

Supporting Information

Time Resolved Resonance Raman Study of the Triplet State of the p-Hydroxyacetophenone and p-Hydroxyphenacyl Diethyl Phosphate Phototrigger Compound

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Experimental		Calculated			
normal	¹³ C	No.	Frequency	¹⁶ O	Assignment descriptions
Raman	IR	normal	¹³ C	¹⁶ O	
		v ₉	415	415	ring C-C o.p. deformation (16a)
482	484	v ₁₀	462	460	skeleton deformation
a	499	v ₁₁	496	494	ring C-H o.p. bending + ring C-C o.p. deformation (16b)
559	574	v ₁₂	567	566	ring C-C i.p. deformation + C(7)-O(2) i.p. bending
	592	v ₁₃	588	580	ring C-H o.p. bending + C(4)-C(7) o.p. bending
630	638	v ₁₄	639	639	ring C-C i.p. deformation (6b)
684	698	v ₁₅	678	676	C(4)-C(7) stretching + ring C-C i.p. deformation
723	725	v ₁₆	722	722	ring C-C o.p. deformation + CH3 rocking
	783	v ₁₇	792	792	ring C-H o.p. bending
816	818	v ₁₈	830	830	ring C-C breathing (1) + C(1)-O(1) stretching
835	837	v ₁₉	839	839	ring C-H o.p. bending
	956	v ₂₀	924	924	ring C-H o.p. bending
		v ₂₁	937	929	C(7)-C(8) stretching + C(7)-O(2) i.p. bending + CH3 rocking
		v ₂₂	981	981	ring C-H o.p. bending
		v ₂₃	1004	1005	ring C-C stretching + ring C-H i.p. bending (18a)
1024	1012	v ₂₄	1026	1015	CH3 rocking + C(4)-C(7) o.p. bending
1068	1084	v ₂₅	1068	1064	CH3 rocking + C(7)-C(8) stretching + ring C-H i.p. bending (18a)
	1115	v ₂₆	1105	1105	ring C-H i.p. bending (18b)
1159	1171	v ₂₇	1167	1166	ring C-H i.p. bending (9a)
	b	v ₂₈	1176	1176	O(1)-H i.p. bending + ring C-H i.p. bending
1212	1235	v ₂₉	1257	1239	C(4)-C(7) stretching + ring C-C stretching + ring C-H i.p. bending (18a)
1268	1252	v ₃₀	1278	1278	C(1)-O(1) stretching + ring C-C stretching + ring C-H i.p. bending (18a)
	1287	v ₃₁	1304	1304	ring C-H i.p. bending + ring C-C stretching (3)
	1310	v ₃₂	1346	1347	ring C-C stretching (14) + O(1)-H i.p. bending
	1366	v ₃₃	1357	1356	CH3 umbrella
	1387	v ₃₄	1440	1439	ring C-C stretching (19b) + O(1)-H i.p. bending
1419	b	v ₃₅	1444	1443	CH3 deformation
1436	1441	v ₃₆	1452	1452	CH3 deformation
1510	1514	v ₃₇	1513	1513	ring C-C stretching (19a) + C(1)-O(1) + C(4)-C(7) stretching
1568	1587	v ₃₈	1590	1589	ring C-C stretching (8b)
1596	1605	v ₃₉	1619	1618	ring C-C stretching (8a)
1654	1647	v ₄₀	1720	1681	C(7)-O(2) stretching
		v ₄₁	2973	2973	methyl group C-H stretching (sym.)
		v ₄₂	3029	3029	methyl group C-H stretching (asym.)
		v ₄₃	3082	3082	methyl group C-H stretching (asym.)
		v ₄₄	3091	3091	ring C-H stretching (asym.)
		v ₄₅	3128	3128	ring C-H stretching (asym.)
		v ₄₆	3130	3130	ring C-H stretching (asym.)
		v ₄₇	3142	3142	ring C-H stretching (sym.)
		v ₄₈	3749	3749	O(1)-H stretching

