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STRUCTURE AND THERMODYNAMICS OF PHOSPHORUS OXIDE CAGED CLUSTERS

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The structure and thermodynamics of the following phosphorus oxide caged clusters were calculated in the gas phase at STP via both the local density approximation (LDA) and a generalized gradient approximation (BLYP) of density functional theory: the experimentally characterized trioxide (P_4O_6) and pentoxide (P_4O_{10}), and in order of thermodynamic preference, the hypothetical $P_{24}O_{60}$, P_8O_{20} , $P_{24}O_{48}$, and $P_{20}O_{20}$. All of the hypothetical oxides would dissociate to the pentoxide at equilibrium. Secondly, the LDA calculation of the enthalpy of formation was unexpectedly superior to the BLYP calculation.

Keywords: density functional theory, phosphorus oxide clusters, LDA, GGA.

INTRODUCTION

Clusters of elements besides carbon are interesting both intrinsically and for their potential applications as superconductors and for their storage capacity. The pnictogens, both with and without chalcogens, have the greatest potential to form large inorganic-based clusters, referred to as endohedral fullerane complexes. There has been much interest, both experimentally and computationally, in clusters composed of group V elements, from nitrogen [1] down to bismuth [2]. Within the cage, the fullerenes will be composed entirely of σ bonds, with no π interactions, in contrast to carbon-based fullerenes, such as C_{60} , which have substantial π interactions.

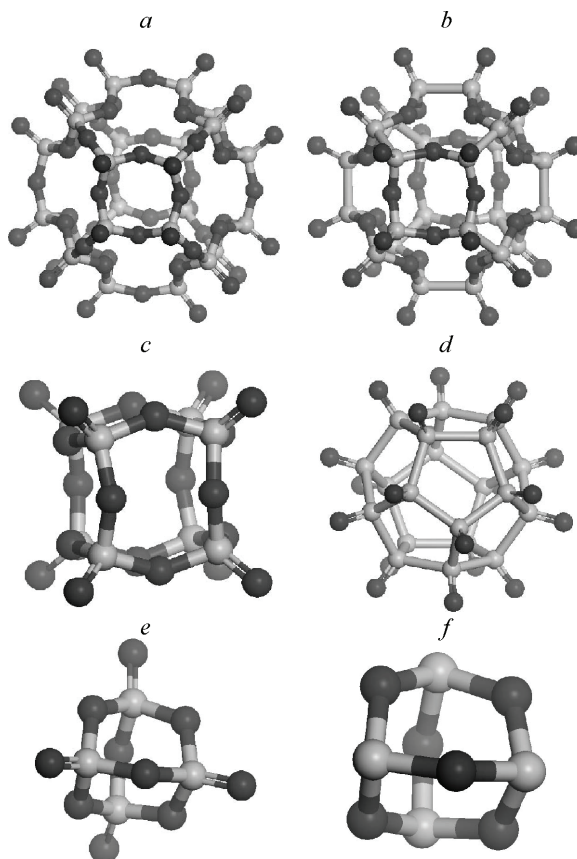
A variety of V-VI cage compounds have been investigated, both computationally and experimentally. Small cage compounds of phosphorus or arsenic with sulfur or selenium, such as P_4S_3 and P_4Se_3 and the As analogues, have been investigated [3]. A larger phosphorus selenium cage molecule, P_8Se_3 , has been characterized as an adduct on Cu, which acts to stop polymerization and provide a support for crystallization [4]. Large V-VI cage molecules (excluding oxygen) that have been experimentally characterized are very rare, though.

Phosphorus oxide fullerenes are the most common V-VI cage compounds studied. The trioxide (P_4O_6) and its fully oxidized and more stable variant, pentoxide (P_4O_{10}), are tetrahedral cages [5] with a framework resembling adamantane (Fig. 1). Along with smaller phosphorus oxides, e.g., P_2O_4 , P_2O_5 , and P_2O_6 [6], cage structures larger than the pentoxide, e.g., P_4O_{18} [7] (from the trioxide and ozone) and P_8O_{12} [8] (the dimer of the trioxide), have also been synthesized and characterized. Synthesis of group V clusters has been accomplished primarily through laser ablation or by quenching vapor in a cold gas, of which both are non-equilibrium techniques. An As_{20} cluster has been synthesized and characterized, although the As_{20} moiety is not standalone, but is part of $As@Ni_{12}@As_{20}$ [9]. Neutral phosphorus clusters have been synthesized up to P_{40} by laser ablation [10, 11]. Neutral clusters have been shown to have "magic" sizes (maxima in the mass spectrum) at P_8 , P_{10} , P_{14} , and P_{40} [10, 12]. Although the hypothetical P_{20} dodecahedron would not be one of these maxima (and would have a positive enthalpy of formation with respect to 5 P_4) [13, 14], the cation mass spectrum has a magic size at P_{21}^+ , which is speculated as being P_{20} stabilized by an additional phosphorus [10]. In addition to the

