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Supplementary Information

Unexpected Higher Stabilisation of Two Classical Antiaromatic Frameworks with a Ruthenium Fragment over Osmium Couterpart: Origin Probed by DFT Calculations

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Computational details

The density functional theory B3LYP[1] was applied to optimize all of the structures in the gas phase. Frequency calculations at the same level of theory have also been performed to identify all stationary points as minima (zero imaginary frequency). In the B3LYP calculations, the effective core potentials (ECPs) of Hay and Wadt with a double-δ valence basis set (LanL2DZ)[2] were used to describe the Ru, Os, P and Cl atoms, whereas the 6-311++G(d,p)[3] basis set was used for the C and H atoms. Polarization functions were added for P (ξ(d) = 0.340), Cl (ξ(d) = 0.514), Ru (ξ(f) = 1.235), Os (ξ(f) = 0.886),[4] Nucleus-independent chemical shift (NICS)[5] values were calculated at the B3LYP-GIAO/6-311++G(d,p) level. To examine the effect of the density functional, we calculated isomerization stabilization energy (ISE) values of **1** (Table 1) at M05/6-311++G(d,p)[6] and TPSS/6-311++G(d,p)[7] levels. The computed ISE values are -28.5 and -28.0 kcal mol^{-1}, respectively, which are comparable to that (-29.5 kcal mol^{-1} in Table 1) at the B3LYP/6-311++G(d,p) level, indicating that the functional dependence is very small. The T_1 states of complexes **1-6** are also optimized at the B3LYP/6-311++G(d,p) level. The results show that all these complexes in the T_1 state are higher in energy than their S0 state. Specifically, the energy gaps including the zero-point energy corrections between the S_0 and T_1 states (ΔE_{S-T}) of complexes **1-6** are 27.8, 28.0, 28.1, 28.5, 28.3, and 28.6 kcal/mol, respectively, indicating all these complexes have a close shell ground state. To gain an insight into the chemical bonding, natural bond orbital (NBO) analysis[8] and electron localization function (ELF)[9] methods were employed. All the optimizations were performed with the Gaussian 03 software package[10] at 298K, whereas the canonical molecular orbital (CMO) NICS calculations were carried out with the Gaussian 09 program. Structures were visualized by the CYLview program.[11]

References:

1. a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; b) B. Miehlich, A. Savin, H. Stoll, H. Preuss, *Chem. Phys. Lett.* **1989**, *157*, 200; c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*. **1988**, *37*, 785.
2. P. J. Hay, W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 299.
3. W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257.
4. a) A. W. Ehlers, M. Bohme, S. Dapprich, A. Gobbi, A. Hollwarth, V. Jonas, K. F. Kohler, R. Stegmann, A. Veldkamp, G. Frenking, *Chem. Phys. Lett.* **1993**, *208*, 111; b) C. E. Check, T. O. Faust, J. M. Bailey, B. J. Wright, *J. Phys. Chem. A* **2001**, *105*, 8111; c) A. Höllwarth, H. Böhme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp, G. Frenking, *Chem. Phys. Lett*. **1993**, *208*, 237.
5. a) P. v. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N. J. R. v. E. Hommes, *J. Am. Chem. Soc*. **1996**, *118,* 6317; b) H. Fallah-Bagher-Shaidaei, C. S. Wannere, C. Corminboeuf, R. Puchta, P. v. R. Schleyer, *Org. Lett.* **2006**, *8*, 863; c) Z. Chen, C. Wannere, C. Corminboeuf, R. Puchta, P. v. R. Schleyer, *Chem. Rev.* **2005**, *105*, 3842.
6. a) Y. Zhao, N. E. Schultz, D. G. Truhlar, *J. Chem. Phys.* **2005**, *123*, 161103; b) Y. Zhao, D. G. Truhlar, *J. Chem. Theory Comput*. **2006**, *2*, 1009; c) Y. Zhao, D. G. Truhlar, *J. Chem. Theory Comput*. **2008**, *4*, 1849; d) Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc*. **2008**, *120*, 215.
7. J. Tao, J. P. Perdew, V. N. Staroverov, G. E. Scuseria, *Phys. Rev. Lett.* **2003**, *91*, 146401.
8. E. D. Glendening, A. E. Reed, J. E. Carpenter, F. Weinhold, NBO, Version 3.1.
9. a) A. D. Becke, K. E. Edgecombe, *J. Chem. Phys.* **1990**, *92*, 5397; b) A. Savin, A. D. Becke, J. Flad, R. Nesper, H. Preuss, H. G. von Schnering, *Angew. Chem., Int. Ed. Engl.* **1991**, *30*, 409; c) B. Silvi, A. Savin, *Nature* **1994**, *371*, 683; d) A. Savin, B. Silvi, F. Can. Colonna, *J. Chem.* **1996**, *74*, 1088; e) M. Kohout, A. Savin, *Int. J. Quantum Chem.* **1996**, *60*, 875; f) A. Savin, R. Nesper, S. Wengert, T.

Fässler, *Angew. Chem., Int. Ed. Engl.* **1997**, *36*, 1809; g) D. Marx, A. Savin, *Angew. Chem., Int. Ed. Engl*. **1997**, *36*, 2077; h) S. Noury, F. Colonna, A. Savin, B. Silvi, *J. Mol. Struct*. **1998**, *450*, 59; i) Y. Yang, *J. Phys. Chem. A* **2010**, *114*, 13257; j) Y. Yang, *Polyhedron* **2012**, *33*, 310.

10. Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.
11. Gaussian 09, Revision D. 01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
12. C. Y. Legault, CYLview, 1.0b; Université de Sherbrooke, 2009 (http://www.cylview.org).

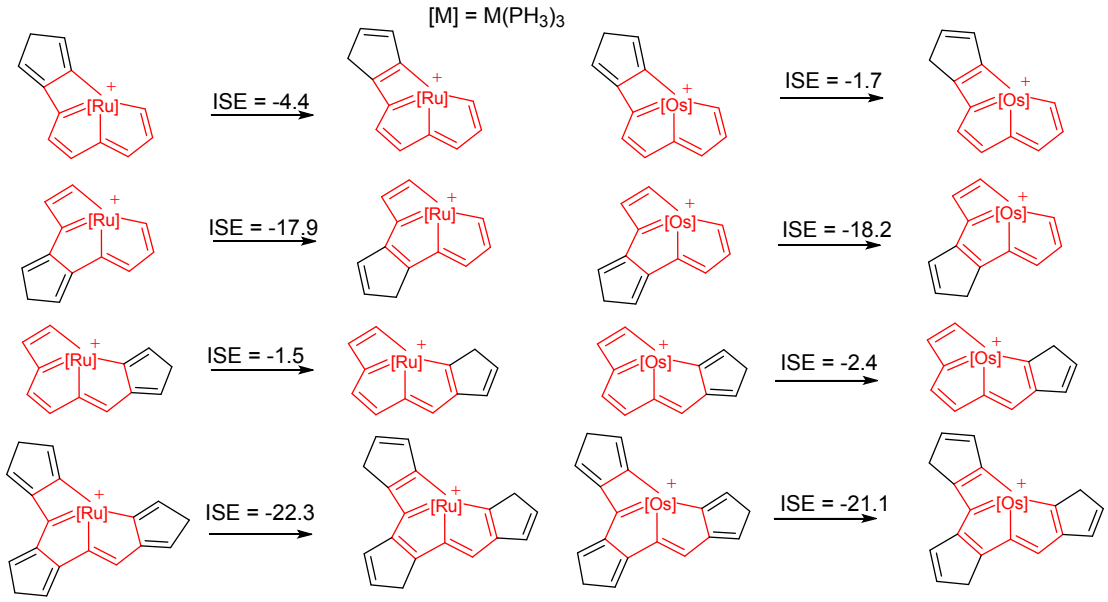

Fig. S1 Indene-isoindene ISE evaluations of the aromaticity of complexes **3** and **4**. The energies (kcal mol^{-1}) include the zero-point energy corrections.

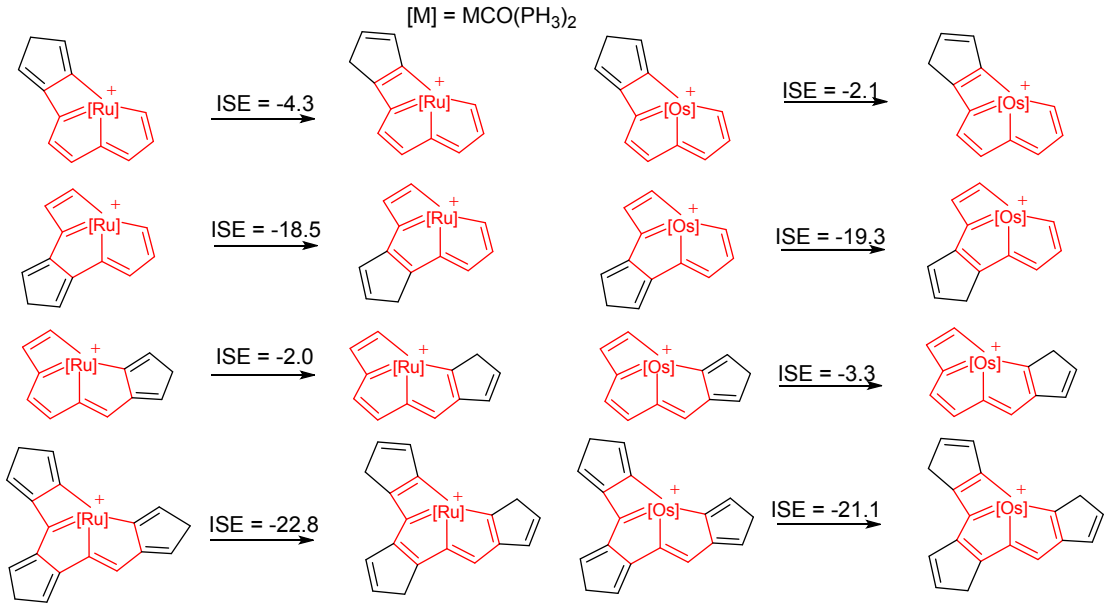

Fig. S2 Indene-isoindene ISE evaluations of the aromaticity of complexes **5** and **6**. The energies (kcal mol^{-1}) include the zero-point energy corrections.

Cartesian coordinates (including numbers of atoms) and electronic energies for all the species calculated in this study

1 E = -472.6553815 a.u.

C	-1.78575100	0.63397100	-0.00021400
C	-2.03382100	1.99931400	-0.00040200
H	-3.04931400	2.39653700	-0.00049500
C	-0.99574300	-1.73986700	0.00008600
Cl	2.72589300	0.43086000	0.00011800
P	0.25033700	-0.00928900	2.36937600
H	1.44564300	0.43714800	2.99732000
H	-0.69843200	0.79122600	3.07040000
H	0.06113100	-1.23519200	3.07437300
P	0.25093300	-0.01009000	-2.36931800
H	-0.69923600	0.78826800	-3.07091100
H	1.44551500	0.43846600	-2.99712200
H	0.06435400	-1.23663900	-3.07389200
C	1.06704700	-2.01819800	0.00056800
C	-0.03990800	-2.79188900	0.00036600
C	-2.38074900	-1.64578100	-0.00007500
C	-2.81241300	-0.32275000	-0.00021200
C	0.27915200	2.08618800	-0.00032400
C	-0.88342300	2.81617400	-0.00044300
H	1.24230200	2.59095400	-0.00037600
H	-0.92857100	3.90224700	-0.00057500
H	-3.86334800	-0.03757900	-0.00034700
H	-3.04224500	-2.50775500	-0.00006000
H	2.11769300	-2.29116800	0.00089500
H	-0.18165100	-3.87306800	0.00044900
Ru	0.22137700	-0.02955300	0.00003100

2 E = -469.8720451 a.u.

C	-1.82845900	0.62290200	-0.00027700
C	-2.09913500	1.98870100	-0.00041600
H	-3.11944700	2.37006700	-0.00052300
C	-1.01411700	-1.72421500	0.00010400
Cl	2.67078700	0.49422000	0.00015900
P	0.22138100	-0.03979400	2.36865200
H	1.40257900	0.43200600	3.00556300
H	-0.75736000	0.71432200	3.07888000
H	0.07322700	-1.29519800	3.02848700
P	0.22194600	-0.04059300	-2.36860200
H	-0.75717200	0.71255700	-3.07933800
H	1.40294800	0.43181700	-3.00542100
H	0.07484700	-1.29634500	-3.02801100
C	1.06861800	-1.99586100	0.00048200
C	-0.03863600	-2.77137300	0.00048300
C	-2.40301900	-1.65818500	-0.00009600
C	-2.85131000	-0.34135300	-0.00031600
C	0.21150700	2.09124100	-0.00029600
C	-0.96196200	2.81530000	-0.00041100
H	1.16099300	2.62111100	-0.00027200
H	-1.01312600	3.90001200	-0.00050800
H	-3.90329600	-0.06459400	-0.00046900
H	-3.05016900	-2.52994000	-0.00004800
H	2.11413100	-2.28733400	0.00070600
H	-0.17457600	-3.85212000	0.00066500
Os	0.18410800	-0.01599000	0.00001700

CBD E = -154.7211828 a.u.

C	-0.78863200	0.66669200	0.00000600
C	0.78861600	0.66667900	-0.00000300
C	0.78863100	-0.66669600	-0.00000300
H	1.55145700	-1.43291300	0.00003300
C	-0.78865000	-0.66670200	-0.00000200
H	-1.55130100	-1.43309400	-0.00001500
H	-1.55120700	1.43311800	0.00000600
H	1.55126100	1.43304500	-0.00000900

CBD-isoindene E = -270.292038 a.u.

C	0.30521500	-0.73628600	-0.00004500
C	0.30523700	0.73585300	0.00001600
C	-1.88735900	0.00012900	0.00004500
H	-2.54849400	0.00004800	-0.87773100
H	-2.54856000	-0.00002200	0.87777300
C	1.79261200	0.68414100	-0.00003900
H	2.57947800	1.42663900	-0.00003200
C	1.79328000	-0.68405000	-0.00009400
H	2.58011100	-1.42640200	-0.00015200
C	-0.94427600	-1.21239400	0.00003800

H	-1.29433700	-2.23621800	-0.00012500
C	-0.94386400	1.21250100	0.00013500
H	-1.29327200	2.23659500	-0.00006900

CBD-indene E = -270.2416624 a.u.