Table1S(a)

Experimental	Frequency		Assignment descriptions
	IR	No.	
			ring C-C o.p. deformation + ring C-D o.p. bending (16b)
			skeleton deformation
552			ring C-D o.p. bending + C(4)-C(7) o.p. bending
569			ring C-C i.p. deformation (6a) + C(7)-O(2) i.p. bending
			ring C-C i.p. deformation (6b)
			ring C-D o.p. bending (10a)
			ring C-C o.p. deformation + ring C-H o.p. bending + CH3 rocking
671			ring C-C i.p. deformation + C(4)-C(7) + C(7)-C(8) stretching
			ring C-C o.p. deformation (17b)
			ring C-C o.p. deformation
737			ring C-H i.p. bending + C(1)-O(1) + C(4)-C(7) stretching + ring C-C stretching
			ring C-D o.p. bending + ring C-C o.p. deformation
791			ring C-D i.p. bending (18b)
818			ring C-D i.p. bending + O(1)-C(1) stretching + ring C-C stretching
847			ring C-D i.p. bending + C(1)-O(1) stretching + ring C-C stretching
943			C(7)-C(8) stretching + CH3 rocking + ring C-H i.p. bending (3)
969			ring C-D i.p. bending (3) + O(1)-H i.p. bending + CH3 rocking
			CH3 rocking + C(4)-C(7) o.p. bending
			ring C-C stretching (13) + CH3 rocking + C(4)-C(7) stretching
1200			O(1)-H i.p. bending + ring C-C stretching + C(4)-C(7) stretching
1229			O(1)-H i.p. bending + ring C-C stretching + C(7)-C(8) stretching
1310			O(1)-H i.p. bending + ring C-C stretching + C(7)-C(8) stretching
1342			C(4)-C(7) stretching + ring C-C stretching + C(1)-O(1) stretching
1365			ring C-C stretching (14) + O(1)-H i.p. bending
			CH3 umbrella
			ring C-C stretching (19b) + O(1)-H i.p. bending + CH3 deformation
b			ring C-C stretching (19a) + C(4)-C(7) + C(1)-O(1) stretching + CH3 deformation
1401			CH3 deformation
1426			CH3 deformation
1561			ring C-C stretching (8b) + O(1)-H i.p. bending
1588			ring C-C stretching (8a)
1640			C(7)-O(2) stretching
2251			ring C-H stretching (asym.)
2271			ring C-H stretching (asym.)
2288			ring C-H stretching (asym.)
			ring C-H stretching (sym.)
a			methyl C-H stretching (sym.)
			methyl C-H stretching (asym.)
			methyl C-H stretching (asym.)
			O(1)-H stretching

Table 1S(b) ^ashoulder band; ^bbroad unresolved band; i.p.: in-plane; o.p.: out-of-plane.