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Fig. 1. Phosphorus oxide molecules.

a–f correspond to $P_{24}O_{60}$, $P_{24}O_{48}$, P_8O_{20} , $P_{20}O_{20}$, P_4O_{10} , and P_4O_6 , respectively. The dark and light spheres correspond to oxygen and phosphorus atoms, respectively



experimental work, a large number of modeling papers have been published on group V clusters. There have been investigations of clusters of nitrogen [1], arsenic [9, 15], antimony [2], and bismuth [2]. Nitrogen clusters (up to N_{20}) have been found at energy minima but with positive enthalpies of formation with respect to N_2 [1], while recent work on arsenic clusters (up to As_{60}) indicates all but As_{20} will dissociate into As_4 units [15]. Of special interest here are clusters of phosphorus and various phosphorus oxides, for which there already have been numerous computational investigations [13–15, 16–21].

Recently Wang et al. [22] discussed the stability of the hypothetical P_{20} dodecahedron and its fully oxidized form $P_{20}O_{20}$, observing "unprecedented high stability" for the latter, but omitting a comparison of their findings with those of other hypothetical clusters or with the experimentally characterized phosphorus oxides. Therefore we were motivated to calculate the thermochemistry of phosphorus-oxygen clusters of comparable size to see if any might be produced in the gas phase. In particular we examined the following hypothetical molecules: $P_{20}O_{20}$, previously discussed in [22], $P_{24}O_{48}$, a fully oxidized form of an octahedral framework discussed earlier by us [23], $P_{24}O_{60}$ in which the P–P bonds in $P_{24}O_{48}$ are replaced by bridging oxygen, and P_8O_{20} , a tetrahedral structure which was relaxed from its octahedral isomer, also fully oxidized. For comparison we also examined the experimentally characterized trioxide and pentoxide [19, 24]. All of these are illustrated in Fig. 1. The "open shell" phosphorus oxides (e.g., the PO radical) were not considered here because of their reactivity or transience [20, 21].

CALCULATION METHODOLOGY

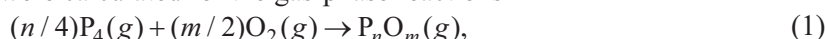
We employed the DMol³ code [25] for the density functional theory (DFT) calculations of the structure and gas-phase thermodynamics, employing local density approximation (LDA) and the BLYP generalized gradient approximation (GGA). All of the molecules discussed here are "closed shell" except for the oxygen molecule, which was calculated with unrestricted spin. The LDA calculations used the local functional parameterized by Perdew and Wang [26] instead of the venerable but more often employed parameterization by Vosko, *et al.* [29]. The BLYP calculations employed the gradient corrected exchange potential due to Becke [27] and the gradient corrected correlation potential due to Lee, Yang, and Parr [28]. The following remarks apply to both the LDA and the BLYP calculations. The DNP (double numerical with polarization) basis set [25] was always generated with a radial cutoff of 4.2 Å and expansion of the angular momentum up through octupole. No pseudopotentials were employed in these all-electron calculations. The SCF calculations were converged with a tolerance of 10^{-6} Hartrees. The geometry optimization was converged with the following tolerances: maximum displacement of 0.005 Å, maximum force component magnitude of 0.002 Hartrees/Å and total energy variation between steps of 10^{-5} Hartrees. The thermal contributions from translations, rotations and (harmonic) vibrations (including the zero-point vibrational energies) were combined into H_{298} and G_{298} for the enthalpy and Gibbs free energy, respectively [30]. For these the formulae of Hi-

rano [31] were employed, with the frequencies obtained from the phonon matrix whose entries were numerically computed from finite differences of analytic first derivatives, with displacements of 0.00529 Å (i.e., 0.001 Bohr). All structures are minima (no imaginary frequencies).

RESULTS

Tables 1 and 2 show the bond lengths in Å, the contributions of the total energy in Hartrees, and the thermal contributions at standard temperature and pressure (STP, H_{298} , G_{298}) in kcal/mol needed to calculate the subsequent formation energies in Table 3 (e.g., [30]). The results of the reference calculations were included in Table 2 for the sake of completeness and reproducibility.