C	-0.39471000	0.78056500	0.00123100
C	-0.34264900	-0.74782100	0.00098600
C	-1.68012300	-0.82684800	-0.00060300
H	-2.42104600	-1.61635200	-0.00250700
C	-1.74288400	0.76972100	-0.00023100
H	-2.53511800	1.50633200	-0.00084800
C	0.95807900	1.25279400	0.00002700
H	1.29945900	2.28041500	-0.00087600
C	1.78741500	0.17253000	-0.00077000
H	2.86949500	0.25096800	-0.00227700
C	1.08964200	-1.20418500	0.00029300
H	1.36976600	-1.80044000	0.87857000
H	1.36882200	-1.80145000	-0.87765200

Pentlene E = -308.4476423 a.u.

C	2.16998400	-0.06087000	-0.00006000
C	1.46536800	1.09537900	-0.00013000
C	0.03802200	0.72801500	-0.00004700
C	-0.03802200	-0.72801500	0.00003600
C	-2.16998400	0.06087000	0.00005500
C	-1.46536800	-1.09537900	0.00014000
C	1.22335900	-1.21968100	0.00000200
C	-1.22335900	1.21968100	0.00000100
H	1.53383500	-2.25721300	0.00005400
H	-1.53383500	2.25721300	-0.00003900
H	1.87022800	2.09733100	-0.00020300
H	3.24693700	-0.15768800	-0.00007600
H	-1.87022800	-2.09733100	0.00021700
H	-3.24693700	0.15768800	0.00006800

Pentlene-isoindene E = -539.539624 a.u.

C	2.01545900	0.86583200	-0.00011100
C	1.70706900	-0.58741900	-0.00019700
C	0.25719600	-0.69755200	-0.00004200
C	-0.25715900	0.69757700	0.00008000
C	-2.01545900	-0.86582700	0.00002800
C	-1.70703700	0.58743900	0.00013100
C	0.75950900	1.60601100	0.00004300
C	-0.75946700	-1.60598700	-0.00000500
H	0.66491800	2.68332100	0.00006900
H	-0.66485700	-2.68329700	-0.00005500
C	-3.35415400	-1.04404200	-0.00002200
C	3.35416300	1.04403700	-0.00026600
H	-3.90243400	-1.97621600	-0.00011000
H	3.90241700	1.97621600	-0.00042100
C	2.85529500	-1.29311700	-0.00039200
C	-2.85530900	1.29308300	-0.00000900
C	4.01434100	-0.31913100	0.00041000
H	4.66289100	-0.46299100	-0.87554600
H	4.66206000	-0.46287100	0.87701500
C	-4.01441600	0.31911600	0.00019700
H	-4.66266800	0.46288000	-0.87600600
H	-4.66247600	0.46287300	0.87654500
H	-2.97566800	2.36812600	0.00017100
H	2.97564300	-2.36816500	-0.00072200

Pentlene-indene E = -539.5124584 a.u.

C	2.00025700	-0.81826100	-0.00003500
C	1.73813000	0.52193600	-0.00010000
C	0.28665100	0.68856200	-0.00004300
C	-0.28665100	-0.68856100	0.00006600
C	-2.00025500	0.81826300	0.00009900
C	-1.73812900	-0.52193600	0.00012600
C	0.72332200	-1.59221500	0.00008800
C	-0.72332100	1.59221700	-0.00003300
H	0.64417900	-2.67169900	0.00008900
H	-0.64417700	2.67170100	-0.00001500
C	-3.02724500	-1.28015300	-0.00001200
C	-3.43766500	1.03992500	0.00009200
C	-4.05635000	-0.16583400	-0.00019100
H	-5.12369700	-0.33996100	-0.00011700
C	3.43766500	-1.03991700	-0.00001200
C	3.02724500	1.28014900	0.00001400
C	4.05634400	0.16582700	-0.00002700
H	5.12369100	0.33994900	-0.00013700
H	-3.13971100	-1.92974700	-0.87801300
H	-3.93089900	2.00344700	-0.00000400
H	3.13979400	1.92964900	0.87807500
H	3.93090100	-2.00343700	-0.00012100
H	-3.13999900	-1.93001200	0.87773000
H	3.13992500	1.93009700	-0.87767100

1-4MR-isoindene E = -588.1824324 a.u.

C	1.78848300	1.37755400	-0.00025700
C	3.14194000	1.05383200	-0.00043500
H	3.91764400	1.81941700	-0.00056200
C	-0.67870600	1.62159400	0.00018500
Cl	-0.16356800	-2.70442100	0.00006200
P	0.29302600	-0.29222600	2.37017800
H	0.16849100	-1.58795400	2.93915400
H	1.39688300	0.20022500	3.12721700
H	-0.75883400	0.37771700	3.06014300
P	0.29177400	-0.29225000	-2.37016600
H	1.39508600	0.20032700	-3.12792300
H	0.16702800	-1.58799300	-2.93905700
H	-0.76060700	0.37757800	-3.05944100
C	-1.81978100	-0.27153900	0.00035800
C	-2.03706300	1.16084400	0.00037100
C	-0.04624600	2.84789600	0.00009600
C	1.34250400	2.70195600	-0.00018900
C	2.25875100	-1.08350400	-0.00030700
C	3.40773600	-0.32380700	-0.00049300
C	-3.35865600	1.48168300	0.00024300
H	-3.83391900	2.45437500	0.00018600
C	-3.00937200	-0.89932300	0.00019700
H	-3.20973800	-1.96215000	0.00013500
C	-4.10337800	0.16459700	0.00019300
H	-4.76265000	0.08170300	-0.87638700
H	-4.76282300	0.08164700	0.87663500
H	2.32423300	-2.16867200	-0.00034000
H	4.41253200	-0.73863900	-0.00065200
H	2.03456200	3.54265100	-0.00030700
H	-0.56476100	3.80228000	0.00022300
Ru	0.35291500	-0.20774800	-0.00000100

1-4MR-indene E = -588.1926977 a.u.

C	1.73954200	1.38752400	-0.00020700
C	3.08938600	1.09755200	-0.00017700
H	3.84520500	1.88344100	-0.00027900
C	-0.75653400	1.59912000	-0.00020500
Cl	-0.15480800	-2.72095300	0.00029200
P	0.37749600	-0.25475600	2.36649500
H	0.38733900	-1.52995500	2.99644300
H	1.46823500	0.35419900	3.05347700
H	-0.69347000	0.35004800	3.09096200
P	0.37737000	-0.25538500	-2.36645100
H	1.46778500	0.35387800	-3.05367500
H	0.38774400	-1.53074800	-2.99605500
H	-0.69392000	0.34873600	-3.09100800
C	-1.81618800	-0.25147400	0.00010500
C	-2.06294100	1.09620700	-0.00009200
C	-3.08472200	-0.95531600	0.00025500
H	-3.20619500	-2.02960900	0.00042600
C	-4.08238000	-0.03014900	0.00007800
H	-5.14385100	-0.24866000	0.00011300
C	-0.12212300	2.84410900	-0.00038400
C	1.25435100	2.71340900	-0.00038400
C	-3.54207300	1.38745300	-0.00007400
H	-3.88488200	1.94745300	0.87905000
H	-3.88493200	1.94724900	-0.87930500
C	2.29004900	-1.07404200	0.00010100
C	3.40470300	-0.28491200	-0.00000200
H	2.37125000	-2.15777300	0.00023500
H	4.42459700	-0.66098800	0.00004200
H	1.93353300	3.56476200	-0.00051400
H	-0.64920700	3.79374900	-0.00049900
Ru	0.34802500	-0.21941700	0.00002000

1-5MR1-isoindene E = -588.1599418 a.u.

C	-0.99715700	1.23646800	-0.00084700
C	-0.73815900	2.56742400	-0.00184700
H	-1.53485000	3.31135700	-0.00240100
C	-0.97571400	-1.35977400	-0.00038100
Cl	3.22242400	-0.51407700	0.00180700
P	0.77599800	0.04976100	2.36480600
H	2.06799600	0.16807700	2.94492500
H	0.12705400	1.16229400	2.96980200
H	0.25035100	-0.98862700	3.19568500
P	0.77865100	0.04606500	-2.36473100
H	0.12779300	1.15600600	-2.97246200
H	2.07110700	0.16659500	-2.94334700
H	0.25659700	-0.99498600	-3.19454700
C	0.87862800	-2.24566800	0.00203200
C	-0.42887600	-2.64911000	0.00009000
C	-2.29516600	-0.82336700	-0.00026400
C	-2.32146800	0.64014100	-0.00043000
C	-3.56002600	-1.33161900	-0.00002000
H	-3.85843700	-2.37144600	0.00016300
C	1.49859800	1.87639100	-0.00157500
C	0.65402900	2.92906700	-0.00221600
C	-4.51126000	-0.17103400	0.00003800

H	-5.17992300	-0.21042600	-0.87351700
H	-5.17967400	-0.21029600	0.87378800
C	-3.61948700	1.04629500	-0.00018800
H	-3.99941400	2.05839800	-0.00017900
H	2.57653000	1.99925500	-0.00178800
H	0.98426900	3.96633300	-0.00293100
H	1.78220500	-2.85043600	0.00435200
H	-0.89906800	-3.63168600	-0.00016400
Ru	0.70006500	-0.12999500	0.00010100

1-5MR1-indene E = -588.1901915 a.u.

C	-1.01382000	1.18152400	-0.00028300
C	-0.82228600	2.55400100	-0.00050200
H	-1.65693100	3.25569200	-0.00066200
C	-0.94750700	-1.37016700	0.00021300
Cl	3.24728100	-0.38639000	0.00018100
P	0.74485600	-0.05763000	2.36735700
H	2.00982200	0.09367600	2.99979100
H	0.01354500	0.94748400	3.06626300
H	0.26838500	-1.20086300	3.07621700
P	0.74513800	-0.05873800	-2.36721500
H	0.01312400	0.94546600	-3.06669900
H	2.01005700	0.09323600	-2.99957700
H	0.26963200	-1.20268800	-3.07556400
C	0.94991100	-2.22361000	0.00064100
C	-0.33166000	-2.65045100	0.00058500
C	-2.23347200	-0.85258800	0.00000200
C	-2.26322500	0.55032900	-0.00027800
C	-3.60973000	-1.36030900	0.00005200
H	-3.89129000	-2.40505200	0.00028100
C	-4.45939600	-0.31533100	-0.00035600
H	-5.54021900	-0.37529600	-0.00047300
C	-3.70651500	1.00352300	-0.00046900
H	-3.94917300	1.61531200	0.87673700
H	-3.94898800	1.61496600	-0.87796100
C	1.41071100	1.92217500	-0.00030000
C	0.52643700	2.97173100	-0.00051500
H	1.88036600	-2.78245000	0.00089100
H	-0.77058200	-3.64832800	0.00076700
H	2.48153500	2.10959500	-0.00028700
H	0.81875500	4.01902900	-0.00067900
Ru	0.71458200	-0.07342300	0.00006900

1-5MR2-isoindene E = -588.1865589 a.u.

C	-0.01455500	1.86627600	-0.00005600
C	1.28815300	2.29682000	-0.00006700
H	1.54766000	3.35484500	-0.00010000
C	-2.30737900	0.86625000	-0.00001400
Cl	0.10494700	-2.69594100	0.00001200
P	-0.36260300	-0.29831800	2.36489100
H	0.41110500	-1.35561900	2.91486600
H	0.20638100	0.80214900	3.07175800
H	-1.54930000	-0.45236300	3.14652800
P	-0.36265600	-0.29847300	-2.36486900
H	0.20591300	0.80213300	-3.07185600
H	0.41140000	-1.35554700	-2.91478500
H	-1.54933100	-0.45299900	-3.14644100
C	-2.36859000	-1.19056000	0.00008500
C	-3.26255700	-0.16084000	0.00004200
C	-2.34685500	2.26523300	-0.00007200
C	-1.08222900	2.80777000	-0.00009400
C	1.69490000	-0.10541200	0.00000500
C	2.26287500	1.26185100	-0.00003300
C	3.62441700	1.23862900	-0.00003100
H	4.29853000	2.08608200	-0.00005400
C	4.05083700	-0.19946800	0.00001200
H	4.67371700	-0.43671100	-0.87538400
H	4.67371800	-0.43666100	0.87542000
C	2.73993000	-0.96081600	0.00003300
H	2.68807300	-2.03992500	0.00006600
H	-2.54990800	-2.26216000	0.00013800
H	-4.35164600	-0.12722600	0.00004900
H	-3.26864900	2.83997400	-0.00009100
H	-0.89165300	3.87979800	-0.00013600
Ru	-0.48942900	-0.22675700	0.00001400

1-5MR2-indene E = -588.1958271 a.u.

C	-0.05350100	1.86780200	-0.00002000
C	1.27105700	2.29809800	-0.00002500
H	1.52387200	3.35832300	-0.00002400
C	-2.30902600	0.77735800	-0.00001800
Cl	0.24816500	-2.67965400	-0.00001000
P	-0.44949400	-0.23109600	2.36761700
H	0.14814100	-1.34265900	3.02529700
H	0.19751200	0.82756300	3.07019300
H	-1.70138900	-0.20941300	3.05107700
P	-0.44957200	-0.23125100	-2.36759600
H	0.19672400	0.82777600	-3.07027300

H	0.14874600	-1.34247300	-3.02523000
H	-1.70151000	-0.21041700	-3.05100400
C	-2.31904600	-1.29699400	0.00011200
C	-3.23076800	-0.30572900	0.00003800
C	-2.39046900	2.15548900	-0.00005200
C	-1.12925800	2.75799700	-0.00004600
C	1.67816200	-0.01677900	-0.00001000
C	2.22490500	1.27354200	-0.00001900
C	3.68806000	1.22108600	-0.00001000
H	4.34582600	2.08168500	-0.00000500
H	-2.43501200	-2.37574700	0.00018800
H	-4.32087700	-0.30810700	0.00003100
H	-3.33069200	2.70031500	-0.00006600
H	-0.98323200	3.83698400	-0.00006700
C	2.84721900	-0.96548900	-0.00003400
H	2.80467100	-1.64371000	0.86073100
H	2.80465900	-1.64369200	-0.86081200
C	4.06472700	-0.07166400	-0.00002800
H	5.08242000	-0.44118700	-0.00003900
Ru	-0.44466000	-0.22259600	0.00001200

1-isoindene E = -819.2179168 a.u.