Experimental	Calculation frequency	Assignment description
484	v25 407	ring C-C o.p. deformation (16a)
527	v26 428	ring deformation + skeleton deformation
544	v27 474	ring deformation + skeleton deformation
shoulder	v28 475	ring deformation + skeleton deformation
	v29 489	ring C-H o.p. bending (16b) + skeleton deformation
571	v30 528	ring C-H o.p. bending (16b) + skeleton deformation
615	v31 561	ring C-H and C-C o.p. deformation (16b) + C(13)-C(11) o.p. bending
	v32 604	ring C-C i.p. deformation (6a)
	v33 630	ring C-C i.p. deformation (6b)
698	v34 691	$\nu^s(\text{P}(1)\text{O}3) + \text{C}(7/9)\text{H}3$ rocking
	v35 709	ring C-H o.p. bending (5)
745	v36 758	C(10)-C(11) and ring C-C stretching + $\nu^s(\text{P}(1)\text{O}3) + \text{C}(8/6)\text{H}2$ rocking + C(9/7)H3 rocking
760	v37 779	C(9/7)H3 rocking + C(8/6)H2 rocking + $\nu^{\text{as}}(\text{O}3)-\text{P}(1)-\text{O}(4)$
774	v38 783	ring C-H bending o.p. bending
shoulder	v39 794	C(9)H3 rocking + C(8)H2 rocking
826	v40 798	C(7)H3 rocking + C(6)H2 rocking
841	v41 801	P(1)-O(5) stretching + $\nu^s(\text{O}(3)-\text{P}(1)-\text{O}(4)) + \text{ring C-C i.p. stretching} + \text{C}(7)\text{H}3$ rocking + C(6)H2 wagging
860	v42 824	ring C-C stretching + C(6)-O(19) + C(10)-C(11) stretching
	v43 830	ring C-H o.p. bending
	v44 910	ring C-H o.p. bending
shoulder	v45 930	P(1)-O(4) + C(8)-C(9) stretching + C(9)H3 rocking
978	v46 946	P(1)-O(3) + C(6)-C(7) stretching + C(7)H3 rocking
994	v47 952	ring C-C stretching + C(10)-C(11) stretching + $\nu^{\text{as}}(\text{P}(1)-\text{O}(5)-\text{C}(10))$
	v48 967	ring C-H o.p. bending + C(10)H2 rocking
	v49 988	C(10)H2 rocking + ring C-H o.p. bending
	v50 995	ring C-C stretching (18a)
1038	v51 1013	$\nu^{\text{as}}(\text{P}(1)-\text{O}(4)-\text{C}(8)) + \nu^{\text{as}}(\text{O}(4)-\text{C}(8)-\text{C}(9)) + \nu^{\text{as}}(\text{P}(1)-\text{O}(3)-\text{C}(6)) + \nu^{\text{as}}(\text{O}(3)-\text{C}(6)-\text{C}(7))$

1069	v52	1040	$v^{as}(P(1)-O(3)-C(6)) + v^{as}(O(3)-C(6)-C(7)) + v^{as}(P(1)-O(4)-C(8)) + v^{as}(O(4)-C(8)-C(9))$
shoulder	v53	1082	$C(9)H3$ rocking + $v^s(O(3)-C(6)-C(7)) + C(10)-O(5) +$ ring C-H i.p. bending (18b)
shoulder	v54	1090	$C(7)H3$ rocking + $v^s(O(3)-C(6)-C(7)) + C(10)-O(5) +$ ring C-H i.p. bending (18b)
1105	v55	1092	$v^{as}(C(10)-O(5)-P(1)) +$ ring C-H i.p. bending (18b) + $C(7(9)H3$ rocking
1117	v56	1097	ring C-H i.p. bending (18b)
shoulder	v57	1144	$C(7)H3$ rocking + $C(6)H2$ wagging
	v58	1157	$C(9)H3$ rocking
1171	v59	1158	ring C-H i.p. bending (9a) + $O(19)-H$ i.p. bending
shoulder	v60	1163	ring C-H i.p. bending (9a) + $O(19)-H$ i.p. bending
1237	v61	1215	$C(13)-C(11)$ stretching + ring C-H i.p. bending (18a) + $C(10)H2$ wagging
1250	v62	1260	$C(10)H2$ twisting + $P(1)-O(2)$ stretching
1260	v63	1265	$C(10)H2$ twisting + $P(1)-O(2)$ stretching
shoulder	v64	1267	$C(16)-O(19)$ stretching + ring C-C stretching and C-H i.p. bending (18a)
	v65	1269	$C(6)H2$ twisting
shoulder	v66	1284	$C(8)H2$ twisting
1293	v67	1294	ring C-C stretching and C-H bending (3)
1350	v68	1334	ring C-C stretching (14) + $O(19)-H$ i.p. bending (i.p.)
1374	v69	1351	$C(10)H2$ wagging + $C(10)-C(11) + C(10)-O(5)$ stretching
shoulder	v70	1357	$C(8)H2$ wagging + $C(9)H3$ umbrella
	v71	1360	$C(6)H2$ wagging + $C(7)H3$ umbrella
shoulder	v72	1381	$C(8)H2$ wagging + $C(9)H3$ umbrella + $C(8)-C(9)$ stretching
1397	v73	1384	$C(6)H2$ wagging + $C(7)H3$ umbrella + $C(6)-C(7)$ stretching
	v74	1425	ring C-C stretching (19a) + $C(10)H2$ scissor + $O(19)-H$ i.p. bending
	v75	1428	$C(10)H2$ scissor + ring C-C stretching (19a) + $O(19)-H$ i.p. bending
1441	v76	1438	$C(7)H3$ deformation
shoulder	v77	1440	$C(9)H3$ deformation
1457	v78	1453	$C(9)H3$ deformation + $C(8)H2$ scissor
shoulder	v79	1458	$C(7)H3$ deformation + $C(6)H2$ scissor
1480	v80	1475	$C(8)H2$ scissor + $C(9)H3$ deformation
	v81	1481	$C(6)H2$ scissor + $C(7)H3$ deformation