The energies (ΔE , at zero temperature and pressure), enthalpies (ΔH at STP), and Gibbs free energies (ΔG at STP) of formation were calculated for the gas-phase reactions



and listed in Table 3. For example, $\Delta G(P_4O_{10}) = G(P_4O_{10}) - (G(P_4) + 5G(O_2))$, where $G = E_{\text{total}} + G_{298}$ is found from Table 1. This formulation is appropriate because molecular oxygen (O_2) and molecular

Table 1

*Results for phosphorus oxides; symmetry is indicated in the parenthesis.
P—P, P—O, and P=O bond lengths are listed in Å. E_{total} is listed in Hartrees.
The combined thermal contributions at STP (H_{298} , G_{298}) are listed in kcal/mol*

Molecule	Method	P—P	P—O	P=O	E_{total}	H_{298}	G_{298}
P ₂₄ O ₆₀ (<i>O_h</i>)	LDA		1.62 (1.58 ^a)	1.44	-12650.0163465	247	126
	BLYP		1.65 (1.61 ^a)	1.46	-12710.4443951	238	114
P ₂₄ O ₄₈ (<i>O_h</i>)	LDA	2.21	1.62	1.45	-11752.4186561	199	93.1
	BLYP	2.28	1.65	1.47	-11806.7670118	192	83.1
P ₈ O ₂₀ (<i>T_h</i>)	LDA		1.62	1.44	-4216.6446289	80.4	32.1
	BLYP		1.62	1.46	-4236.7963214	78.5	29.5
P ₂₀ O ₂₀ (<i>I_h</i>)	LDA	2.28		1.48	-8297.6590108	101	12.1
	BLYP	2.48		1.50	-8332.8101463	96.2	-3.82
	B3LYP ^b	2.32		1.53			
P ₄ O ₁₀ (<i>T_d</i>)	LDA		1.61	1.44	-2108.3292111	40.2	9.81
	BLYP		1.65	1.46	-2118.4149223	38.5	7.57
	expt ^c		1.60	1.43			
P ₄ O ₆ (<i>T_d</i>)	LDA		1.66		-1809.2055972	24.6	-2.14
	BLYP		1.69		-1817.2663984	23.4	-3.89
	expt ^d		1.64				

^a With bridging oxygens; ^b ref [22]; ^c ref [34]; ^d ref [35].

Table 2

Results for the reference gas-phase molecules P₄ and O₂. Column headings as in Table 1

Molecule	Method	Bond	E_{total}	H_{298}	G_{298}	Molecule	Method	Bond	E_{total}	H_{298}	G_{298}
P ₄ (<i>T_d</i>)	LDA	2.19	-1360.5535879	7.30	-14.1	O ₂	LDA	1.21	-149.3287560	4.83	-9.99
	BLYP	2.24	-1365.5352936	7.10	-14.5		BLYP	1.24	-150.3906375	4.19	-10.2
	expt ^a	2.21					expt ^a	1.21			

^a ref [24].

Table 3

Gas-phase formation energies of phosphorus oxides from oxygen and phosphorus, with the symmetry indicated in parenthesis. All of the energies are listed in kcal/mol for the gas-phase reaction 1. ΔE was calculated at zero temperature and pressure. ΔH and ΔG were calculated at STP. The experimental ΔH was calculated by subtracting the enthalpy of formation of the sublimation of the solid white phosphorus (14.1 kcal/mol) from the standard enthalpy of formation [24]

Molecule	Method	ΔE	ΔH	ΔG	Molecule	Method	ΔE	ΔH	ΔG
P ₂₄ O ₆₀ (O _h)	LDA	-4287	-4216	-3777	P ₄ O ₁₀ (T _d)	LDA	-710	-699	-636
	BLYP	-3460	-3390	-2953		BLYP	-581	-571	-508
P ₂₄ O ₄₈ (O _h)	LDA	-3267	-3217	-2850	P ₄ O ₆ (T _d)	expt ^a		-708	
	BLYP	-2623	-2580	-2208		LDA	-418	-414	-356
P ₈ O ₂₀ (T _h)	LDA	-1412	-1390	-1252	BLYP	BLYP	-351	-347	-289
	BLYP	-1142	-1119	-981		expt ^a		-543	
P ₂₀ O ₂₀ (I _h)	LDA	-1006	-986	-824					
	BLYP	-770	-751	-599					

^a ref [24].

phosphorus (the P₄ tetrahedron) are the actual species in the gas phase for a wide range of non-ionizing temperatures [13, 32]. We neglected P₂ formation because it does not appear below $T = 1000$ K [32]. The standard allotrope of phosphorus is "white phosphorus", the molecular solid of P₄, so conversion of the experimental enthalpy of formation to that for reaction 1 involves subtracting the enthalpy of the sublimation of white phosphorus ($\Delta H = 14.1$ kcal/mol at STP [24] for the reaction $4P(s) \rightarrow P_4(g)$).

The pentoxide remains the most stable of the molecules in Table 3. To be explicit, we show ΔG for representative dissociation reactions of the hypothetical molecules in Table 4, employing both the LDA and BLYP calculations. These results indicate that all of the hypothetical clusters would spontaneously dissociate into the pentoxide at equilibrium at STP. They also indicate that P₂₄O₆₀ and P₈O₂₀ would be the least unstable with respect to decomposition to pentoxide, while the P₂₀O₂₀ would be the most unstable. Of course these results do not address the rate at which such decomposition would occur.