C	-0.40512900	1.81259400	-0.03549400
C	-1.63548100	2.35916200	-0.14335800
H	-1.78638400	3.43514500	-0.21484600
C	1.73395400	0.38936000	-0.08537500
Cl	-1.13977700	-2.68510900	0.57434800
P	-0.48099800	-0.68906300	-2.27432300
H	-1.21832700	-1.84802800	-2.63531100
H	-1.20242800	0.30663600	-2.99055300
H	0.63587100	-0.83652000	-3.15341800
P	-0.24476100	-0.28740000	2.42784900
H	0.19071100	0.88429500	3.11864800
H	-1.53523000	-0.43139300	3.00137400
H	0.46842800	-1.27035400	3.16983000
C	1.49411600	-1.79086500	-0.09157500
C	2.53143100	-0.78846200	-0.18667900
C	2.02614900	1.77950000	-0.05855900
C	0.81954100	2.60033700	0.00296600
C	3.14242300	2.56152500	-0.04073800
H	4.17583200	2.24322900	-0.07215000
C	-2.30927500	0.01488600	-0.06418300
C	-2.72497900	1.43253400	-0.17224100
C	-4.07267000	1.53671800	-0.27142900
H	-4.65752600	2.44374600	-0.35560700
C	3.77471600	-1.33609800	-0.30653600
H	4.74116800	-0.85223300	-0.37462800
C	2.05488900	-3.01049800	-0.15412800
H	1.57440000	-3.97742700	-0.09811300
C	-4.64733200	0.14797800	-0.24239300
H	-5.34682400	0.00349100	0.59411900
H	-5.22026100	-0.08299500	-1.15274700
C	2.69383600	3.99222400	0.04830100
H	3.10842300	4.48245500	0.94233900
H	3.07376200	4.57854800	-0.80234400
C	3.56546500	-2.83150400	-0.29772400
H	4.11596800	-3.29172900	0.53676700
H	3.97346000	-3.29363400	-1.20888900
C	-3.42885300	-0.74042300	-0.11102000
H	-3.49026900	-1.81623000	-0.04719000
C	1.18545400	3.90526200	0.07393700
H	0.54388500	4.77314300	0.13899900
Ru	-0.15162700	-0.39458400	0.05350600

1-indene E = -819.265738 a.u.

C	0.39820800	1.74177000	-0.00018600
C	1.66974400	2.28618100	-0.00015600
H	1.83518300	3.36337400	-0.00022700
C	-1.78731000	0.41156900	-0.00019200
Cl	1.17629800	-2.77354400	0.00015500
P	0.21549100	-0.40436300	2.36418000
H	0.93564500	-1.43938700	3.02470400
H	0.75465200	0.72198900	3.05277100
H	-1.02090800	-0.50994600	3.06958200
P	0.21552600	-0.40519300	-2.36409600
H	0.75247600	0.72196700	-3.05309700
H	0.93775100	-1.43903000	-3.02420400
H	-1.02063400	-0.51349200	-3.06950300
C	-1.53739000	-1.69728900	0.00038900
C	-2.53961500	-0.76945700	0.00005800
C	-2.12595700	-3.02421100	0.00073200
H	-1.57588000	-3.95446200	0.00102200
C	-3.47914900	-2.88351500	0.00061000
H	-4.19661500	-3.69547100	0.00079300
C	-1.97915300	1.78643000	-0.00041200
C	-0.77717100	2.50361500	-0.00038900
C	-3.10086500	2.72974600	-0.00060500
H	-4.14790000	2.45599300	-0.00065800

C	-2.61491900	3.98661500	-0.00071400
H	-3.20283200	4.89554500	-0.00087100
C	-1.09636100	3.98371000	-0.00059600
H	-0.68579100	4.49782300	0.87683600
H	-0.68566000	4.49761200	-0.87809000
C	-3.89689900	-1.42426300	0.00015300
H	-4.50613100	-1.18016100	0.87954700
H	-4.50600900	-1.18067900	-0.87947100
C	2.30069600	0.01753400	0.00004200
C	2.71743100	1.34673900	-0.00003000
C	4.17884600	1.43756700	0.00003700
H	4.74906900	2.35884100	0.00000300
C	4.68092200	0.18787800	0.00013900
H	5.72938400	-0.08219000	0.00020500
C	3.55526700	-0.81840400	0.00014900
H	3.58256600	-1.49610300	0.86176900
H	3.58263300	-1.49618800	-0.86140400
Ru	0.20065300	-0.41013100	0.00005100

2-4MR-isoindene E = -585.4029135 a.u.

C	-1.72010900	1.42204900	0.00024900
C	-3.08025800	1.11400200	0.00047500
H	-3.84763900	1.88609600	0.00058600
C	0.73593300	1.64172900	-0.00015100
Cl	0.18605500	-2.66905800	-0.00005500
P	-0.23486000	-0.26722500	-2.37107900
H	-0.11953000	-1.56426100	-2.93998700
H	-1.33782500	0.23973300	-3.11828700
H	0.82845700	0.39999500	-3.04404300
P	-0.23390100	-0.26724700	2.37110700
H	-1.33647600	0.23982100	3.11881800
H	-0.11845700	-1.56430100	2.93994800
H	0.82979200	0.39985600	3.04358900
C	1.86702400	-0.25515000	-0.00032000
C	2.09926600	1.17840100	-0.00034600
C	0.11804400	2.88063600	-0.00007100
C	-1.26860200	2.74862000	0.00014900
C	-2.20711000	-1.03090000	0.00034400
C	-3.35415000	-0.25878600	0.00051400
C	3.42076700	1.48728400	-0.00042100
H	3.90243500	2.45674900	-0.00044100
C	3.05475500	-0.88896600	-0.00039100
H	3.24765000	-1.95342800	-0.00042200
C	4.15817100	0.16428500	-0.00031600
H	4.81698100	0.07476100	0.87599800
H	4.81710900	0.07471700	-0.87652500
H	-2.30156500	-2.11371700	0.00035900
H	-4.35993400	-0.66900000	0.00066700
H	-1.95550900	3.59199800	0.00025400
H	0.64848900	3.82748100	-0.00017300
Os	-0.29984000	-0.17308700	0.00002500

2-4MR-indene E = -585.4082073 a.u.

C	1.68540400	1.42315200	-0.00022000
C	3.04262400	1.14140700	-0.00019800
H	3.79246300	1.93160600	-0.00031000
C	-0.79791200	1.61920000	-0.00022200
Cl	-0.17566400	-2.68377200	0.00035100
P	0.28609900	-0.21227100	2.36581400
H	0.27871700	-1.48398500	3.00379500
H	1.36524700	0.40335100	3.06439500
H	-0.80683100	0.40386800	3.04515100
P	0.28598800	-0.21290900	-2.36577200
H	1.36498400	0.40272200	-3.06458100
H	0.27880300	-1.48479500	-3.00341100
H	-0.80709400	0.40284600	-3.04521100
C	-1.86355800	-0.23384800	0.00007800
C	-2.11383600	1.11155100	-0.00009900
C	-3.13128000	-0.94141000	0.00023300
H	-3.25167700	-2.01600400	0.00038500
C	-4.13261200	-0.02098800	0.00002300
H	-5.19333800	-0.24173600	0.00002100
C	-0.17732700	2.87222700	-0.00040600
C	1.20122900	2.75007800	-0.00040500
C	-3.59195200	1.39716800	-0.00005400
H	-3.93632100	1.95709200	0.87875500
H	-3.93641700	1.95707500	-0.87884000
C	2.24055900	-1.02770300	0.00009700
C	3.36114500	-0.23467700	-0.00001900
H	2.34642200	-2.10951200	0.00024200
H	4.37937400	-0.61214600	0.00002200
H	1.87784000	3.60217400	-0.00053300
H	-0.71236700	3.81652800	-0.00052600
Os	0.30303000	-0.18505500	0.00001600

2-5MR1-isoindene E = -585.3769898 a.u.

C	-1.10411100	1.24659100	0.00002800
C	-0.86992300	2.58656400	0.00008400

H	-1.67999100	3.31438200	0.00010900
C	-1.06093100	-1.32774200	-0.00002100
Cl	3.11031300	-0.42693200	-0.00007600
P	0.66540600	0.01691100	2.36819800
H	1.95329800	0.14635500	2.95531600
H	-0.01378600	1.09898000	2.99466000
H	0.15423000	-1.06629400	3.14714700
P	0.66534500	0.01707600	-2.36819600
H	-0.01379200	1.09923500	-2.99456200
H	1.95323100	0.14647800	-2.95533700
H	0.15407900	-1.06603900	-3.14721400
C	0.81218500	-2.21768300	-0.00008600
C	-0.49471300	-2.62008300	0.00001900
C	-2.39130600	-0.81742600	-0.00001800
C	-2.42784900	0.64640900	-0.00000500
C	-3.65206900	-1.33377400	-0.00001800
H	-3.94494100	-2.37505300	-0.00000900
C	1.36946900	1.92038600	0.00008800
C	0.51376900	2.96892900	0.00012900
C	-4.61091900	-0.17823800	0.00001800
H	-5.27893300	-0.21885100	-0.87381200
H	-5.27887000	-0.21883000	0.87389900
C	-3.72793900	1.04517400	-0.00004800
H	-4.11438700	2.05492300	-0.00006500
H	2.44331800	2.07675900	0.00011500
H	0.83147700	4.00897400	0.00018600
H	1.70882600	-2.83141200	-0.00011900
H	-0.96137200	-3.60271800	0.00006500
Os	0.59364500	-0.09649300	-0.00000200

2-5MR1-indene E = -585.406446664 a.u.

C	-1.12707300	1.18757100	-0.00000900
C	-0.95074100	2.56699100	-0.00001500
H	-1.79251100	3.25830800	-0.00002100
C	-1.04186600	-1.34415000	-0.00002100
Cl	3.13664700	-0.32266200	0.00002800
P	0.63365400	-0.08428200	2.36638000
H	1.89530400	0.06132400	3.00751200
H	-0.11306600	0.90173600	3.07518800
H	0.15890900	-1.25477400	3.02880800
P	0.63370500	-0.08430700	-2.36637500
H	-0.11291300	0.90176800	-3.07521200
H	1.89538300	0.06118000	-3.00748100
H	0.15887100	-1.25476600	-3.02879600
C	0.87283800	-2.20672000	0.00001300
C	-0.41199000	-2.62814400	-0.00002100
C	-2.33791500	-0.84625700	-0.00001900
C	-2.37758200	0.55530600	-0.00001900
C	-3.70923400	-1.36345600	0.00002700
H	-3.98415500	-2.41011200	0.00005100
C	-4.56687100	-0.32439600	0.00004400
H	-5.64721100	-0.39216100	0.00008700
C	-3.82253300	0.99961300	-0.00004600
H	-4.07176000	1.60893300	0.87716600
H	-4.07170900	1.60868300	-0.87745600
C	1.28191700	1.94122000	0.00000700
C	0.38998200	2.99252400	-0.00000600
H	1.78969700	-2.78733800	0.00003700
H	-0.85104600	-3.62465900	-0.00003700
H	2.34822600	2.15242600	0.00000700
H	0.68036700	4.03919300	-0.00000600
Os	0.60777200	-0.05310900	0.00000000

2-5MR2-isoindene E = -585.4009411 a.u.

C	0.08728900	1.89205700	-0.00006600
C	1.39468200	2.31084900	-0.00008600
H	1.66421800	3.36560800	-0.00011900
C	-2.20539500	0.93138700	-0.00001800
Cl	0.17559700	-2.65092900	0.00007800
P	-0.33264400	-0.25958200	2.36356100
H	0.25765800	-1.41538400	2.94471400
H	0.38564200	0.75642200	3.05943900
H	-1.55220100	-0.21448600	3.10697300
P	-0.33267900	-0.25974000	-2.36354100
H	0.38559900	0.75621500	-3.05949900
H	0.25761200	-1.41558300	-2.94462500
H	-1.55224700	-0.21469000	-3.10693700
C	-2.29610400	-1.13858500	0.00005400
C	-3.17410000	-0.08663300	0.00002800
C	-2.23528200	2.33442900	-0.00006600
C	-0.96536200	2.85799900	-0.00009200
C	1.77463200	-0.09620500	-0.00000700
C	2.35861100	1.26557900	-0.00005200
C	3.71912200	1.23139100	-0.00004700
H	4.39894700	2.07423500	-0.00007000
C	4.13426100	-0.20947600	-0.00001300
H	4.75560200	-0.45139700	-0.87533200
H	4.75560800	-0.45135100	0.87531400

C	2.81708200	-0.95775800	0.00001200
H	2.75910800	-2.03636100	0.00004000
H	-2.52064200	-2.20201100	0.00009400
H	-4.26114800	-0.03703100	0.00003700
H	-3.15031800	2.91831500	-0.00007900
H	-0.75360400	3.92487300	-0.00012900
Os	-0.41173400	-0.19094700	0.00000900

2-5MR2-indene E = -585.4118601 a.u.

C	0.04392600	1.90023600	-0.00003000
C	1.37526500	2.32142200	-0.00001500
H	1.64001100	3.37761300	-0.00003000
C	-2.20927700	0.84379400	0.00000500
Cl	0.30762200	-2.63448300	-0.00001100
P	-0.41896900	-0.20666800	2.36622700
H	0.18314600	-1.31242200	3.03036000
H	0.19537600	0.86371900	3.07941900
H	-1.69370600	-0.21057300	3.00475800
P	-0.41910700	-0.20676600	-2.36622800
H	0.19482900	0.86380400	-3.07949700
H	0.18333300	-1.31233900	-3.03036700
H	-1.69388700	-0.21112100	-3.00467100
C	-2.26056700	-1.24890800	0.00008200
C	-3.15002500	-0.23460800	0.00007400
C	-2.28528200	2.22521300	-0.00002900
C	-1.01811200	2.81165900	-0.00005700
C	1.73839600	-0.00042000	-0.00005100
C	2.31016200	1.28460600	-0.00001200
C	3.77043200	1.20842400	-0.00004600
H	4.44024200	2.05963400	-0.00006900
H	-2.42559100	-2.32134000	0.00012900
H	-4.23904100	-0.21599300	0.00010200
H	-3.21981600	2.77810300	-0.00002400
H	-0.85373700	3.88688100	-0.00007500
C	2.89898600	-0.96570400	0.00007200
H	2.85128400	-1.64165700	0.86185600
H	2.85130900	-1.64178900	-0.86160800
C	4.12840200	-0.08909400	0.00000900
H	5.14023300	-0.47419400	0.00004000
Os	-0.37192500	-0.18211000	-0.00000200

2-isoindene E = -816.437189 a.u.