1516	v82	1499	ring C-C stretching (19a) + C(13)-C(11) + C(16)-O(19) stretching
1579	v83	1572	ring C-C stretching (8b) + O(19)-H i.p. bending
1609	v84	1601	ring C-C stretching (8a) + C(11)-C(13) + C(16)-O(19) stretching
1660	v85	1707	C(11)-O(12) stretching

Table 2S ^a shoulder band; ^b broad unresolved band; i.p.: in-plane; o.p.: out-of-plane.

Experimental	Calculated			
	normal	Frequency		Assignment description
		¹³ C	¹³ C	
416		415	415	ring C-C o.p. deformation (16a)
		467	464	skeleton i.p. deformation
		492	489	skeleton i.p. deformation
472		499	498	ring C-H o.p. bending + ring C-C o.p. deformation (16b)
472	?	640	640	ring C-C i.p. deformation (6b)
668	667	685	683	ring C-C i.p. deformation + C(7)-C(8) stretching?
		691	690	ring C-C o.p. deformation
shoulder		772	772	ring C-H i.p. deformation ?
762	768	788	788	ring C-C stretching (1)
		816	816	ring C-H o.p. bending (17b)
		910	910	ring C-H o.p. bending
~920	912	947	943	ring C-H o.p. bending + ring C-C deformation + ν^2 (O(2)-C(7)-C(8))
		953	953	ring C-H o.p. bending
963	953	975	972	CH3 rocking
		1004	1004	Ring C-C i.p. deformation (18a) + C(7)-C(8) stretching
		1022	1019	CH3 rocking
~1095		1120	1115	Ring C-H i.p. bending (18b) + O(1)-H i.p. bending
1158	1159	1155	1144	C(7)-C(8) stretching + ring C-H i.p. bending (9a) + O(1)-H i.p. bending
		1183	1183	O(1)-H i.p. bending + ring C-H i.p. bending + ring C-C stretching
		1220	1207	ring C-H i.p. bending (9a) + C(7)-O(2) stretching
1257	1256	1294	1293	C(1)-O(1) stretching + ring C-H i.p. bending (18a)
1296	a	1315	1312	ring C-C stretching + ring C-H i.p. bending (3)
1325	a	1361	1361	O(1)-H i.p. bending + ring C-C stretching (14)
a		1374	1352	C(4)-C(7) stretching + ring C-C stretching (19a) + C(1)-O(1) stretching
1378	1358	1392	1492	CH3 umbrella
a	a	1448	1448	ring C-C stretching
a	a	1468	1468	CH3 deformation
1449	1446	1479	1479	CH3 deformation + ring C-C stretching (19a)
1506	1504	1509	1504	ring C-C stretching (19a) + C(1)-O(1) + C(4)-C(7) stretching + CH3 deformation
a	a	1547	1547	ring C-C stretching (8b) + O(1)-H i.p. bending
1594	1594	1575	1573	ring C-C stretching (8a) + O(1)-C(1) stretching + O(1)-H i.p. bending