Table 5 shows our results for the unoxidized P₂₀ dodecahedron, the starting point for the investigation of phosphorus oxide clusters by Wang *et al.* [22]. Our LDA results incorrectly (but not surprisingly) predict a negative ΔH for the P₂₀ dodecahedron, while our BLYP results are comparable to the well established MP2 results of Häser *et al.* [13] and Hu *et al.* [14], for which the ΔH of P₂₀ is about +20 kcal/mol. On the one hand, a positive enthalpy of formation is in itself not by any means prohibitive, since many molecules also have positive enthalpies of formation (e.g., the standard enthalpy of formation for C₆₀ is +635 kcal/mol [24]). On the other hand, we were interested only in clusters with negative gas-phase enthalpies, so we did not calculate H₂₉₈ or G₂₉₈ for P₂₀. Wang *et al.* [22] obtained a negative enthalpy for P₂₀ with their B3LYP DFT calculation only because their entry (in their Table 1) for the enthalpy is actually the binding (or atomization) enthalpy for the reaction $20P \rightarrow P_{20}$, rather

Table 4

Gas-phase equilibria with hypothetical phosphorus oxide molecules and the pentoxide at STP. ΔG is listed in kcal/mol

Reaction	Method	ΔG	Reaction	Method	ΔG
P ₈ O ₂₀ \rightarrow 2P ₄ O ₁₀	LDA	-21	P ₂₄ O ₄₈ \rightarrow 4P ₄ O ₁₀ + P ₄ O ₆ + P ₄ + O ₂	LDA	-71
	BLYP	-35		BLYP	-134
P ₂₄ O ₆₀ \rightarrow 6P ₄ O ₁₀	LDA	-42	P ₂₀ O ₂₀ \rightarrow 2P ₄ O ₁₀ + 3P ₄	LDA	-438
	BLYP	-97		BLYP	-415

Table 5

Results for the hypothetical P_{20} (I_h). The P—P bond length is listed in Å and E_{total} is listed in Hartrees; The binding (or atomization) energy E_{bind} and ΔE are listed in kcal/mol; E_{bind} is included for comparison to ref [22]

Method	Bond	E_{total}	E_{bind}	ΔE	Method	Bond	E_{total}	E_{bind}	ΔE
LDA	2.24	-6802.8325593	-1789	-41	B3LYP ^c	2.29			38
BLYP	2.31	-6827.6408985	-1324	22	BLYP ^d				6.2
MP2 ^a		-6812.6389200		19	B3LYP ^e	2.29		-1231	
MP2 ^b	2.24	-6817.5120560		23					

^a ref [13]; ^b ref [14]; ^c ref [17]; ^d ref [18]; ^e ref [22].

than the thermodynamically relevant enthalpy of formation evaluated with respect to the tetramer actually present in the gas phase, i.e., $5P_4 \rightarrow P_{20}$.

DISCUSSION AND CONCLUSIONS

LDA results are now published much less frequently because such calculations almost always underestimate the atomization or binding energy, even though it is well known that they also provide excellent structures, i.e., bond lengths and angles. Nevertheless we included the LDA results for the energies here because the LDA predictions of ΔH for both the trioxide and the pentoxide (Table 3) are superior to the results from the GGA (BLYP) calculations, which suggests that they might also be better for the hypothetical oxides. The result is also interesting in view of the failure of the LDA to predict the positive enthalpy of formation for P_{20} from P_4 (Table 5) even though the reaction $5P_4 \rightarrow P_{20}$ is isodesmic, while none of the phosphorus oxides reactions (1) are isodesmic.

The choice of approximations employed in the calculations turned out to be inessential for ranking the oxides; instead, what was crucial was the appropriate description of the gas-phase thermochemistry. We emphasize this formulation because sometimes we see in the literature that conclusions about molecular stability have been drawn from the binding (or atomization) energies, or hybrids thereof, instead of the thermodynamically relevant formation energies, each of which is referenced to the species actually in the gas phase (i.e., P_4 and O_2).

The calculations show that all of the proposed hypothetical phosphorus oxide clusters possess a negative free energy with respect to the pentoxide, and therefore would spontaneously dissociate into the pentoxide in gas-phase equilibria. On the other hand, we have nothing to say here about the rate at which such a dissociation would occur; they might remain metastable for long times (e.g., C_{60}). A nonequilibrium technique (e.g., laser ablation, or a quench from a thermal plasma [33]) might produce bulk quantities of these clusters. In that case, the results of Tables 3 and 4 indicate that $P_{24}O_{60}$ would be the most preferred among the hypothetical species, and that all of the octahedral and tetrahedral species would be preferred over $P_{20}O_{20}$. We note that, in common with the pentoxide, the most preferred species possess no P—P bonds.

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