C	-0.37828800	1.85571200	-0.01757800
C	-1.60601000	2.41926700	-0.08689800
H	-1.74832000	3.49700900	-0.12944000
C	1.74682900	0.43942400	-0.06755800
Cl	-1.14713500	-2.64345800	0.41304100
P	-0.42965600	-0.58211700	-2.30870900
H	-1.17089400	-1.72502500	-2.71142100
H	-1.12520600	0.44434500	-3.00693400
H	0.71306900	-0.71808300	-3.15255900
P	-0.23825300	-0.32620000	2.41177800
H	0.17676700	0.83806000	3.12368600
H	-1.52705400	-0.51434100	2.97688200
H	0.49862900	-1.31850700	3.11764800
C	1.51126600	-1.73564400	-0.07542100
C	2.55870900	-0.73764000	-0.14264100
C	2.04975300	1.82986900	-0.04403300
C	0.84402900	2.65021300	0.00832400
C	3.16538800	2.60926200	-0.03566400
H	4.19861000	2.29044300	-0.06511900
C	-2.28757400	0.07786200	-0.05110300
C	-2.70158500	1.50056500	-0.11630500
C	-4.04962500	1.61633700	-0.19398200
H	-4.62806200	2.52963900	-0.24818700
C	3.79849800	-1.28750300	-0.23873500
H	4.76635700	-0.80530900	-0.29645300
C	2.07277400	-2.95692200	-0.12720300
H	1.58764600	-3.92257600	-0.08995100
C	-4.63302500	0.23199900	-0.19611300
H	-5.32349600	0.06635800	0.64414000
H	-5.21894900	0.02885000	-1.10499200
C	2.71711100	4.04262100	0.03317400
H	3.12984400	4.54619100	0.92044900
H	3.09443600	4.61790700	-0.82591000
C	3.58662700	-2.78495200	-0.23779500
H	4.12272000	-3.25325900	0.60131300
H	4.00491700	-3.24332200	-1.14621900
C	-3.41943800	-0.66470400	-0.10486600
H	-3.49045400	-1.74119400	-0.07464800
C	1.20852800	3.95604500	0.05935800
H	0.56682200	4.82490000	0.11034400
Os	-0.13435900	-0.34538700	0.03420900

2-indene E = -816.4806191 a.u.

C	0.36539800	1.79327600	-0.00027300
C	1.63517000	2.35387800	-0.00030000
H	1.79165900	3.43141600	-0.00043900

C	-1.79561300	0.45396100	-0.00015100
Cl	1.18540100	-2.69654500	0.00041200
P	0.15970600	-0.36749200	2.36277100
H	0.89243200	-1.39014200	3.02964200
H	0.65699900	0.77147200	3.06152000
H	-1.09538400	-0.50973900	3.02616000
P	0.15976000	-0.36834300	-2.36266600
H	0.65649600	0.77062400	-3.06180800
H	0.89301200	-1.39086000	-3.02916000
H	-1.09524500	-0.51145500	-3.02602800
C	-1.54518600	-1.66119200	0.00028200
C	-2.55032200	-0.73707400	0.00005500
C	-2.13202200	-2.98999900	0.00052300
H	-1.58199100	-3.92058100	0.00072900
C	-3.48547500	-2.85528200	0.00043200
H	-4.20089800	-3.66873700	0.00055900
C	-2.00772700	1.82749800	-0.00037800
C	-0.81166400	2.55438600	-0.00043600
C	-3.13599200	2.76125700	-0.00054800
H	-4.18121200	2.48018200	-0.00054700
C	-2.66010100	4.02233700	-0.00070700
H	-3.25526400	4.92650900	-0.00085500
C	-1.14126100	4.03109800	-0.00065200
H	-0.73621800	4.55001600	0.87668500
H	-0.73615500	4.54978000	-0.87810100
C	-3.90366000	-1.39577400	0.00012700
H	-4.51421500	-1.15277000	0.87915900
H	-4.51414300	-1.15311600	-0.87905000
C	2.26637500	0.08637000	0.00003300
C	2.68363200	1.42203200	-0.00013200
C	4.14288700	1.51713400	-0.00009700
H	4.70846500	2.44120500	-0.00020400
C	4.65083300	0.27030200	0.00009700
H	5.70028800	0.00447700	0.00017500
C	3.53053300	-0.74140800	0.00019100
H	3.56374100	-1.41745300	0.86255200
H	3.56380000	-1.41767400	-0.86199600
Os	0.18296300	-0.35251500	0.00005300

3 E = -465.7769319 a.u.

C	-1.82440700	-0.49044300	0.01381200
C	-2.18375300	-1.82796000	0.03828900
H	-3.22589100	-2.14282900	0.04935300
C	-0.80801700	1.80478500	0.01389000
P	0.00679900	-0.01714700	-2.38418000
H	1.15646100	0.05109600	-3.22344200
H	-0.64278200	-1.13569300	-2.97291800
H	-0.75121200	1.04275400	-2.95330800
P	0.13165400	0.02279700	2.39245300
H	-0.86587900	-0.78867000	2.99687600
H	1.25487500	-0.38084800	3.17035000
H	-0.14248900	1.26979800	3.02008300
C	1.30266800	1.92564600	-0.02980800
C	0.24457800	2.76243300	0.00034900
C	-2.19025900	1.84093300	0.01647200
C	-2.74991300	0.56321100	0.01441600
C	0.12635000	-2.13648000	0.04580800
C	-1.10539600	-2.73879800	0.05698300
H	0.99025900	-2.80074900	0.06481000
H	-1.24823800	-3.81494100	0.07861100
H	-3.82301900	0.38423200	0.01653600
H	-2.76688400	2.76095200	0.01628700
H	2.34813000	2.22778300	-0.06129200
H	0.19563200	3.84998400	0.00685200
Ru	0.24749600	-0.00976700	-0.00052000
P	2.64873100	-0.55724900	-0.07026200
H	3.39447000	-0.07337700	-1.18165200
H	3.47068100	-0.05283900	0.97635600
H	3.08721100	-1.91285600	-0.07203200

3-4MR-isoindene E = -581.3133754 a.u.

C	-1.84091400	1.28304700	0.00015200
C	-3.17002300	0.89457500	0.00026300
H	-3.98484100	1.61601900	0.00029600
C	0.63702000	1.58977300	-0.00002500
P	-0.42826700	-0.11382900	-2.39082900
H	0.29614900	-1.04896500	-3.18431800
H	-1.70568300	-0.22286600	-3.00457200
H	0.03124500	1.09422800	-2.98352200
P	-0.42789100	-0.11379700	2.39096100
H	-1.70525000	-0.22254200	3.00487300
H	0.29640800	-1.04910200	3.18436000
H	0.03197700	1.09415200	2.98359700
C	1.88620000	-0.29281000	-0.00011100
C	2.00001300	1.16030200	-0.00006200
C	-0.03325100	2.79783900	0.00003800
C	-1.41738200	2.61890000	0.00009700
C	-2.21768000	-1.23848400	0.00024000

C	-3.37489100	-0.49990500	0.00029300
C	3.29768900	1.56805400	0.00002600
H	3.69750000	2.57318700	0.00003900
C	3.12582500	-0.82167400	-0.00010100
H	3.44243300	-1.85713900	-0.00004300
C	4.13518800	0.31851500	-0.00126800
H	4.80027900	0.28309000	0.87313100
H	4.79851900	0.28329000	-0.87703200
H	-2.33392700	-2.32192600	0.00024700
H	-4.36497800	-0.94628300	0.00035900
H	-2.12498600	3.44548500	0.00014000
H	0.45520300	3.76727200	0.00002900
Ru	-0.34626300	-0.25657300	0.00006200
P	0.42226100	-2.56335600	0.00002500
H	1.23745900	-2.98602900	-1.08413300
H	1.23752400	-2.98602200	1.08413700
H	-0.52777000	-3.63071100	0.00005300

3-4MR-indene E = -581.3201038 a.u.

C	-1.77574600	1.33483200	0.00018500
C	-3.11342600	1.01092900	0.00026800
H	-3.89058100	1.77316000	0.00036900
C	0.72736000	1.56785700	0.00011700
P	-0.45156300	-0.10234800	-2.38547700
H	-0.02690200	-1.19159900	-3.20115100
H	-1.72967300	0.12735400	-2.96214900
H	0.29248900	0.93966700	-3.00635000
P	-0.45114800	-0.10292200	2.38552900
H	-1.72899600	0.12774600	2.96239400
H	-0.02739800	-1.19280900	3.20082500
H	0.29389700	0.93822700	3.00667000
C	1.87184600	-0.27990600	-0.00013500
C	2.03870200	1.08507700	0.00001700
C	3.18780500	-0.89467400	-0.00028000
H	3.41790800	-1.95216500	-0.00041700
C	4.12478300	0.09391000	-0.00020200
H	5.19666800	-0.05997600	-0.00026300
C	0.07966600	2.80321800	0.00022300
C	-1.29642400	2.66406700	0.00025500
C	3.49460900	1.46347100	-0.00001300
H	3.80145900	2.04596200	-0.87747200
H	3.80154900	2.04576300	0.87754500
C	-2.28558400	-1.16996500	0.00013200
C	-3.39671900	-0.38025900	0.00024500
H	-2.44355100	-2.24757100	0.00012100
H	-4.40974700	-0.77149100	0.00030900
H	-1.97946300	3.51094200	0.00033200
H	0.59746700	3.75712100	0.00026500
Ru	-0.34965100	-0.25819100	0.00000200
P	0.28963200	-2.62467000	-0.00035800
H	1.08936800	-3.09212700	-1.08037900
H	1.08942000	-3.09244200	1.07948900
H	-0.70431100	-3.64759600	-0.00048000

3-5MR1-isoindene E = -581.2865366 a.u.

C	0.93734900	1.24616400	0.08681800
C	0.62723000	2.55785100	0.21695200
H	1.39212100	3.32804100	0.29396200
C	0.98536300	-1.37207300	0.11399300
P	-0.31216100	0.23851100	-2.33694000
H	-1.08288900	-0.40795800	-3.34976700
H	-0.45227200	1.58662700	-2.76035000
H	0.98629000	-0.05620000	-2.83630500
P	-0.85003300	-0.12351500	2.37767900
H	-0.17955300	0.95602300	3.01051600
H	-2.12377500	-0.01614200	3.00517400
H	-0.32464700	-1.21872900	3.12482400
C	-0.84184100	-2.30769700	-0.13783200
C	0.45147200	-2.66903400	0.11223700
C	2.27793200	-0.79727700	0.07020000
C	2.27155800	0.66785600	0.03569300
C	3.56142100	-1.27293500	0.04924300
H	3.88910000	-2.30379400	0.06432700
C	-1.61799300	1.81688600	0.21551700
C	-0.77384800	2.86903900	0.28782500
C	4.47499600	-0.09061300	-0.00386900
H	5.16559600	-0.09053700	0.85373200
H	5.13206200	-0.13834100	-0.88584500
C	3.55606900	1.10429400	-0.01614700
H	3.91238600	2.12398400	-0.05245700
H	-2.68360200	2.02395700	0.31879400
H	-1.12525400	3.89105500	0.40775200
H	-1.64413500	-3.00085400	-0.39075000
H	0.93030500	-3.64273500	0.18310500
Ru	-0.71897400	-0.16569200	-0.01051800
P	-3.12098700	-0.43568500	-0.39048400
H	-3.66086600	-1.70954500	-0.72958900
H	-3.99064000	-0.09114200	0.68242100

H	-3.71591200	0.35231900	-1.41435800

3-5MR1-indene E = -581.3160783 a.u.

C	1.01578400	1.18134700	0.01723700
C	0.83277400	2.55173700	0.04907900
H	1.66873600	3.24899200	0.06401200
C	0.90046700	-1.37560400	0.00072400
P	-0.51892200	0.06433700	-2.38013300
H	-1.55670500	-0.41441300	-3.23226600
H	-0.33102600	1.35149300	-2.95314100
H	0.57988400	-0.62928500	-2.95879300
P	-0.60363000	-0.05111400	2.38769300
H	-0.02966200	1.09772700	2.99650400
H	-1.78332600	-0.15710400	3.18045000
H	0.17081500	-1.07348800	3.00410000
C	-1.03010700	-2.24512900	-0.04056600
C	0.25865300	-2.64494200	-0.01872500
C	2.19254000	-0.88541900	0.00253000
C	2.25065100	0.52178100	0.00976900
C	3.55676300	-1.42179900	-0.00402400
H	3.81801600	-2.47086900	-0.01020100
C	4.42169800	-0.39020700	0.00027800
H	5.50084500	-0.46880100	-0.00149000
C	3.69924800	0.94298600	0.00914400
H	3.95286600	1.55559200	-0.86430600
H	3.95685300	1.54595000	0.88815300
C	-1.42821200	1.96064900	0.05490000
C	-0.51316700	2.98064100	0.06997600
H	-1.89690400	-2.90298800	-0.07242900
H	0.68895000	-3.64491100	-0.02113800
H	-2.47784900	2.25232900	0.07656100
H	-0.78926700	4.03074400	0.09640000
Ru	-0.74094500	-0.05504500	-0.00064200
P	-3.16500100	-0.43065900	-0.06242100
H	-3.68424200	-1.16840900	-1.16337000
H	-3.74104300	-1.19162500	0.99382300
H	-4.07460600	0.66634300	-0.07363700

3-5MR2-isoindene E = -581.313705 a.u.

C	-0.05350400	1.84183600	0.00001800
C	1.24637800	2.28162400	-0.00015400
H	1.49722200	3.34064300	-0.00016200
C	-2.33148600	0.78843300	0.00033100
P	-0.44591500	-0.13698700	2.39005600
H	0.12570600	-1.20331400	3.14289800
H	0.26335800	0.94884700	2.97155000
H	-1.68428100	-0.01661200	3.08346600
P	-0.44659500	-0.13683600	-2.38995700
H	0.26236300	0.94913600	-2.97157900
H	0.12496700	-1.20303200	-3.14302900
H	-1.68517100	-0.01658800	-3.08301400
C	-2.36093900	-1.29643400	0.00030600
C	-3.25477300	-0.27265000	0.00044900
C	-2.39909000	2.17628300	0.00034900
C	-1.13999800	2.75058800	0.00018700
C	1.73972300	-0.13311800	-0.00018400
C	2.23671400	1.26884100	-0.00025300
C	3.59844100	1.31379700	-0.00035800
H	4.22311200	2.19739200	-0.00040600
C	4.10673200	-0.08896000	-0.00042600
H	4.74269200	-0.28985500	-0.87457000
H	4.74286200	-0.28987200	0.87359000
C	2.84202900	-0.91956000	-0.00031800
H	2.91063100	-1.99959300	-0.00034400
H	-2.61523500	-2.35494200	0.00031400
H	-4.34269700	-0.26529600	0.00060300
H	-3.33142000	2.73224300	0.00048000
H	-0.97802000	3.82651900	0.00016500
P	0.23981200	-2.60372900	-0.00018200
H	1.03861600	-3.06233900	-1.08339700
H	1.03879900	-3.06252000	1.08282100
H	-0.74624400	-3.63038000	-0.00017900
Ru	-0.48132100	-0.26593700	0.00005400

3-5MR2-indene E = -581.3159129 a.u.