Table 3S(a)

Experimental	Calculated	
	Frequency	Assignment description
HA-D ₄	V ₁₀	ring C-C o.p. deformation (16a)
	V ₁₁	ring C-D o.p. bending
	V ₁₂	skeleton i.p. deformation
	V ₁₃	skeleton i.p. deformation
	V ₁₄	ring C-D o.p. bending
	V ₁₅	ring C-D o.p. bending
	V ₁₆	ring C-C i.p. deformation (6b)
	V ₁₇	skeleton i.p. deformation
	V ₁₈	ring C-C o.p. deformation (17b)
	V ₁₉	ring C-D o.p. bending
	V ₂₀	ring C-C i.p. stretching (1)
	V ₂₁	ring C-C o.p. deformation
	V ₂₂	ring C-D i.p. bending
	V ₂₃	ring C-D i.p. bending (18b)
	V ₂₄	ring C-D i.p. bending (9a)
	V ₂₅	CH ₃ rocking + v ^{as} (O(2)-C(7)-C(8)) + ring C-C stretching
	V ₂₆	CH ₃ rocking + ring C-C stretching
	V ₂₇	ring C-D i.p. bending (3) + CH ₃ rocking
	V ₂₈	CH ₃ rocking
	V ₂₉	ring C-C stretching + C(7)-O(2) stretching + O(1)-H i.p. bending
	V ₃₀	ring C-C stretching + O(1)-H i.p. bending + C(7)-C(8) stretching
	V ₃₁	v ^{as} (O(2)-C(7)-C(8)) + ring C-C stretching + O(1)-H i.p. bending
	V ₃₂	O(1)-H i.p. bending + ring C-C stretching
	V ₃₃	C(4)-C(7) stretching + C(1)-O(1) stretching + ring C-C stretching (13)
	V ₃₄	ring C-C stretching + CH ₃ umbrella
1413	V ₃₅	CH ₃ umbrella
b	V ₃₆	ring C-C stretching (19a) + C(4)-C(7) stretching + CH ₃ deformation
1476	V ₃₇	CH ₃ deformation
b	V ₃₈	CH₃ deformation
b	V ₃₉	ring C-C stretching (8b) + O(1)-H i.p. bending
1573	V ₄₀	ring C-C stretching (8a) + O(1)-H i.p. bending

Table 3S(b) ^ashoulder band, ^bbroad unresolved band. i.p.: in-plane; o.p.: out-of-plane.

