250297
O	−1.257354	−0.629312	−0.411054
C	4.752539	0.393711	0.271571
C	3.324123	−0.083695	−0.016940
C	0.425186	0.015959	−0.102087
C	−3.880524	−1.104717	0.240184
C	−2.976313	1.591843	−0.461702
H	5.398336	0.179271	−0.590781
H	5.151109	−0.173136	1.126173
H	4.789718	1.463479	0.507687
H	0.917779	−0.891313	−0.431057
H	0.365512	0.855883	−0.782758
H	0.316146	0.194132	0.962173
H	−4.730576	−0.650168	0.768388
H	−4.159764	−1.305721	−0.802924
H	−3.837200	1.998342	0.088225
H	−3.600205	−2.043455	0.734890
H	−3.252223	1.430366	−1.512744
H	−2.212505	0.310403	1.660714
H	−2.145622	2.307858	−0.406886

$T_{7m3\text{-}9}$

25

P	−2.315748	0.028175	0.000928
O	3.414676	1.349508	−0.002304
O	2.602560	−0.764117	−0.010226
O	−1.006872	0.853003	−0.007164
C	4.977806	−0.475144	0.009429
C	3.557174	0.101084	−0.004901
C	0.664727	0.088539	−0.008040
C	−3.705624	1.178483	0.008361
C	−2.479405	−1.033447	−1.453502
C	−2.462990	−1.031535	1.458507

H	5.567875	−0.021693	−0.799041
H	5.464798	−0.204556	0.957840
H	4.982266	−1.566040	−0.096911
H	1.170161	1.046629	−0.008938
H	0.567350	−0.449907	0.926169
H	0.565165	−0.451085	−0.941328
H	−4.654618	0.624425	0.015201
H	−3.656247	1.809876	−0.888642
H	−3.644533	1.812065	0.903092
H	−3.450882	−1.546900	−1.436237
H	−3.435129	−1.544006	1.453224
H	−2.408089	−0.418596	−2.360746
H	−2.380526	−0.415617	2.364089
H	−1.679981	−1.786604	−1.461126
H	−1.664431	−1.785643	1.457867

$T_{7p3\text{-}9}$

46

P	0.634191	−0.016702	−0.230511
O	−4.855023	−0.689370	−2.282388
O	−4.324402	0.261257	−0.290936
O	−0.513271	−0.206369	−1.286568
C	4.662599	0.029098	−2.505032
C	4.590700	0.573093	−1.209997
C	3.510739	−0.497810	−3.115221
C	3.368436	0.592857	−0.519768
C	2.283234	−0.485901	−2.433558
C	2.210578	0.064029	−1.134437
C	1.517855	−2.577114	2.892303
C	1.457642	−1.428569	2.086994
C	0.818382	2.742794	0.168591
C	0.815612	−3.738975	2.523277
C	0.684275	−1.444300	0.903012
C	0.565775	3.940269	0.854596
C	0.432979	1.506797	0.741745
C	0.054313	−3.758509	1.342189
C	−6.643281	−0.069970	−0.789392
C	−5.160850	−0.176927	−1.172751
C	−2.289411	0.008623	−0.804481

C	−0.473398	2.690765	2.672185
C	−0.226283	1.486763	1.993075
C	−0.074748	3.914675	2.106720
C	−0.010882	−2.615958	0.527868
H	5.621210	0.018186	−3.041425
H	5.488521	0.990449	−0.734583
H	3.565134	−0.919760	−4.127811
H	3.323450	1.029414	0.487040
H	2.115318	−2.561962	3.813782
H	2.008860	−0.527779	2.390165
H	1.382425	−0.894380	−2.910032
H	1.314836	2.774431	−0.810460
H	0.872977	4.896165	0.409568
H	0.865554	−4.633412	3.159075
H	−7.236845	0.252738	−1.658140
H	−7.005844	−1.069310	−0.494522
H	−6.800909	0.619985	0.051271
H	−2.647180	−0.418073	−1.736634
H	−2.277925	−0.610921	0.086861
H	−2.241738	1.086827	−0.694473
H	−0.980098	2.669734	3.646317
H	−0.595460	−2.637305	−0.400185
H	−0.549139	0.538159	2.440361
H	−0.492523	−4.665213	1.050358
H	−0.267524	4.854035	2.642750