C	-0.06226300	1.84788900	-0.00000900
C	1.25730000	2.27355100	-0.00001400
H	1.51354600	3.33163300	-0.00001700
C	-2.31567900	0.74373700	-0.00001900
P	-0.48381500	-0.07906000	2.38709000
H	0.00572700	-1.14850400	3.19217400
H	0.25048100	0.99048600	2.96726800
H	-1.74627900	0.11386900	3.01391100
P	-0.48386300	-0.07916500	-2.38708300
H	0.25008000	0.99060800	-2.96728800
H	0.00605700	-1.14847300	-3.19211900
H	-1.74638200	0.11331400	-3.01393400
C	-2.34645800	-1.35329000	0.00005800

C	-3.23360900	-0.34088600	0.00001200
C	-2.40404800	2.11887100	-0.00003300
C	-1.14685300	2.72923600	-0.00002500
C	1.71489800	-0.05184600	-0.00003200
C	2.21884000	1.25192600	-0.00001900
C	3.68294100	1.26091600	-0.00002200
H	4.29857000	2.15066300	-0.00001100
H	-2.57372100	-2.41614100	0.00011200
H	-4.32186100	-0.33878800	0.00000900
H	-3.34687600	2.65732500	-0.00004100
H	-1.00891600	3.80821600	-0.00003200
C	2.93755000	-0.95330900	-0.00001100
H	2.96173100	-1.61705800	0.87472300
H	2.96167200	-1.61710600	-0.87470900
C	4.11636900	-0.00961700	-0.00011300
H	5.14506700	-0.34375200	-0.00016200
Ru	-0.44788100	-0.25211500	0.00000600
P	0.24653600	-2.62180000	0.00006000
H	1.04859700	-3.09325400	-1.07744200
H	1.04854700	-3.09320400	1.07762100
H	-0.73603900	-3.64946500	0.00006100

3-isoindene E = -812.3575346 a.u.

C	-0.46598200	1.77500000	-0.03748400
C	-1.72376700	2.25691100	-0.10494300
H	-1.93317500	3.32219800	-0.17393200
C	1.73383100	0.38755700	-0.07513400
P	-0.42234300	-0.58570400	-2.27402500
H	-1.06804000	-1.74318300	-2.79154100
H	-1.19082500	0.42980800	-2.90059400
H	0.73412000	-0.57848300	-3.10783600
P	-0.19992500	0.14932700	2.42502300
H	0.61333200	1.23800000	2.84120900
H	-1.45444700	0.56229400	2.94854500
H	0.16920000	-0.80032900	3.42537800
C	1.51932600	-1.85036200	-0.04835500
C	2.51722300	-0.79432000	-0.15525600
C	1.97921200	1.77929000	-0.09306000
C	0.75126600	2.57801000	-0.04622800
C	3.07758400	2.59568800	-0.12011800
H	4.11927000	2.30576200	-0.15531400
C	-2.34058800	-0.13516300	-0.07260200
C	-2.77567000	1.28464600	-0.14080300
C	-4.11973000	1.36388900	-0.28863100
H	-4.71571800	2.26306700	-0.36802000
C	3.77670000	-1.29687700	-0.31204700
H	4.71478500	-0.76816600	-0.42009200
C	2.14515300	-3.03902600	-0.14181300
H	1.73990800	-4.04253900	-0.10883200
C	-4.67394700	-0.02664100	-0.36100800
H	-5.41335500	-0.22931800	0.42641000
H	-5.19582200	-0.20874600	-1.31123800
C	2.59290900	4.01073100	-0.08331900
H	3.01042600	4.54889800	0.78148500
H	2.95399400	4.57184500	-0.95903800
C	3.64021100	-2.79199700	-0.31097700
H	4.23061700	-3.23919400	0.50217100
H	4.04511200	-3.22625100	-1.23628000
C	-3.44825600	-0.89918200	-0.22278100
H	-3.53446100	-1.97743900	-0.25281400
C	1.08895000	3.89104700	-0.03545300
H	0.43021400	4.74739400	-0.00283100
Ru	-0.15952600	-0.41062500	0.09144900
P	-0.94309000	-2.62303000	0.66669900
H	-2.23488800	-2.81726300	1.22962800
H	-0.99357800	-3.59215800	-0.37373100
H	-0.17371300	-3.34279900	1.61814300

3-indene E = -812.3937115 a.u.

C	-0.42382400	1.71527000	-0.00037900
C	-1.69909500	2.22911900	-0.00124800
H	-1.88836900	3.30103600	-0.00182500
C	1.77399200	0.40419200	0.00114600
P	-0.17484400	-0.25296500	-2.37921100
H	-0.73396200	-1.28423100	-3.19045900
H	-0.85679600	0.86008800	-2.94162900
H	1.08413600	-0.12417100	-3.03141300
P	-0.17467900	-0.25327500	2.37985500
H	-0.84659300	0.86619900	2.94162800
H	-0.74436400	-1.27911300	3.19062800
H	1.08482600	-0.13636700	3.03331800
C	1.59515400	-1.74866700	-0.00067800
C	2.54440800	-0.75957000	0.00063800
C	2.28082900	-3.03052400	-0.00249500
H	1.83805900	-4.01746000	-0.00403600
C	3.62273800	-2.80118000	-0.00213600
H	4.38788400	-3.56716700	-0.00315400
C	1.95635200	1.78083300	0.00119900

C	0.74974300	2.48747700	0.00023800
C	3.07323700	2.72989100	0.00159100
H	4.12177600	2.46567600	0.00230700
C	2.57204800	3.98000700	0.00098800
H	3.14945300	4.89501600	0.00114300
C	1.05592000	3.96590200	0.00007300
H	0.64101900	4.47717400	-0.87680600
H	0.63997300	4.47759400	0.87621400
C	3.93737700	-1.32584800	-0.00002800
H	4.53032800	-1.03993900	-0.87754000
H	4.53028300	-1.04237300	0.87830300
C	-2.35148300	-0.05904200	-0.00021700
C	-2.73877000	1.27388700	-0.00126500
C	-4.19741900	1.40977600	-0.00210100
H	-4.73295200	2.35022700	-0.00300400
C	-4.74072800	0.18227700	-0.00149000
H	-5.79410400	-0.06307900	-0.00180000
C	-3.64699400	-0.85772000	0.00001300
H	-3.73505600	-1.51608600	-0.87445500
H	-3.73575100	-1.51384000	0.87611100
Ru	-0.19510400	-0.44081400	0.00031400
P	-1.13519300	-2.70455400	0.00107800
H	-1.98738600	-3.07893800	1.07788500
H	-1.98254300	-3.08160800	-1.07867900
H	-0.29545700	-3.84738600	0.00451500

4 E = -462.9912892 a.u.

C	1.86655700	-0.49240500	-0.06825000
C	2.23285900	-1.82934600	-0.18202000
H	3.27428500	-2.14070800	-0.22030800
C	0.84836300	1.78868300	0.09691700
P	0.06154800	-0.16881100	2.37677600
H	-1.07880800	-0.14061200	3.23014700
H	0.71234900	-1.32726700	2.88082300
H	0.83801800	0.85563400	2.98314800
P	-0.13548700	0.26467100	-2.37610700
H	1.04123200	-0.18759400	-3.03171000
H	-1.11688000	-0.35572400	-3.20041300
H	-0.21706100	1.59832900	-2.86470800
C	-1.27170000	1.90318600	0.19602000
C	-0.21439100	2.74300900	0.20405400
C	2.23144100	1.83423000	0.07632000
C	2.79368700	0.55858000	-0.01243700
C	-0.07745600	-2.11761200	-0.19048500
C	1.15592200	-2.73083400	-0.24884900
H	-0.93714000	-2.78514100	-0.24384500
H	1.28854800	-3.80359200	-0.34024000
H	3.86583900	0.38171900	-0.04096800
H	2.80679900	2.75243500	0.13344400
H	-2.31476600	2.20255900	0.27431800
H	-0.16856000	3.82714500	0.27656700
P	-2.60469500	-0.58667700	0.04746400
H	-3.33706000	-0.21362600	1.20873300
H	-3.44058000	-0.00032200	-0.94269300
H	-3.01367000	-1.94493300	-0.06841000
Os	-0.20282500	-0.01711800	0.00021700

4-4MR-isoindene E = -578.5302212 a.u.

C	1.78359000	1.33891600	0.03103700
C	3.12010600	0.96509100	0.05815300
H	3.92805300	1.69220900	0.07952400
C	-0.69180800	1.62663000	0.01381800
P	0.29569000	-0.15381700	2.39306600
H	-0.12972200	-1.29925200	3.12420700
H	1.54440800	0.08928900	3.02584700
H	-0.51192700	0.83774300	3.01347400
P	0.39786600	-0.01153300	-2.38808100
H	1.65698700	-0.24018500	-3.00692000
H	-0.43181200	-0.83411700	-3.20229000
H	0.07338700	1.26437600	-2.92277700
C	-1.92019200	-0.25627400	-0.00884100
C	-2.06092800	1.19655400	0.00770600
C	-0.03101500	2.84239000	0.02227500
C	1.35434400	2.67365200	0.03027600
C	2.16794500	-1.16831300	0.03837600
C	3.32912200	-0.42488900	0.06390800
C	-3.36226000	1.58110000	0.01729600
H	-3.77884300	2.57925100	0.03175600
C	-3.15230200	-0.80487000	-0.01106300
H	-3.45108600	-1.84573300	-0.02041700
C	-4.18153400	0.31697900	0.00424600
H	-4.84644600	0.28002600	-0.87014000
H	-4.84363500	0.25967500	0.87960700
H	2.30049400	-2.24959600	0.04470900
H	4.31776500	-0.87202900	0.08580600
H	2.05648000	3.50362500	0.03843300
H	-0.52695700	3.80724000	0.02311200
P	-0.43343700	-2.54397800	-0.09960300

H	-1.25092300	-3.01366000	0.96335700
H	-1.23831900	-2.92342400	-1.20673600
H	0.53607700	-3.58984600	-0.13564300
Os	0.29689200	-0.21220400	-0.00169400

4-4MR-indene E = -578.532667 a.u.

C	-1.72631300	1.37476100	0.00315100
C	-3.07140200	1.05801500	0.01600000
H	-3.84510700	1.82246200	0.01588000
C	0.77273700	1.60182000	0.01940600
P	-0.40929400	-0.02005700	-2.37598700
H	0.17528000	-1.01693000	-3.21027400
H	-1.70495900	0.04529700	-2.95641900
H	0.18990700	1.13749000	-2.94477900
P	-0.30116200	-0.08583700	2.39035600
H	-1.40294100	0.58426400	2.98752300
H	-0.29861700	-1.27423800	3.17600400
H	0.78550300	0.60051900	3.00169900
C	1.91022700	-0.24621100	-0.01738000
C	2.09284800	1.11459800	0.01013900
C	3.21928800	-0.87769500	-0.05102500
H	3.43747400	-1.93752800	-0.07845300
C	4.16825700	0.09835300	-0.03948500
H	5.23804500	-0.06715900	-0.05351200
C	0.13096700	2.84067700	0.01583900
C	-1.24823000	2.70386200	0.00315800
C	3.55109200	1.47456700	-0.00042800
H	3.85335000	2.07303500	-0.86885300
H	3.87730200	2.03449900	0.88482900
C	-2.23172100	-1.11470400	0.04161100
C	-3.35374800	-0.32824700	0.03686500
H	-2.40086800	-2.19052900	0.06183800
H	-4.36352600	-0.72472800	0.04992100
H	-1.92925100	3.55129800	-0.00278100
H	0.64964600	3.79335200	0.01553400
P	0.31799700	-2.59516400	-0.04893700
H	1.09999800	-3.04099200	-1.15034800
H	1.12310600	-3.09318900	1.01273300
H	-0.69604200	-3.59521100	-0.06074400
Os	-0.30507100	-0.21558700	0.00541600

4-5MR1-isoindene E = -578.5000732 a.u.

C	1.06710300	1.26006300	0.00635500
C	0.79279700	2.58951400	0.01317900
H	1.57571100	3.34388000	0.01679600
C	1.08514500	-1.34151400	-0.00134700
P	-0.49002700	0.04978900	-2.38496100
H	-1.69967700	0.10536600	-3.13476600
H	0.16301800	1.20570800	-2.88722900
H	0.18298000	-0.97376800	-3.11260500
P	-0.50335900	0.02001200	2.38623800
H	0.18461300	1.14767600	2.90608200
H	-1.71669000	0.10992000	3.12645600
H	0.12852700	-1.03346800	3.10816600
C	-0.79124400	-2.26375600	-0.01205300
C	0.52380700	-2.63562400	-0.00711700
C	2.39027800	-0.79531000	-0.00022100
C	2.39835600	0.67095600	0.00329900
C	3.66869300	-1.28409800	-0.00245200
H	3.98674800	-2.31789600	-0.00514500
C	-1.46093700	1.89213400	0.01159200
C	-0.59999800	2.93714600	0.01604200
C	4.59369300	-0.10913300	-0.00069200
H	5.26873900	-0.13969600	0.86847000
H	5.26609800	-0.13582300	-0.87210100
C	3.68847400	1.09528200	0.00302900
H	4.05643700	2.11151200	0.00490900
H	-2.52293200	2.13933700	0.01512700
H	-0.93388600	3.97094600	0.02189100
H	-1.63225800	-2.95526700	-0.02100100
H	0.99327400	-3.61510400	-0.00927800
P	-3.04531800	-0.37935000	-0.01076700
H	-3.62262800	-1.67922800	-0.01840400
H	-3.75797300	0.20494200	1.07274300
H	-3.74907400	0.21368500	-1.09541100
Os	-0.60167700	-0.12044000	-0.00026400

4-5MR1-indene E = -578.530247 a.u.