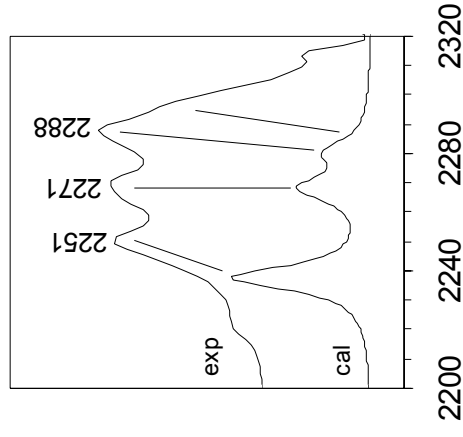
Experimental	frequency	calculation Assignment description
	v25 407	ring deformation + skeleton deformation
	v26 416	ring deformation
	v27 455	ring deformation. + skeleton deformation
	v28 466	ring CCC bending
	v29 504	C-H bending (o.p.) + skeleton deformation + ring boat deformation
	v30 510	C-H bending (o.p.) + ring boat deformation + skeleton deformation
	v31 538	skeleton deformation
	v32 586	CCC bending (ring) + CC(11)C bending (o.p.) + P-O(5) stretching (minor)
	v33 640	ring C-C i.p. deformation (6b)
	v34 701	ring C-C o.p. deformation
	v35 703	ring C-C stretching + $\nu^s(\text{C}(13)\text{-C}(11)\text{-C}(10))$
a	v36 739	$\nu^s(\text{P}(1)\text{O}3)$
	v37 784	ring C-H o.p. bending (10a)
768	v38 805	ring C-C stretching (1)
	v39 810	ring C-C stretching (1) + $\nu^{\text{as}}(\text{P}(1)\text{-O}(4)\text{-C}(8))$ + C(9)H3 rocking
	v40 816	$\nu^{\text{as}}(\text{O}(4)\text{-P}(1)\text{-O}(3))$ + C(7)H3 rocking
	v41 824	C(8)H2 rocking + C(9)H3 rocking
	v42 825	C(6)H2 rocking + C(7)H3 rocking
	v43 828	ring C-H o.p. bending (17b)
913	v44 913	C(10)-O(5) stretching
	v45 923	ring C-H o.p. bending
921	v46 958	ring C-H o.p. bending + C(10)H2 rocking
	v47 960	ring C-H o.p. bending
	v48 968	$\nu^s(\text{O}(4)\text{-P}(1)\text{-O}(3))$ + C(6)-C(7) + C(8)-C(9) stretching
947	v49 979	$\nu^{\text{as}}(\text{O}(4)\text{-P}(1)\text{-O}(3))$ + C(6)-C(7) + C(8)-C(9) stretching
	v50 989	ring C-C stretching + C(10)H2 rocking
989	v51 1008	ring C-C stretching + C(10)-C(11) stretching

1097	v52 1050	Asymmetric stretching of the two ethyl groups
1162	v53 1081	Asymmetric stretching of the two ethyl groups
	v54 1123	C(9)H3 rocking
	v55 1124	C(7)H3 rocking
	v56 1125	ring C-C stretching + ring C-H i.p. bending (18b)
	v57 1167	ring C-H i.p. bending (9a) + C(11)-C(10) stretching + O(19)-H i.p. bending
	v58 1178	C(8)H2 rocking + C(9)H3 rocking
	v59 1179	C(6)H2 rocking + C(7)H3 rocking
	v60 1186	ring C-H i.p. bending (9a) + O(19)-H i.p. bending + ring C-C stretching
1257	v61 1228	C(10)H2 twisting + C(11)-O(12) stretching + ring C-H i.p. bending (9a)
1297	v62 1263	C(10)H2 twist + C(13)-C(11) stretching + ring C-H i.p. bending (9a)
	v63 1295	P(1)-O(2) stretching + C(10/6)H2 wagging + C(8)H2 twisting
1330	v64 1299	C(16)-O(19) stretching + ring C-H i.p. bending (18a) + ring C-C stretching
	v65 1311	C(6)H2 twisting + C(7)H3 rocking
1330	v66 1316	ring C-C stretching + ring C-H i.p. bending (3) + C(11)-C(10) stretching
	v67 1319	C(8)H2 twisting + C(9)H3 rocking
	v68 1364	ring C-C stretching (14) + O(19)-H i.p. bending + C(10)H2 wagging
1371	v69 1371	C(11)-C(13) stretching + C(10)H2 twisting + C(10)-O(12) stretching + ring C-C stretching + ring C-H and O(19)-H i.p. bending
a	v70 1379	C(10)H2 wag + ring C-C stretching (14) + ν^{as} (C(13)-C(11)-O(12)) + O(19)-H i.p. bending
	v71 1403	C(6)H2 wag + C(7)H3 umbrella
	v72 1406	C(8)H2 wag + C(9)H3 umbrella
	v73 1429	C(6)H2 wag + C(7)H3 umbrella
	v74 1434	C(8)H2 wag + C(9)H3 umbrella
1453	v75 1457	ring C-C stretching (19b) + C(10)H2 scissor
1453	v76 1482	C(10)H2 scissor + ring C-C stretching (19a)
	v77 1483	C(7)H3 deformation
1498	v78 1484	C(9)H3 deformation
	v79 1503	C(9)H3 deformation + C(10/8)H2 scissor + ring C-C stretching (19a)
	v80 1504	C(7)H3 deformation + C(6)H2 scissor

v81	1504	ring C-C stretching (19a) + C(13)-C(11) stretching + C(10/8)H2 scissor + C(9)H3 deformation
v82	1527	C(6)H2 scissor
v83	1529	C(8)H2 scissor
v84	1551	ring C-C stretching (8b) + O(19)-H i.p.bending
v85	1582	ring C-C stretching (8a) + C(16)-O(19) stretching + O(19)-H i.p.bending
1606		
1612		

Table 4S ^aShoulder band. i.p.: in-plane; o.p.: out-of-plane.

5 Comparison of experimental FT-IR spectrum of HA-D₄ with corresponding DFT calculated IR spectrum.



6. The Cartesian coordinates, total energies of the stationary points found for the ground and triplet state of HA and HPDP obtained by DFT calculation with B3LYP/6-311G** basis set are included in this supporting information.

(A) Ground state of HA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.172792	-2.137677	0.000000
2	6	0	1.077915	-1.513093	0.000000
3	6	0	1.157426	-0.125883	0.000000
4	6	0	0.000000	0.661683	0.000000
5	6	0	-1.246422	0.015163	0.000000
6	6	0	-1.339809	-1.364510	0.000000
7	1	0	1.983442	-2.112630	0.000000
8	1	0	2.136123	0.338248	0.000000
9	6	0	0.027164	2.155184	0.000000
10	1	0	-2.137669	0.630698	0.000000
11	1	0	-2.298957	-1.867480	0.000000
12	8	0	-0.319645	-3.489136	0.000000
13	1	0	0.547684	-3.908638	0.000000
14	8	0	-1.005733	2.798100	0.000000
15	6	0	1.372282	2.863368	0.000000
16	1	0	1.196193	3.937707	0.000000
17	1	0	1.960812	2.592487	0.881750
18	1	0	1.960812	2.592487	-0.881750

E(RB+HF-LYP) = -460.241045328

Zero-point correction= 0.141576 (Hartree/Particle)

Sum of electronic and zero-point Energies= -460.099470

(B) Triplet state of HA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.680039	0.049838	-0.037894
2	6	0	0.106253	1.248878	-0.081267
3	6	0	1.480772	1.203248	-0.064606
4	6	0	2.149913	-0.030037	0.003585
5	6	0	1.404831	-1.219564	0.065599
6	6	0	0.024956	-1.188028	0.070117
7	1	0	-0.403066	2.200536	-0.163656
8	1	0	2.070852	2.110116	-0.123419
9	8	0	3.514840	-0.011347	0.003192
10	1	0	1.921004	-2.174181	0.124742
11	1	0	-0.523159	-2.117808	0.154204
12	1	0	3.846015	-0.915172	0.029952
13	6	0	-2.095268	0.119278	-0.053969
14	8	0	-2.659506	1.280593	0.207357
15	6	0	-3.040206	-1.052196	-0.116503

16	1	0	-2.609383	-1.850440	-0.724419
17	1	0	-3.268103	-1.448416	0.881907
18	1	0	-3.984101	-0.747106	-0.574079

E(UB+HF-LYP) = -460.126898862

Zero-point correction= 0.137459 (Hartree/Particle)