C	1.13297600	1.18698700	0.07954100
C	0.96477800	2.56264000	0.16869200
H	1.80622300	3.25077900	0.20603200
C	1.00005000	-1.35511300	-0.07990100
P	-0.43211700	0.20086900	-2.37014300
H	-1.54078300	-0.08498800	-3.21873100
H	-0.08754300	1.49030600	-2.85879000
H	0.55920500	-0.59546900	-3.00669700
P	-0.45650500	-0.26921900	2.37325500
H	0.59099800	0.45762900	3.00101800

H	-1.53860600	0.10698000	3.21920300
H	-0.20292200	-1.57713100	2.87411200
C	-0.94421700	-2.21207500	-0.20069200
C	0.34254900	-2.62141300	-0.19734100
C	2.29907100	-0.88074500	-0.04662600
C	2.36533800	0.52533000	0.03973800
C	3.65911900	-1.42195700	-0.09087500
H	3.91518400	-2.47011900	-0.16020500
C	4.53043500	-0.39718000	-0.02892500
H	5.60905000	-0.48215400	-0.03912700
C	3.81599000	0.93733800	0.06159700
H	4.07431000	1.59970400	-0.77324000
H	4.08086600	1.48299400	0.97525200
C	-1.29210600	1.96817500	0.15725300
C	-0.37378400	2.99418800	0.20934300
H	-1.81238300	-2.86195400	-0.28753500
H	0.76494400	-3.62083800	-0.26934900
H	-2.33778800	2.27211100	0.19201600
H	-0.65192400	4.04064200	0.27958700
P	-3.06434700	-0.37833800	-0.04234100
H	-3.61474600	-0.95579900	-1.22101600
H	-3.62946700	-1.26095900	0.91942100
H	-3.94208100	0.73190100	0.11000400
Os	-0.62827900	-0.03342600	0.00283700

4-5MR2-isoindene E = -578.5262359 a.u.

C	0.04638200	1.87768100	-0.00011600
C	1.35026700	2.30894200	-0.00026400
H	1.61165800	3.36464800	-0.00034200
C	-2.24096200	0.86157700	0.00028300
P	-0.39839200	-0.09818600	2.38594200
H	0.28866900	-1.09467300	3.13743000
H	0.17490300	1.06506000	2.96828300
H	-1.65435100	-0.12245600	3.05797700
P	-0.39912900	-0.09804600	-2.38590900
H	0.17345400	1.06549700	-2.96836100
H	0.28813900	-1.09416600	-3.13769700
H	-1.65528300	-0.12283000	-3.05756400
C	-2.28703500	-1.22862500	0.00032300
C	-3.17540800	-0.19183400	0.00047100
C	-2.29502600	2.25353100	0.00017800
C	-1.02851500	2.80733900	-0.00003500
C	1.80672400	-0.11110000	-0.00002300
C	2.32852300	1.28344100	-0.00020100
C	3.68965300	1.30811100	-0.00015300
H	4.32660600	2.18285600	-0.00023400
C	4.17779000	-0.10177700	-0.00001000
H	4.81132200	-0.31116800	-0.87396500
H	4.81134300	-0.31095400	0.87397800
C	2.90075800	-0.91188400	0.00011500
H	2.95482900	-1.99272600	0.00027600
H	-2.56248200	-2.28159800	0.00032300
H	-4.26186100	-0.17641200	0.00065100
H	-3.21868600	2.82231800	0.00026900
H	-0.84758700	3.87931400	-0.00015400
P	0.29311600	-2.57231700	-0.00035300
H	1.08424200	-3.03759900	-1.08575900
H	1.08396600	-3.03810700	1.08504100
H	-0.71908900	-3.57049700	-0.00069700
Os	-0.40477100	-0.21882400	0.00002600

4-5MR2-indene E = -578.530001 a.u.

C	0.04068700	1.88804200	-0.00005600
C	1.36782900	2.30605600	-0.00005400
H	1.63748800	3.35968100	-0.00005700
C	-2.21940200	0.81274800	-0.00001700
P	-0.45541400	-0.04568200	2.38453000
H	0.25228400	-0.98412700	3.18983500
H	0.02495600	1.16209100	2.95873900
H	-1.74006000	-0.13346500	2.98932100
P	-0.45560100	-0.04579600	-2.38452800
H	0.02397200	1.16227500	-2.95877700
H	0.25267500	-0.98379900	-3.18983800
H	-1.74021200	-0.13440800	-2.98927400
C	-2.28149200	-1.29543000	0.00012400
C	-3.15417100	-0.26851900	0.00006500
C	-2.29756600	2.19058300	-0.00007600
C	-1.03211900	2.78553800	-0.00008900
C	1.76674600	-0.02665100	0.00001000
C	2.30676200	1.26964900	-0.00001000
C	3.76862400	1.24135300	0.00005400
H	4.40519800	2.11617500	0.00006900
H	-2.53329700	-2.35238900	0.00020400
H	-4.24128600	-0.25276700	0.00008100
H	-3.23303000	2.74032500	-0.00009400
H	-0.87989600	3.86167300	-0.00013100
C	2.97229300	-0.95511500	0.00002600
H	2.98354500	-1.61784500	0.87550000

H	2.98357100	-1.61782800	-0.87546100
C	4.17219200	-0.03863100	0.00003500
H	5.19254600	-0.39717600	0.00004300
P	0.29459000	-2.58830300	-0.00001700
H	1.08558900	-3.07306600	-1.07926200
H	1.08544700	-3.07312100	1.07931000
H	-0.72029300	-3.58073500	-0.00011100
Os	-0.36914600	-0.20345400	0.00000100

4-isoindene E = -809.5724296 a.u.

C	-0.42770400	1.82956300	-0.03942600
C	-1.67793300	2.33776700	-0.09436200
H	-1.87087900	3.40593700	-0.15121800
C	1.75321900	0.43002500	-0.07180600
P	-0.39244300	-0.52287700	-2.29762500
H	-1.08729300	-1.64869200	-2.82068000
H	-1.10508500	0.53379100	-2.92268400
H	0.77986600	-0.56899800	-3.10535700
P	-0.17841300	0.14753900	2.41875700
H	0.61692100	1.24888600	2.83408300
H	-1.43750400	0.51925400	2.96308600
H	0.22907500	-0.81833400	3.38688700
C	1.52326600	-1.79079100	-0.06813000
C	2.54388700	-0.75379400	-0.15118800
C	2.01614200	1.82131000	-0.08777900
C	0.79392900	2.62810300	-0.04681100
C	3.11934300	2.62731200	-0.11561000
H	4.15878900	2.32948700	-0.14891700
C	-2.31028500	-0.04521800	-0.07648000
C	-2.74125500	1.37783500	-0.13264000
C	-4.08472300	1.46785000	-0.27587100
H	-4.67431100	2.37203100	-0.34449700
C	3.79280000	-1.27510600	-0.29484400
H	4.74099900	-0.76194700	-0.38728200
C	2.12960200	-2.99058700	-0.16313600
H	1.70591900	-3.98692700	-0.14698000
C	-4.64886300	0.08235800	-0.36079900
H	-5.38972100	-0.12380400	0.42454300
H	-5.17306600	-0.08800900	-1.31204500
C	2.64521900	4.04758100	-0.08646400
H	3.06328400	4.58787600	0.77645700
H	3.00972200	4.60193500	-0.96484800
C	3.63165400	-2.77067300	-0.30896400
H	4.20268500	-3.23651600	0.50722800
H	4.03932100	-3.20363500	-1.23345600
C	-3.42926700	-0.79734600	-0.23189800
H	-3.52448800	-1.87447400	-0.27393700
C	1.14019200	3.93851900	-0.04166400
H	0.48723400	4.79962600	-0.01577200
P	-0.96186000	-2.58438300	0.60629200
H	-2.24947400	-2.76253800	1.17915300
H	-1.03151600	-3.53645600	-0.44920500
H	-0.18391700	-3.31895300	1.53820100
Os	-0.14383100	-0.35607900	0.07425200

4-indene E = -809.607021 a.u.

C	-0.46963700	1.76873000	0.01894700
C	-1.76345100	2.25614000	-0.01765100
H	-1.98373100	3.32072900	-0.04518300
C	1.75087800	0.50488200	-0.05056000
P	-0.19822400	-0.29844600	-2.35118800
H	-0.82652200	-1.32988500	-3.10879500
H	-0.82392800	0.83336000	-2.94153500
H	1.06427600	-0.26771900	-3.00786900
P	-0.06652900	-0.06142400	2.39303000
H	0.85363500	0.92719200	2.83648600
H	-1.24387100	0.36914900	3.06584300
H	0.31256500	-1.13433800	3.25304700
C	1.63632800	-1.66323000	-0.04474500
C	2.55567200	-0.65039600	-0.09219800
C	2.35465700	-2.93040300	-0.06596100
H	1.93529800	-3.92780700	-0.04321000
C	3.68804700	-2.66773300	-0.13082600
H	4.47244100	-3.41245900	-0.16990000
C	1.90793800	1.88377100	-0.03716500
C	0.68338000	2.56753500	0.00561600
C	3.00139200	2.85795500	-0.06022600
H	4.05530900	2.61815300	-0.09531000
C	2.47397900	4.09708400	-0.03277100
H	3.03200700	5.02399100	-0.04203000
C	0.95903700	4.05135100	0.01295300
H	0.50788000	4.56553700	-0.84416700
H	0.56148300	4.54543100	0.90759300
C	3.95883400	-1.18337100	-0.15205500
H	4.50571500	-0.88785000	-1.05605700
H	4.58189200	-0.87730200	0.69753800
C	-2.30439000	-0.05348900	-0.01746600
C	-2.76100700	1.26652100	-0.04749500

C	-4.22043700	1.32739100	-0.12840200
H	-4.80260800	2.23913900	-0.15873100
C	-4.69987000	0.07369400	-0.15928200
H	-5.73840100	-0.22309700	-0.21593400
C	-3.55942600	-0.91139000	-0.07980900
H	-3.55621200	-1.59951700	-0.93595000
H	-3.66846400	-1.54490100	0.81029600
P	-0.87678900	-2.71903300	0.24163000
H	-2.22382700	-3.10754800	0.47038900
H	-0.58441300	-3.58683200	-0.84713500
H	-0.26143600	-3.45637800	1.28897300
Os	-0.18680900	-0.37465500	0.03163300

5 E = -570.8209338 a.u.

C	1.78007400	-0.44436300	-0.00022700
C	2.16521700	-1.77382600	-0.00040100
H	3.21298400	-2.06985900	-0.00052300
C	0.69751500	1.82607800	0.00009300
P	-0.13933600	-0.01677500	2.40255800
H	-1.20802700	-0.55011800	3.17361300
H	0.95002900	-0.73402000	2.96320000
H	0.01800600	1.24356300	3.04120000
P	-0.14000300	-0.01599900	-2.40254700
H	0.95048000	-0.73123900	-2.96357600
H	-1.20794400	-0.55111900	-3.17340800
H	0.01496000	1.24471200	-3.04103800
C	-1.42136200	1.87724200	0.00052000
C	-0.38884800	2.74502700	0.00036900
C	2.07807000	1.89971100	-0.00006800
C	2.67450200	0.63629200	-0.00023700
C	-0.14442800	-2.16033700	-0.00030300
C	1.10856000	-2.71369600	-0.00044100
H	-0.99349400	-2.84097800	-0.00033600
H	1.28322200	-3.78554800	-0.00058100
H	3.75278900	0.49022000	-0.00036600
H	2.62953300	2.83510900	-0.00003700
H	-2.48293700	2.10239800	0.00079500
H	-0.38118900	3.83345500	0.00047100
Ru	-0.30742900	-0.02465300	0.00002900
C	-2.24157200	-0.56136700	0.00018500
O	-3.33347600	-0.86185400	0.00027600

5-4MR-isoindene E = -686.3592002 a.u.

C	-1.85967500	1.20435700	-0.04120700
C	-3.17425100	0.76939900	-0.05698800
H	-4.01487800	1.46003600	-0.08666000
C	0.62083200	1.56047800	-0.03793300
P	-0.39489200	-0.28233400	-2.39747900
H	-0.04569300	-1.46981400	-3.09575300
H	-1.64897400	0.00274400	-2.99879200
H	0.43814100	0.65234400	-3.07037200
P	-0.49006500	-0.06773200	2.40096000
H	-1.76241200	-0.29866200	2.98829400
H	0.32478000	-0.88748300	3.22864100
H	-0.18074100	1.21100700	2.93688000
C	1.89151000	-0.32280000	0.01868300
C	1.98678500	1.13225000	-0.02602300
C	-0.07479100	2.75355700	-0.06497100
C	-1.45884600	2.54789600	-0.06507800
C	-2.16873500	-1.35167700	-0.01245800
C	-3.33811600	-0.63332600	-0.04277300
C	3.28727400	1.53270700	-0.04156300
H	3.69069600	2.53590800	-0.07364000
C	3.11978600	-0.86336700	0.03262800
H	3.41458900	-1.90378700	0.06451600
C	4.12334900	0.28066500	-0.00412200
H	4.78798000	0.27279300	0.87116100
H	4.78661200	0.21896000	-0.87822000
H	-2.24046200	-2.43695400	-0.00511500
H	-4.31711200	-1.10374200	-0.05483400
H	-2.17844700	3.36420300	-0.08478900
H	0.39131200	3.73394000	-0.08328100
Ru	-0.33719800	-0.30245100	0.00919800
C	0.40253600	-2.14228100	0.10576100
O	0.81496700	-3.19997500	0.16266200

5-4MR-indene E = -686.3660071 a.u.