Sum of electronic and zero-point Energies= -459.989440

(C) Ground state of HPDP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	2.251669	-0.152028	0.673222
2	8	0	1.560267	-0.278190	1.966309
3	8	0	3.404062	-1.233978	0.457149
4	8	0	3.027642	1.197206	0.333667
5	8	0	1.266042	-0.347210	-0.608037
6	6	0	4.201012	-1.309465	-0.751592
7	6	0	5.116499	-2.509195	-0.625478
8	6	0	2.397201	2.512576	0.412546
9	6	0	2.271054	3.103925	-0.976192
10	6	0	-0.068096	-0.804785	-0.423702
11	6	0	-1.050649	0.361399	-0.269038
12	8	0	-0.645519	1.505741	-0.227737
13	6	0	-2.499164	0.037191	-0.178952
14	6	0	-3.414942	1.098649	-0.085860
15	6	0	-4.774207	0.866359	0.003004
16	6	0	-5.254173	-0.449333	0.005234
17	6	0	-4.358698	-1.519168	-0.083139
18	6	0	-2.994771	-1.273200	-0.174812
19	8	0	-6.597958	-0.621652	0.095896
20	1	0	-6.806149	-1.562212	0.095651
21	1	0	1.865582	4.117678	-0.907415
22	1	0	1.590953	2.503158	-1.580435
23	1	0	3.245416	3.154511	-1.468143
24	1	0	5.739629	-2.596652	-1.519856
25	1	0	4.537426	-3.428195	-0.513983
26	1	0	5.769270	-2.405064	0.243443

27	1	0	3.054351	3.105695	1.050185
28	1	0	1.422859	2.421298	0.891694
29	1	0	4.766312	-0.380148	-0.851729
30	1	0	3.529498	-1.405700	-1.609399
31	1	0	-0.143199	-1.451003	0.455857
32	1	0	-0.326171	-1.386809	-1.311809
33	1	0	-5.484886	1.680420	0.074514
34	1	0	-4.729208	-2.539733	-0.076906
35	1	0	-2.323495	-2.121085	-0.236076
36	1	0	-3.025903	2.109209	-0.083994

SCF Done: E(RB+HF-LYP) = -1260.56851391

Zero-point correction=

0.285518 (Hartree/Particle)

Sum of electronic and zero-point Energies=

-1260.282996

(D) triplet of HPDP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	2.457277	-0.113033	-0.602534
2	8	0	2.851139	-0.840991	-1.820136
3	8	0	3.246985	1.248074	-0.361066
4	8	0	2.667376	-0.854225	0.803538
5	8	0	0.893114	0.319909	-0.568843
6	6	0	3.020290	2.108679	0.784717
7	6	0	3.938329	3.305044	0.649039
8	6	0	2.173309	-2.209041	0.999006
9	6	0	2.348730	-2.557643	2.461567
10	6	0	-0.031509	-0.069944	-1.631080
11	6	0	-1.177139	-0.867436	-1.090921
12	8	0	-0.968461	-2.151091	-0.905101
13	6	0	-2.374521	-0.315984	-0.544592
14	6	0	-3.480742	-1.167281	-0.231604
15	6	0	-4.651652	-0.655244	0.278664
16	6	0	-4.776532	0.723155	0.516185
17	6	0	-3.692047	1.577209	0.246340
18	6	0	-2.506675	1.071328	-0.244784
19	8	0	-5.962277	1.172768	1.008302
20	1	0	-5.929481	2.130448	1.107603
21	1	0	2.003708	-3.579363	2.641846
22	1	0	1.769119	-1.881213	3.093331
23	1	0	3.399485	-2.491391	2.751876

24	1	0	3.797242	3.979522	1.498239
25	1	0	3.725341	3.854158	-0.270362
26	1	0	4.982704	2.987763	0.627811
27	1	0	2.747433	-2.876921	0.352782
28	1	0	1.122401	-2.253351	0.701524
29	1	0	3.231355	1.539112	1.692542
30	1	0	1.968651	2.407779	0.793187
31	1	0	0.518226	-0.640489	-2.380464
32	1	0	-0.412624	0.850284	-2.077581
33	1	0	-5.499975	-1.296045	0.486659
34	1	0	-3.782950	2.641290	0.446132
35	1	0	-1.666175	1.736736	-0.394232
36	1	0	-3.395655	-2.225429	-0.441636

E(UB+HF-LYP) = -1260.45808957

Zero-point correction= 0.281821 (Hartree/Particle)

Sum of electronic and zero-point Energies= -1260.176269