C	-1.77520900	1.27301300	0.01577400
C	-3.10434500	0.91874600	0.02998900
H	-3.89930500	1.66241500	0.04413500
C	0.73756600	1.53415500	0.03314700
P	-0.49361900	-0.06761800	-2.39019700
H	0.18040200	-0.98471400	-3.24412200
H	-1.79741100	-0.12255400	-2.94991900
H	-0.02464300	1.15684400	-2.93828900
P	-0.42862000	-0.22018600	2.39722000
H	-1.65070500	0.22948100	2.96302000
H	-0.23486900	-1.41124600	3.14983700

H	0.49423700	0.63409700	3.06172200
C	1.86723000	-0.31979900	-0.01087800
C	2.04624800	1.04417100	0.02831100
C	3.15734300	-0.96906300	-0.03736400
H	3.34926000	-2.03301700	-0.07050900
C	4.11150700	0.00447900	-0.01023800
H	5.18045100	-0.16900300	-0.01613900
C	0.07150500	2.76104600	0.04114700
C	-1.30428300	2.60750100	0.02905200
C	3.51102300	1.38857700	0.03337800
H	3.82831600	1.98901100	-0.82805000
H	3.83560200	1.93697100	0.92620300
C	-2.25601900	-1.26913800	0.02708300
C	-3.36610400	-0.47984900	0.03694400
H	-2.39087300	-2.34796200	0.03860700
H	-4.37546400	-0.88093700	0.05072200
H	-1.99281700	3.45020000	0.03200600
H	0.57613800	3.72204800	0.05183100
Ru	-0.33492100	-0.30777300	-0.00390400
C	0.19561600	-2.23158900	-0.07995700
O	0.51741500	-3.31825700	-0.12786700

5-5MR1-isoindene E = -686.3305499 a.u.

C	0.86782100	1.24658500	0.06044400
C	0.54010500	2.55661000	0.15372900
H	1.29334000	3.33930800	0.21718300
C	0.93143500	-1.37740500	0.10718100
P	-0.39289600	0.18162300	-2.36256000
H	-1.17806000	-0.50051200	-3.33599400
H	-0.54671100	1.52057300	-2.80526400
H	0.90429600	-0.12073900	-2.85767400
P	-0.88954300	-0.05236200	2.38417400
H	-0.26093700	1.08094300	2.96052000
H	-2.16160900	0.00817200	3.01504900
H	-0.29775600	-1.09829500	3.14968900
C	-0.92103800	-2.32404100	-0.07177400
C	0.38520100	-2.67077000	0.12402000
C	2.21814100	-0.79555800	0.07279700
C	2.20576400	0.67133700	0.02879300
C	3.50653200	-1.26490900	0.06471300
H	3.83923900	-2.29409000	0.08915200
C	-1.71448900	1.80995400	0.15162200
C	-0.86547800	2.85743300	0.20349600
C	4.41279300	-0.07897000	0.01243000
H	5.09839000	-0.07308300	0.87436300
H	5.07793400	-0.13009000	-0.86364400
C	3.48893900	1.11187800	-0.01370700
H	3.84195600	2.13255900	-0.05316400
H	-2.78401000	1.98234700	0.22213200
H	-1.22563600	3.87968300	0.29408400
H	-1.74648400	-3.01077800	-0.24513700
H	0.85973700	-3.64643500	0.19757200
Ru	-0.78690800	-0.17400900	-0.01645900
C	-2.73989000	-0.45442600	-0.30958700
O	-3.84352000	-0.63479500	-0.49547800

5-5MR1-indene E = -686.3612072 a.u.

C	-0.92508600	1.18723700	0.02111200
C	-0.69731900	2.55031300	0.05763800
H	-1.50911800	3.27540100	0.07773900
C	-0.86749500	-1.37821000	-0.00504100
P	0.67060300	-0.08150300	2.39611800
H	1.86586400	-0.14155500	3.16428000
H	0.05653500	1.05097400	2.99374200
H	-0.06502100	-1.13173200	3.01063600
P	0.57569900	0.05625100	-2.39384100
H	0.45709500	1.35773900	-2.95005200
H	1.59025200	-0.47849200	-3.23555000
H	-0.56389400	-0.57604800	-2.96057100
C	1.05368900	-2.28179500	-0.05382500
C	-0.24193300	-2.65606800	-0.03107500
C	-2.14785300	-0.85791400	0.00262900
C	-2.17456600	0.55301700	0.01550600
C	-3.52375300	-1.36273200	-0.00360500
H	-3.80875400	-2.40546800	-0.01368000
C	-4.36467000	-0.31142500	0.00665900
H	-5.44529900	-0.36529300	0.00687100
C	-3.61284800	1.00513600	0.01972800
H	-3.85459600	1.61061300	0.90166600
H	-3.85377600	1.62803100	-0.85013900
C	1.56332800	1.91271700	0.05784500
C	0.66209900	2.94318800	0.07754500
H	1.93375800	-2.91523000	-0.08875400
H	-0.68308500	-3.65107500	-0.03679100
H	2.62011000	2.17019400	0.07733700
H	0.96207400	3.98680300	0.10720600
Ru	0.80503000	-0.08676300	-0.00450700
C	2.77789600	-0.39979800	-0.05548500

O	3.89663500	-0.58006600	-0.08719800

5-5MR2-isoindene E = -686.361474941 a.u.

C	0.07047600	1.80372500	0.00010100
C	-1.23139200	2.24538000	0.00018800
H	-1.48525600	3.30364300	0.00027500
C	2.33896900	0.70238600	-0.00045600
P	0.43854400	-0.18764700	-2.40382800
H	-0.09223100	-1.28295300	-3.13897500
H	-0.30665200	0.87358400	-2.98312200
H	1.67926300	-0.02610400	-3.08172200
P	0.43891700	-0.18707000	2.40385500
H	-0.30971300	0.87173100	2.98315900
H	-0.08772200	-1.28401700	3.13954400
H	1.67932800	-0.02105300	3.08121600
C	2.32268300	-1.40298100	0.00001000
C	3.22975900	-0.39088900	-0.00049900
C	2.42800700	2.08704100	-0.00035300
C	1.17534900	2.68766700	-0.00000500
C	-1.73382100	-0.17280000	-0.00008700
C	-2.22173300	1.23085600	0.00011800
C	-3.58550000	1.26403900	0.00008900
H	-4.21653500	2.14318400	0.00019000
C	-4.08622500	-0.14295300	-0.00023300
H	-4.72295300	-0.34490000	0.87310600
H	-4.72284100	-0.34451500	-0.87374400
C	-2.82164700	-0.97282500	-0.00035200
H	-2.85934400	-2.05389200	-0.00056800
H	2.53529100	-2.46830100	0.00037400
H	4.31768800	-0.41394800	-0.00075700
H	3.36781700	2.63071300	-0.00047500
H	1.03958200	3.76759400	0.00015400
Ru	0.46789700	-0.31512000	-0.00000600
C	-0.15773100	-2.20188000	0.00046900
O	-0.49103300	-3.28567000	0.00090900

5-5MR2-indene E = -686.364538 a.u.

C	-0.04593400	-1.81333200	-0.00001600
C	1.28289900	-2.22378600	-0.00000100
H	1.55767100	-3.27711100	-0.00000300
C	-2.30314800	-0.67947000	0.00002700
P	-0.46208700	0.10302000	-2.39826800
H	-0.13296100	1.23223700	-3.19815900
H	0.40636100	-0.86282300	-2.97236700
H	-1.69720100	-0.26506800	-2.99748200
P	-0.46213700	0.10322000	2.39826800
H	0.40550500	-0.86333800	2.97238000
H	-0.13194900	1.23220900	3.19803900
H	-1.69752900	-0.26373600	2.99760700
C	-2.32394300	1.44503300	-0.00004500
C	-3.20294400	0.42617800	0.00001400
C	-2.39713800	-2.05155500	0.00002000
C	-1.14064000	-2.67872100	-0.00000800
C	1.69916500	0.10986700	0.00003500
C	2.22748300	-1.18576500	0.00002700
C	3.69201600	-1.14455600	0.00005400
H	4.33703800	-2.01302300	0.00005200
H	-2.52446100	2.51089400	-0.00009300
H	-4.29163200	0.43789100	0.00003700
H	-3.34232400	-2.58657100	0.00002100
H	-1.02144900	-3.76028100	-0.00001600
C	2.87981400	1.05173600	0.00007400
H	2.86884200	1.72042800	-0.87156300
H	2.86880300	1.72040400	0.87172900
C	4.08435300	0.14090300	0.00008700
H	5.10345900	0.50314800	0.00011400
Ru	-0.42856700	0.29691200	-0.00000900
C	0.07803400	2.22840400	-0.00007800
O	0.35400200	3.32842700	-0.00012700

5 Isoindene E = -917.4092932 a.u.

C	-0.49248000	1.74175100	-0.00580900
C	-1.76405700	2.19547400	-0.01794900
H	-2.00519200	3.25605800	-0.03593200
C	1.73494100	0.37112600	-0.02734100
P	-0.38244800	-0.35679800	-2.37174400
H	-0.91581000	-1.49709100	-3.03176900
H	-1.24075600	0.65678400	-2.86867900
H	0.77199400	-0.13750900	-3.17623400
P	-0.30031800	-0.11744200	2.40537400
H	0.60588400	0.80381500	2.99734600
H	-1.53600000	0.39126900	2.88066200
H	-0.12160000	-1.22431700	3.28285000
C	1.50538700	-1.88507900	0.00637100
C	2.50694200	-0.82321500	-0.03527400
C	1.96165400	1.76523300	-0.03794000
C	0.72156800	2.55409700	-0.01813600
C	3.05095900	2.59595200	-0.05807800

H	4.09627500	2.31712400	-0.07668300
C	-2.33678000	-0.21486800	-0.01616300
C	-2.79657900	1.19724900	-0.02387200
C	-4.15092500	1.23821200	-0.04892400
H	-4.77586100	2.12105800	-0.06348000
C	3.76910700	-1.34535300	-0.06502000
H	4.71922400	-0.82818100	-0.09951100
C	2.11381000	-3.07984400	0.00436000
H	1.68000400	-4.07046800	0.03192300
C	-4.67575100	-0.16780700	-0.06274300
H	-5.32524100	-0.37693400	0.79872200
H	-5.28982500	-0.37031000	-0.95136900
C	2.55102800	4.00503800	-0.05095200
H	2.95204400	4.56039700	0.81098100
H	2.92012400	4.55651400	-0.92960300
C	3.61798600	-2.83992600	-0.04055600
H	4.13784100	-3.27117500	0.82723400
H	4.09345700	-3.29724800	-0.92011300
C	-3.42543700	-1.01499300	-0.04110500
H	-3.46439900	-2.09578000	-0.04056100
C	1.04767100	3.86961000	-0.02375500
H	0.38037000	4.71986300	-0.01356700
Ru	-0.16715700	-0.43767800	0.02330900
C	-0.77912200	-2.29767100	0.13471900
O	-1.13071000	-3.37904400	0.20209400

H	-4.35354600	-3.58451100	-0.00067400
C	-1.88821000	1.78818200	-0.00034100
C	-0.66045400	2.47338700	0.00023300
C	-2.98181400	2.76379000	-0.00046200
H	-4.03592200	2.52286400	-0.00087000
C	-2.45344900	4.00254400	-0.00003600
H	-3.01114400	4.92970000	-0.00006300
C	-0.93843400	3.95708100	0.00045100
H	-0.51206600	4.45979100	0.87691000
H	-0.51150200	4.46016300	-0.87552300
C	-3.90675100	-1.34275000	-0.00112400
H	-4.50154300	-1.06148800	0.87660100
H	-4.50084200	-1.06204100	-0.87950000
C	2.33523900	-0.18337300	-0.00043500
C	2.79392100	1.12763500	-0.00036100
C	4.26041300	1.15676400	-0.00090000
H	4.86262500	2.05583100	-0.00092500
C	4.71644300	-0.10781400	-0.00137300
H	5.75177600	-0.42055000	-0.00182200
C	3.55626500	-1.07420700	-0.00110900
H	3.58099800	-1.74158400	0.87111300
H	3.58027700	-1.74128500	-0.87358400
Ru	0.20849700	-0.46511300	0.00025800
C	0.81760300	-2.35123500	0.00178700
O	1.14776400	-3.43889600	0.00283400

5 Indene E = -917.4464411 a.u.

C	0.50080000	1.68302000	0.00041500
C	1.80377600	2.13680400	0.00010300
H	2.04942700	3.19718500	-0.00002100
C	-1.74563200	0.40754700	-0.00051300
P	0.20420300	-0.24088000	2.38971700
H	0.47636200	-1.37174300	3.20993400
H	1.13212600	0.68252500	2.94042400
H	-0.99917800	0.20613700	3.00183300
P	0.20460600	-0.24407900	-2.38957100
H	1.12125400	0.69063700	-2.94005700
H	0.49315500	-1.37244800	-3.20757400
H	-1.00344600	0.18621500	-3.00453700
C	-1.58114500	-1.76520300	-0.00001600
C	-2.51734900	-0.76305800	-0.00072100
C	-2.24532600	-3.04993400	0.00016000
H	-1.77556400	-4.02420900	0.00069600
C	-3.58779100	-2.81929000	-0.00052000

6 E = -568.0391765 a.u.

C	1.85253000	-0.39026500	-0.00129200
C	2.28932700	-1.71022500	-0.00383900
H	3.34524200	-1.97136400	-0.00436300
C	0.68512200	1.83986800	0.00403300
P	-0.10010100	0.02433300	2.40340700
H	-0.99789200	-0.76676200	3.16907700
H	1.13978100	-0.37874400	2.96465500
H	-0.28271200	1.29338000	3.01709900
P	-0.10038500	0.03681600	-2.40324600
H	1.14328800	-0.35231900	-2.96591200
H	-0.99064500	-0.75902500	-3.17277800
H	-0.29438100	1.30695200	-3.01119900
C	-1.44727300	1.82020800	0.00487000
C	-0.44352500	2.72212500	0.00659500
C	2.06263900	1.96596300	0.00377700
C	2.70649400	0.72175400	0.00084700
C	-0.00871300	-2.15018300	-0.00430100

C	1.26446000	-2.67649900	-0.00537800
H	-0.83143500	-2.86258600	-0.00543900
H	1.46311800	-3.74308100	-0.00728300
H	3.78893400	0.61755900	0.00023800
H	2.58198300	2.91891200	0.00578500
H	-2.51493100	2.01142200	0.00566800
H	-0.47637700	3.80898000	0.00911500
C	-2.15593200	-0.63910400	-0.00186100
O	-3.24018500	-0.97296200	-0.00295000
Os	-0.24968400	-0.04314100	-0.00005500

6-4MR-isoindene E = -683.579493607 a.u.

C	-1.80277700	1.27236400	0.00021800
C	-3.12699500	0.85489400	0.00049200
H	-3.96120400	1.55226300	0.00061800
C	0.68780600	1.59733800	-0.00021100
P	-0.36901200	-0.10911800	-2.40420300
H	0.48178800	-0.94815600	-3.17286700
H	-1.62414600	-0.36729200	-3.01620600
H	-0.05154100	1.15993400	-2.95637800
P	-0.36818800	-0.10914500	2.40429900
H	-1.62351100	-0.36577300	3.01656000
H	0.48170600	-0.94934100	3.17269600
H	-0.04896300	1.15944400	2.95653300
C	1.93170000	-0.28878200	-0.00021900
C	2.05966700	1.16624100	-0.00034800
C	0.00281300	2.79946800	-0.00019100
C	-1.38476200	2.61130600	0.00005400
C	-2.12567000	-1.27088400	0.00045500
C	-3.29737000	-0.54328100	0.00062600
C	3.36497300	1.53986300	-0.00048000
H	3.78904900	2.53499900	-0.00058200
C	3.14977900	-0.85355300	-0.00024800
H	3.42332500	-1.90043300	-0.00018300
C	4.17776700	0.26938800	-0.00043500
H	4.84099200	0.22072500	0.87442300
H	4.84080100	0.22057100	-0.87543600
H	-2.21919500	-2.35462600	0.00055200
H	-4.27648700	-1.01174800	0.00084500
H	-2.09253500	3.43718600	0.00010000
H	0.47874100	3.77466500	-0.00033800
C	0.39429100	-2.11837400	-0.00012200
O	0.79035100	-3.18472500	-0.00022600
Os	-0.28803900	-0.25824500	0.00003300

6-4MR-indene E = -683.5827156 a.u.

C	-1.72871900	1.32298400	0.02890900
C	-3.06566500	0.97701800	0.05317700
H	-3.85777900	1.72221300	0.07582700
C	0.78942100	1.57167000	0.04678400
P	-0.43359600	0.03457300	-2.38511100
H	0.43989900	-0.69301700	-3.23973800
H	-1.68579500	-0.24988800	-2.99224700
H	-0.20078000	1.35589200	-2.85006300
P	-0.30603900	-0.18780800	2.39858700
H	-1.38825600	0.51631200	2.98952000
H	-0.36681200	-1.40572400	3.12826400
H	0.80315800	0.43501100	3.03459200
C	1.91086600	-0.28553200	-0.01695100
C	2.10563600	1.07497600	0.03570500
C	3.19302300	-0.95096000	-0.05939600
H	3.37189500	-2.01680100	-0.10554100
C	4.15924800	0.00969700	-0.02696900
H	5.22589100	-0.17564100	-0.03987000
C	0.12912600	2.80242400	0.05961700
C	-1.25114300	2.65474600	0.04665500
C	3.57270800	1.40014300	0.03543300
H	3.89225400	2.00601500	-0.82153600
H	3.91041900	1.93581100	0.93124500
C	-2.20586700	-1.20382500	0.04444300
C	-3.32636400	-0.41742100	0.06259500
H	-2.35136100	-2.28161400	0.05800200
H	-4.33241900	-0.82355600	0.08441500
H	-1.93326500	3.50189300	0.05317700
H	0.63459500	3.76234300	0.07267600
C	0.21703500	-2.18017000	-0.11610200
O	0.52544600	-3.27136500	-0.18760500
Os	-0.29298000	-0.26018800	-0.00320300

6-5MR1-isoindene E = -683.5474462 a.u.

C	1.00137000	1.26190400	0.05957100
C	0.70356100	2.58363000	0.14709800
H	1.47040600	3.35228900	0.20276200
C	1.03261800	-1.35936300	0.07724100
P	-0.29370400	0.18535600	-2.36678400
H	-1.07320200	-0.53057800	-3.31884900
H	-0.47009000	1.51631600	-2.82635300
H	1.01089700	-0.10585100	-2.84678000

P	-0.74100500	-0.05464300	2.39108700
H	-0.05458700	1.04106900	2.97470100
H	-2.00621400	0.05106000	3.02768200
H	-0.18566700	-1.14626000	3.11788900
C	-0.85285700	-2.27809700	-0.05279900
C	0.45786500	-2.64767200	0.07755300
C	2.33035300	-0.79996300	0.05662000
C	2.33434300	0.67040200	0.02939400
C	3.61360200	-1.28270800	0.05053100
H	3.93563000	-2.31532800	0.06678400
C	-1.55599100	1.86383200	0.15146800
C	-0.69605500	2.90746200	0.19772200
C	4.53220000	-0.10570600	0.01714200
H	5.21285300	-0.11605200	0.88293600
H	5.20210700	-0.15323000	-0.85549900
C	3.62323200	1.09577100	-0.00011800
H	3.98868600	2.11256300	-0.02512500
H	-2.62175500	2.06085300	0.21803800
H	-1.04280600	3.93365100	0.28374300
H	-1.69640700	-2.95235900	-0.17652900
H	0.91528900	-3.63189700	0.11762600
C	-2.61904300	-0.38775500	-0.27836400
O	-3.72905200	-0.55408200	-0.45003500
Os	-0.66662200	-0.12861500	-0.01060000

6-5MR1-indene E = -683.5795136 a.u.

C	1.06160400	1.20097500	-0.07999200
C	0.85278900	2.57169000	-0.15706500
H	1.67105000	3.28756700	-0.18795000
C	0.96944200	-1.35664400	0.10721000
P	-0.44625200	-0.28077600	-2.38231200
H	-1.40438600	0.32832400	-3.23685600
H	0.75444300	0.23833700	-2.93299700
H	-0.43342800	-1.60340100	-2.90491400
P	-0.53926100	0.18708100	2.38846600
H	0.02521100	1.39967700	2.86506400
H	-1.73041300	0.13834300	3.16207200
H	0.25092300	-0.77333600	3.07623100
C	-0.97243200	-2.23985000	0.22569600
C	0.32027900	-2.62688700	0.24080800
C	2.25866400	-0.85717500	0.06427900
C	2.30243200	0.55375100	-0.03920300
C	3.62756900	-1.37436800	0.10951400
H	3.90084200	-2.41719800	0.19078800
C	4.48144100	-0.33604400	0.03187700
H	5.56131000	-0.40333500	0.03933600
C	3.74629000	0.98581400	-0.07258900
H	3.99724400	1.52426600	-0.99461500
H	3.99741100	1.66442900	0.75142000
C	-1.40619000	1.93643000	-0.13009200
C	-0.49868600	2.97109200	-0.18222100
H	-1.85749000	-2.86145200	0.30389200
H	0.74774500	-3.62234000	0.33329200
H	-2.45929600	2.20926300	-0.14419700
H	-0.79814600	4.01267800	-0.23846500
C	-2.64808100	-0.35078200	-0.03707600
O	-3.77020100	-0.52502000	-0.05765300
Os	-0.68223000	-0.05242400	-0.00263200

6-5MR2-isoindene E = -683.5776096 a.u.

C	0.03810800	1.84931900	-0.00000400
C	1.34637100	2.27687200	-0.00009100
H	1.61637600	3.33043400	-0.00010500
C	-2.25216400	0.79122000	0.00020400
P	-0.39320200	-0.13802400	2.40168500
H	0.37325200	-1.08948200	3.12742400
H	0.09302500	1.06638100	2.97676600
H	-1.64521100	-0.25894900	3.06779000
P	-0.39424100	-0.13785900	-2.40166800
H	0.09060000	1.06705200	-2.97688100
H	0.37269300	-1.08850300	-3.12797500
H	-1.64649900	-0.25982300	-3.06713400
C	-2.25938200	-1.31921700	0.00034500
C	-3.15844700	-0.29180900	0.00037800
C	-2.31829600	2.18010400	0.00021300
C	-1.05373100	2.75553200	0.00008800
C	1.80375700	-0.14994900	-0.00013500
C	2.32007700	1.24533800	-0.00015200
C	3.68349000	1.25429200	-0.00022300
H	4.32923300	2.12270400	-0.00024700
C	4.15973400	-0.16108200	-0.00027500
H	4.79343500	-0.37280200	-0.87354900
H	4.79359900	-0.37283000	0.87287400
C	2.88042500	-0.96675000	-0.00018200
H	2.89887400	-2.04844700	-0.00020700
H	-2.49502200	-2.37962400	0.00049100
H	-4.24515300	-0.30388300	0.00049200
H	-3.24586300	2.74316900	0.00031800

H	-0.89719300	3.83193700	0.00008800
C	0.20007800	-2.15160800	-0.00016900
O	0.52110400	-3.24085200	-0.00029100
Os	-0.39320300	-0.26047200	0.00002600

6-5MR2-indene E = -683.582936 a.u.

C	0.07229200	1.86340700	-0.00024600
C	1.41291300	2.25771900	-0.00018000
H	1.70889600	3.30419300	-0.00013300
C	-2.20537100	0.76161400	-0.00005100
P	-0.46109900	-0.05551500	2.39666400
H	0.49373000	-0.73788800	3.19844400
H	-0.33884000	1.25994300	2.91455300
H	-1.66999900	-0.48242600	3.01048300
P	-0.46178000	-0.05543200	-2.39665300
H	-0.34547800	1.26078100	-2.91396000
H	0.49626700	-0.73312600	-3.19856300
H	-1.66864700	-0.48756600	-3.01083400
C	-2.26263700	-1.37533900	0.00046800
C	-3.12457400	-0.34060800	0.00027600
C	-2.27897500	2.13653500	-0.00026900
C	-1.00905800	2.74462100	-0.00033400
C	1.75690100	-0.08674100	0.00017100
C	2.32747600	1.20024600	0.00009000
C	3.78799500	1.11412600	0.00049100
H	4.45808000	1.96336000	0.00062100
H	-2.48333700	-2.43682400	0.00074300
H	-4.21233900	-0.33790000	0.00039500
H	-3.21311900	2.68953200	-0.00034900
H	-0.87549500	3.82379000	-0.00052400
C	2.91470100	-1.05933200	0.00043400
H	2.88622600	-1.72667100	0.87252200
H	2.88623800	-1.72691100	-0.87146300
C	4.14350200	-0.18180500	0.00014100
H	5.15191500	-0.57267800	0.00009000
C	0.11932400	-2.17353000	-0.00031600
O	0.37218100	-3.28135800	-0.00053600
Os	-0.34651700	-0.24092100	-0.00002600

6-isoindene E = -914.6288724 a.u.

C	-0.46386300	1.79968900	-0.01627200
C	-1.73004200	2.27490600	-0.03553300
H	-1.95886800	3.33720100	-0.06022000
C	1.75428800	0.42101500	-0.02856200
P	-0.34985600	-0.34383100	-2.37572100
H	-1.08234600	-1.39530300	-2.98768600
H	-1.01217700	0.79325200	-2.90579500
H	0.83300200	-0.36599500	-3.16682600
P	-0.26078700	-0.06556100	2.40926300
H	0.52501900	0.98966000	2.94361300
H	-1.54265600	0.26269100	2.92177500
H	0.11250600	-1.12788100	3.27949400
C	1.52381500	-1.81898600	-0.00210400
C	2.53980100	-0.77110400	-0.04149100
C	1.99085500	1.81691200	-0.04041200
C	0.75333700	2.61036600	-0.02501900
C	3.08192600	2.64162900	-0.05906100
H	4.12602100	2.35832900	-0.07482200
C	-2.31032100	-0.12839400	-0.02267500
C	-2.77056800	1.28477000	-0.03981400
C	-4.12433200	1.33056200	-0.06946800
H	-4.74552400	2.21587200	-0.09016200
C	3.79254900	-1.30542900	-0.07798800
H	4.74824900	-0.79897900	-0.11451600
C	2.11764500	-3.02169800	-0.01140000
H	1.67140800	-4.00697900	0.01294400
C	-4.65493200	-0.07322400	-0.07712000
H	-5.30848700	-0.27590500	0.78294400
H	-5.26755100	-0.27942300	-0.96600300
C	2.58831500	4.05455100	-0.05546000
H	2.98751000	4.61078800	0.80642000
H	2.95932500	4.60304600	-0.93491200
C	3.62546700	-2.80138000	-0.05911100
H	4.14125500	-3.24281100	0.80569000
H	4.09199900	-3.26104100	-0.94192600
C	-3.40764700	-0.92190900	-0.04675400
H	-3.45084500	-2.00284100	-0.04079200
C	1.08417300	3.92417100	-0.03170200
H	0.41957300	4.77671800	-0.02504100
C	-0.78913600	-2.23426000	0.15648900
O	-1.14109000	-3.31556700	0.23803300
Os	-0.15219800	-0.38181700	0.02433100

6-indene E = -914.6634158 a.u.

C	-0.47687000	1.74670600	0.00485000
C	-1.78108600	2.21590900	-0.01086500
H	-2.02123000	3.27654500	-0.02470400
C	1.76270100	0.45726200	-0.03763600

P	-0.14512900	-0.29373100	-2.38130300
H	-0.98995300	-1.15191900	-3.13729000
H	-0.49012300	0.96005400	-2.95224700
H	1.10258900	-0.54461800	-3.01624200
P	-0.11139700	-0.08071500	2.39025200
H	0.80682200	0.90536100	2.83803300
H	-1.30497900	0.35256900	3.02851800
H	0.25031000	-1.16503100	3.23743000
C	1.59195200	-1.71393500	0.00066100
C	2.53759400	-0.72329500	-0.04330700
C	2.24158600	-3.00685600	0.02007600
H	1.76127900	-3.97544700	0.05524900
C	3.58578500	-2.79255900	-0.01718000
H	4.34339200	-3.56553800	-0.01995900
C	1.91493500	1.83793300	-0.03648000
C	0.68765900	2.53114900	-0.01016600
C	3.01129600	2.80872800	-0.04853800
H	4.06426900	2.56340900	-0.06886700
C	2.48936700	4.05026300	-0.03346700
H	3.05189800	4.97444500	-0.04031100
C	0.97436500	4.01272400	-0.00706100
H	0.53627500	4.52457100	-0.87248500
H	0.56664400	4.51354300	0.87932400
C	3.91810900	-1.31856000	-0.06030400
H	4.49751900	-1.06520500	-0.95675400
H	4.53471900	-1.02337700	0.79773500
C	-2.29899900	-0.10404800	-0.01951800
C	-2.76857200	1.21082200	-0.02546700
C	-4.23303700	1.23223400	-0.05587200
H	-4.83907800	2.12861000	-0.06469000
C	-4.68374300	-0.03389800	-0.07246600
H	-5.71747600	-0.35077400	-0.09582200
C	-3.52069900	-0.99635700	-0.04959900
H	-3.52249800	-1.66180400	-0.92365800
H	-3.56388200	-1.66489500	0.82078100
C	-0.81638800	-2.27441200	0.12095500
O	-1.15543300	-3.35888700	0.19448700
Os	-0.19461700	-0.39975800	0.01466000